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LETTER TO THE EDITOR

Threshold and scaling in percolation with restricted valence

J Kertész^{†§¶}, B K Chakrabarti^{†||¶} and J A M S Duarte[‡]

[†] Institute for Theoretical Physics, University of Cologne, D5000 Köln 41, West Germany
[‡] Laboratório de Física, Faculdade de Ciências, Universidade do Porto, 4000 Porto, Portugal

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Abstract. Monte Carlo calculations have been carried out to study the problem of percolation with restricted valence on the square and simple cubic lattices. The results are in full agreement with the expectations: there is no transition when the restriction (v) is equal to two, while even for $v=3$ the transition occurs and the correlation length exponent, determined via finite size scaling, is within the numerical accuracy the same as that in the unrestricted random percolation. The maximum random occupancy as a function of the restriction is also determined.

Recently a new lattice statistical problem was defined: percolation with restricted valence (Gaunt *et al* 1979). In this model lattice sites (bonds) are occupied randomly as in the usual percolation problems, but the occupation is prohibited if it would lead to an occupied site having valence higher than a prescribed value v . (The valence of a site is the number of different paths to neighbouring occupied sites.) The practical use of this model may be the descriptions of steric hindrance effects in gelation (Stauffer *et al* 1981). If the coordinations number is Q , $v \leq Q$ of course. $v=0$ and $v=1$ correspond to the trivial cases of isolated single sites and isolated pairs of sites, respectively; $v=Q$ is the unrestricted model. A number of papers have been devoted to the problem of restricted valence animals. Gaunt *et al* (1979) have shown rigorously that the dominant singularity of the generating function of animals can be characterised by different exponents for $v=2$ than for $v \geq 3$. Furthermore, extensive series analysis for such restricted valence animals on different lattices in 2, 3 and 4 dimensions suggests that there is no change in this exponent for $v \geq 3$ (Gaunt *et al* 1979, 1980, Whittington *et al* 1979, Duarte and Ruskin 1980, Duarte 1981). Family has used real space renormalisation groups to show that lattice animals with $v=2$ are in a different universality class than lattice animals with $v > 2$ (Family 1980 and unpublished).

The animal problem is the zero concentration limit of the general percolation model (Stauffer 1979). It is difficult to go beyond this limit by series expansions, since restricted valence percolation is essentially a correlated percolation where the occupation of a site depends on the environment and so the single cluster approach of the series expansion method seems not to be adequate here (see below for a more detailed discussion of this problem). In this paper we give an account of a Monte Carlo (MC)

§ Permanent address: Research Institute for Technical Physics of the HAS, Budapest, Ujpest 1, Pf 76, H-1325, Hungary.

|| Present address: Saha Institute of Nuclear Physics, Calcutta 700009 India.

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investigation of the site percolation transition (appearance of an infinite cluster) on the square and simple cubic lattices. The natural parameter of the problem is the concentration x of occupied sites. If there is a restriction, the lattice cannot be fully occupied and there must be an $x_m(v)$ maximum occupancy depending on the lattice and the restriction, $x_m(v) \leq 1$ (equality holds only for $v = Q$).

In the computer program each site corresponds to a matrix element M , the absolute value of which is the actual valency of the site plus unity and the sign shows whether it is occupied or not. First the lattice is empty and $M = -1$ is set for each site. Then the lattice is gradually filled until the concentration x has been reached. The main steps during this procedure are as follows. A site is randomly chosen. If the occupation is possible, the absolute value of the neighbouring matrix elements is enlarged by one and the sign of the actual matrix element is set to be positive. Two versions were used.

(i) After visiting a site the algorithm is simply repeated, thus multiple visits are allowed.

(ii) The unvisited sites are stored in a separate array and sites are randomly picked out from there. After the visit the site is dropped from this array independent of whether or not occupation was allowed.

