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LETTER TO THE EDITOR

Monte Carlo renormalisation-group approach to percolation on a continuum: test of universality

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Abstract. It is shown that a Monte Carlo renormalisation-group technique can be employed for direct renormalisation of a system on a continuum, i.e. without restriction to a periodic lattice. For the problem of overlapping discs we find the critical area fraction $s_c = 0.688 \pm 0.005$ and the correlation-length critical exponent $\nu = 1.33 \pm 0.07$. The latter result indicates the regular–irregular lattice universality.

1. Introduction

Almost all discussions of percolation thresholds in real materials use results of calculations on regular lattices with randomly occupied sites or bonds. In this way the structural (topological) disorder of many materials characterised by randomly distributed inhomogeneities in space is described by models possessing substitutional disorder. This simplification is of great computational convenience in many series expansion and Monte Carlo investigations. Furthermore, it makes natural the use of real-space renormalisation-group techniques, where a regular cell is transformed into a new one (for references see Essam (1980)).

Since the critical properties of various lattices have been found to be independent of the lattice geometry (universality), it is usually supposed that the regular–irregular (random) lattice universality also holds. This basic assumption stands behind the extrapolation of results obtained by investigations of regular lattices to the case of percolation in random structures.

On the other hand, evidence has begun to accumulate that some modifications of models on the regular lattices can result in new universality classes. In investigations of the orientated bond percolation (Blease 1977, Kertész and Vicsek 1980) and the correlated site percolation (Kirkpatrick 1980) on two-dimensional lattices new, non-standard values were found for the correlation-length exponent.

In this Letter we will study the scaling behaviour of an irregular lattice consisting of discs of equal radii with randomly distributed centres on a plane (overlapping discs). This model has direct relevance to such physical problems as impurity conduction in lightly doped semiconductors, variable-range hopping in amorphous semiconductors or ferromagnetism in a dilute system of magnetic atoms in a non-magnetic host crystal with long-range interaction between the magnetic atoms, etc. The critical radius at which percolation occurs was firstly determined by the construction of clusters starting from a

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central vertex (Roberts 1967). Pike and Seager (1974) calculated the same quantity by checking percolation between the two opposite edges of a cell having the shape of a square. Fremlin (1976) generated clusters of overlapping discs in order to find the critical density at which the infinite cluster appears. As far as we know, the only work dealing with some scaling properties of the random lattice is the paper of Kurkijärvi (1974) who investigated the conductivity of overlapping spheres in finite cubic cells. Later Shklovskii and Efros (1979) showed that Kurkijärvi's results concerning the standard deviation of the critical radius values may be related to the problem of regular–irregular lattice universality. Webman *et al* (1977) studied the electrical conductivity critical exponent of the continuous percolation simulated by a correlated cubic network.

There are several possibilities for studying scaling properties of a percolation model. The Monte Carlo (large-cell) real-space renormalisation-group method (MS RSRG) (Reynolds *et al* 1978, 1980) proved to be a very appropriate tool for the determination of the correlation-length critical exponent on various percolating lattices. In the following section it will be shown that the regularity of the cells to be renormalised is not an inherent condition for this type of transformation, and after some insignificant modifications the MS RSRG can be employed for our purposes.

2. Renormalisation of the area fraction

The irregular lattice to be considered in this Letter is made up of discs of equal radius r_0. Their centres (the sites of the random lattice) are uniformly distributed on a plane with density ρ. Those sites whose discs intersect are considered as belonging to the same cluster. Since the value of $r_0 = r_c$ at which the infinite cluster appears depends on the density, it is more convenient to introduce the dimensionless variable

$$s = 1 - \exp(-\pi r_0^2 \rho),$$

where s is the so-called area fraction, playing the role of the occupation probability. In the following considerations ρ is regarded as being equal to unity.

We expect that near the percolation threshold the characteristic quantities of the clusters scale with $|s - s_c|$ similarly to the case of the regular lattices. Namely, we can write

$$\xi \sim |s - s_c|^{-\nu}$$

where s_c is the critical area fraction, ξ denotes the correlation length and ν is the corresponding critical exponent.