The percolation transition is indicated by the appearance of a cluster percolating from top to bottom and the multi-labelling technique (Hoshen and Kopelman 1976) was used to find the threshold x_c of the actual realisation. The samples are characterised by their linear size b . In order to see the size effect we studied samples with $b = 20, 50, 100, 180, 240, 360$ on the square lattice and $b = 10, 20, 30, 40, 50$ on the simple cubic lattice. For $v = 2$ no transition was found (except for a few cases on the smallest samples due to fluctuations). For $v = 3$ we found a clear percolation transition. In order to determine the correlation length exponent ν and the infinite size limit of the threshold concentration x_c we applied the usual finite size scaling analysis (see e.g. Reynolds *et al* 1980). For $v = 3$ and for each size b , ρ realisations were generated with $\rho b^2 \geq 5 \times 10^6$ and $\rho b^3 \geq 10^7$ in two and three dimensions, respectively. The mean $\langle x_c(b) \rangle$ and the width $\sigma(b) = (\langle x_c^2(b) \rangle - \langle x_c(b) \rangle^2)^{1/2}$ of the distribution of the actual thresholds x_c were determined. σ and $\langle x_c(b) \rangle$ must scale according to finite size scaling (Reynolds *et al* 1980):

$$\sigma \propto b^{-1/\nu} \quad (1a)$$

$$|\langle x_c(b) \rangle - x_c(\infty)| \propto b^{-1/\nu} \quad (1b)$$

with ν being the critical exponent of the correlation length.

Figure 1 shows a plot of $\ln \sigma$ against $\ln b$ for (a) the square, (b) the simple cubic case with $v = 3$. From the slopes we find effective exponents $\nu_{2D} = 1.35 \pm 0.03$ and $\nu_{3D} = 0.91 \pm 0.08$ in two and three dimensions, respectively. For the unrestricted problem the most accurate available values are $\nu_{2D} = 1.333 \pm 0.002$ (Blöte *et al* 1981) and $\nu_{3D} = 0.88 \pm 0.01$ (Heermann and Stauffer 1981). From our calculations we can conclude that the change over to the unrestricted critical behaviour seems to take place between valences 2 and 3 as in the case of restricted valence animals (Gaunt *et al* 1979, 1980, Whittington *et al* 1979, Duarte and Ruskin 1980, Family 1980, Duarte 1981). In other words: if there is a phase transition in the restricted valence problem ($v \geq 3$), the critical behaviour is probably in the same universality class as that of the unrestricted percolation problem.

In figure 2 the plot according to equation (1b) is shown for determining the critical concentration x_c . We calculated the critical concentrations x_c and the maximum

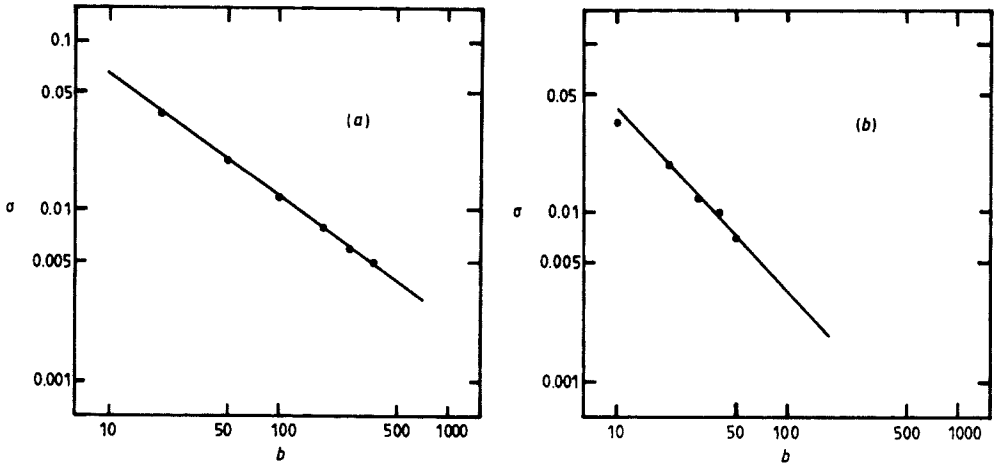


Figure 1. Determination of the critical exponent ν for $\nu = 3$ from the log-log plot σ against b (for definitions see the text). (a) square lattice, $\nu_{2D} = 1.35 \pm 0.03$, (b) simple cubic lattice, $\nu_{3D} = 0.91 \pm 0.08$.

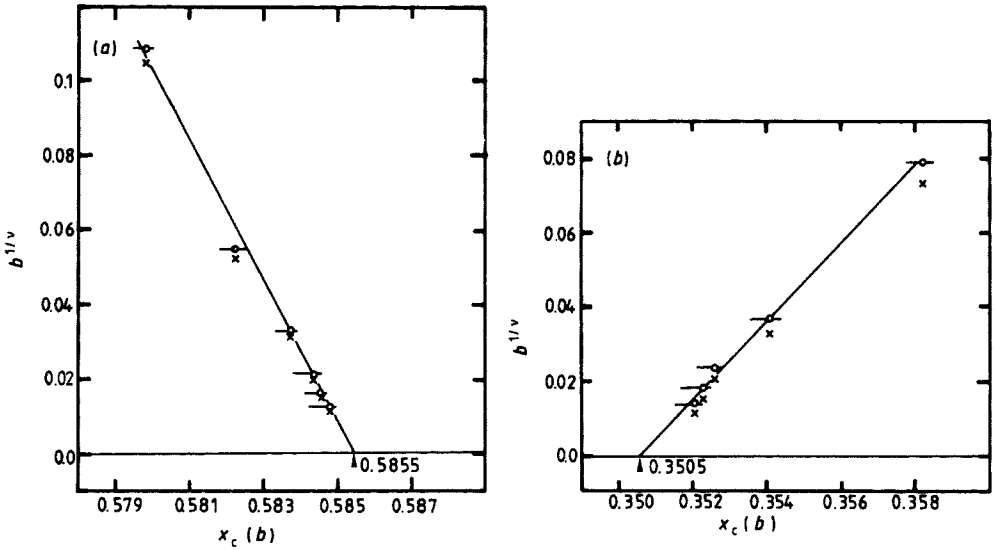


Figure 2. Extrapolation to the infinite system size for determination of the critical concentrations x_c with $\nu = 3$ using $b^{-1/\nu}$ plotted against $x_c(b)$ (for definitions see the text). Plots are taken both with calculated (\circ) and best estimates for the universal value of the exponent (\times) (Blöte *et al* 1981, Heermann and Stauffer 1981); (a) square lattice, $x_c = 0.5855 \pm 0.001$, (b) simple cubic lattice, $x_c = 0.3505 \pm 0.0015$.

random concentrations x_m for all possible restrictions (table 1). Since version (i) of our program becomes infinitely slow at x_m we used version (ii) here. However, the rearranging of the array which stores the unvisited sites takes such a long time that at x_c version (ii) is more than an order of magnitude slower.

Table 1. Critical and maximum concentrations for the square and simple cubic lattices. Note that the 'restricted' threshold is in two dimensions lower and in three dimensions higher than the unrestricted one.

v	Square		Simple cubic	
	x_c	x_m	x_c	x_m
0	—	0.365 ± 0.002	—	0.305 ± 0.002
1	—	0.413 ± 0.002	—	0.344 ± 0.002
2	—	0.526 ± 0.002	—	0.405 ± 0.002
3	0.5855 ± 0.001	0.706 ± 0.002	0.3505 ± 0.0015	0.503 ± 0.002
4	0.5927 ± 0.0002^a	1	0.332 ± 0.002	0.625 ± 0.002
5	—	—	0.330 ± 0.002	0.764 ± 0.002
6	—	—	0.3117 ± 0.0003^b	1

^a Derrida and De Seze (1981).

^b Heermann and Stauffer (1981).

The highest possible concentration x_m is, as far as we know, a new lattice statistical quantity. One can always find a 'crystalline' structure where the concentration is higher (see figure 3(a)), but due to the *random* process of occupation this *regular* maximum occupancy can never be reached. The situation is similar to the case of hexagonal close-packed and randomly close-packed hard spheres. Of course x_m is well defined only in the thermodynamic limit ($b \rightarrow \infty$); in finite systems the actual maximum occupancy has a distribution becoming sharper, the larger the system is. The numbers in table 1 are obtained from estimates at two different sizes.

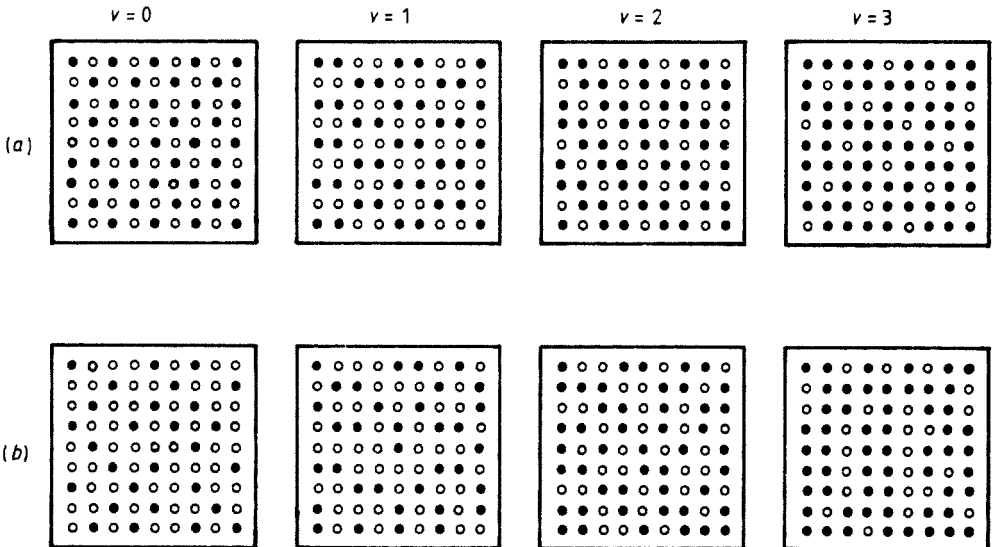


Figure 3. The regular arrangements of maximum occupied sites satisfying the restrictions given an upper limit for the maximum random concentration. Examples are shown on the square lattice. (a) realisations of regular arrangements for $v = 0, 1, 2$ and 3 ; $x_m = \frac{1}{2}, \frac{1}{2}, \frac{2}{3}$ and $\frac{4}{3}$, respectively, (b) realisations for the random arrangements; for the maximum concentrations see table 1. (●) occupied site; (○) empty site.

Finally let us make a few remarks on the other two approximate methods usually used in percolation problems: series expansion and renormalisation group techniques. As already mentioned above, the present problem is clearly seen to be different from simple investigations of the structure of the mean size series as in unrestricted random percolation, where now the mean size is restricted only to the clusters with the pertinent valence restriction. The usual second moment expansion is

$$S^v(p) = \sum_{t, \{s_i\}} s^2 g(s_1, s_2, \dots, s_v; t) p^s (1-p)^t \quad (2)$$

with $s_1 + s_2 + \dots + s_v = s$, where p is the site occupation probability, s_i is the number of sites in the cluster having valence equal to i , t is the number of perimeter sites and $g(s_1, s_2, \dots, s_v; t)$ is simply taken from the perimeter expansions of the extensive tabulations of Gaunt *et al* (1979, 1980), Whittington *et al* (1979), and Duarte and Ruskin (1980). Clearly it is impossible to combine a restricted valence lattice covering (in the Monte Carlo sense above) with the usual meaning of 'perimeter'. The structure of the $S^v(p)$ for $v < 4$ no longer shows a transition for square, triangular and simple cubic site problems although for higher valences on the last two lattices (eleven and ten term long series, respectively) an apparent singularity is obtained near to the unrestricted critical point with comparable values for the exponent γ . This series method is not an approximation to the MC problem studied above but it is a different problem of rather mathematical interest: what is the leading singularity in the mean size series by selecting the terms from the point of view of the valence?

It seems to be plausible to apply a real space renormalisation group (RSRG) transformation (Reynolds *et al* 1980) to the restricted valence problem. If there is more than one parameter this method usually leads to surprisingly good descriptions of the universality classes (Family 1980). However, there are exceptions (Nakanishi *et al* 1981) where the simple RSRG does not work and the restricted valence percolation problem is one of them. A natural way of introducing the second parameter is to say that the valence of a site is restricted to v with a given probability s and unrestricted with $1-s$. However, in a small cell one will find many percolating configurations even if $v = 2$; thus the renormalisation group will predict a transition in this case too, in contradiction with our MC result†. One has to go to bigger cells: the side of the cell must be much larger than the average chain length at the maximum occupancy (see figure 3(b)). But large cells can be treated only by MC techniques and the handling with two parameters is difficult here: the simple MC simulation is the most adequate method for the restricted valence percolation problem.

In conclusion we determined the critical and maximum concentrations for the restricted valence percolation on the square and simple cubic lattices. Our results suggest that whenever there is a phase transition (valence $v \geq 3$) the critical exponents are the same as in the unrestricted problem.

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† Some years ago the Boston University group also arrived at the conclusion that small cell RSRG is not appropriate to investigate restricted valence percolation (W Klein, private communication).

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