When applying the MC RSRG to our system, we firstly partition the irregular lattice into square-shaped cells of sides characterised by the quantity $b = N^{1/2}$, where N is the average number of sites falling into a cell. The actual number of sites in a cell N_i is distributed according to the Poisson distribution: $P_{N_i} = N^{N_i} e^{-N}/N_i!$. The cells of size b are renormalised into smaller ones of characteristic length b' and the rescaling factor is obviously given by b/b'. The renormalisation group is defined by

$$R'(s', b') = R(s, b) \tag{1}$$

where s' plays the role of the renormalised area fraction. Since s can be associated with the occupation probability and a large cell can be regarded as occupied if it contains a cluster spanning the cell, we define $R(s, b)$ as the probability of having a cluster

connecting the two opposite edges of a cell of size b if the area fraction is just equal to s. Therefore

$$R(s, b) = \sum_{k=1}^{\infty} P_k(N) R[s(k), b] \tag{2}$$

where $P_k(N)$ is the probability of finding k discs in the cell for a given N and $R[s(k), b]$ denotes the probability of having a cluster which percolates between the opposite edges of a cell containing k discs. $s(k)$ is the corresponding area fraction determined by the expression

$$s(k) = 1 - (1 - \pi r_0^2/N)^k.$$

In principle, it is possible for relatively small values of N to calculate $R(s, b)$ from (2) approximately, using analytical calculations and numerical integration, because the terms with $k \gg N$ can be neglected and $R[s(k), b]$ may be expressed as a multi-dimensional integral. The value of $R[s(k), b]$ equals that part of the $2k$-dimensional unit hypercube which corresponds to such configurations of the k sites that a percolating path of overlapping discs is present in the cell.

After $R(s, b)$ is determined, the fixed point $s^*_{b,b'}$ of the transformation equation (1) gives an approximation for the critical area fraction s_c. The correlation-length critical exponent can be determined using MC RSRG in several ways. For a particular choice of b and b' it can be obtained from (Reynolds *et al* 1978)

$$\nu_{b,b'} = \ln(b/b')/\ln \lambda_{b,b'}$$

where

$$\lambda_{b,b'} = \left(\frac{\mathrm{d}R(s, b)}{\mathrm{d}s} \Big/ \frac{\mathrm{d}R'(s, b')}{\mathrm{d}s} \right)\Bigg|_{s=s^*_{b,b'}}$$

is the eigenvalue of the linearised transformation equation (1). We obtain better approximations for ν by extrapolating the $\nu_{b,b'}$ values to the $b \to \infty$ limit. Following Reynolds *et al* (1978), we write

$$y = y_{b,b'} + c/\ln(b/b') \tag{3a}$$

or

$$\ln \lambda_{b,b'} = y \ln(b/b') - c \tag{3b}$$

where $y = 1/\nu$ and c is constant. One can either extrapolate y to $b/b' \to \infty$, where the RSRG should become exact, using (3*a*), or one can determine y from the slope of the $\ln \lambda_{b,b'}$ versus $\ln(b/b')$ plot (3*b*). Levinshtein *et al* (1975) showed that when b goes to infinity the standard deviation $\sigma_s(b)$ belonging to the probability distribution function $L(s, b) = \mathrm{d}R(s, b)/\mathrm{d}s$ scales with an exponent equal to ν^{-1}. Therefore ν can also be obtained from the slope of the plot $\ln[\sigma_s(b)]$ versus $\ln(b)$.

3. Calculation and results

The small cells in our model are relatively ill defined because of the uncertainty in the choice of the boundary region to be considered when checking percolation from the upper to the lower edge of a cell. Therefore we consider cells containing N discs, where $N \gg 1$ and $R(s, b)$ will be determined from Monte Carlo experiments. During one run

we first build up a random lattice within a cell of size b. Coordinates of the sites are generated by random numbers distributed uniformly on the interval [0, 1]. The cell is divided into $n \times n$ subcells and after a site is generated it receives an index depending on the position of the subcell into which it fell. Another index labels sites inside one cell. In this way we can distinguish the sites belonging to subcells neighbouring a reference subcell.

n is chosen in such a way that the critical diameter for the possible configurations is always less than the size of a subcell; therefore no discs can overlap belonging to other than nearest-neighbouring subcells. Now the multilabelling technique (Hoshen and Kopelman 1976) can be used for the cluster analysis on the random lattice: the connectivity properties have to be checked only for the sites belonging to the neighbouring subcells. Application of this algorithm results in a program being only six to eight times slower for this irregular lattice than for the regular ones and requiring computing time proportional to N.

The program finds the least radius at which the given configuration percolates. In a series of experiments we thus obtain the density distribution function $L(s, b)$ of volume fractions at which spanning occurs. Integrating $L(s, b)$, we recover $R(s, b)$ and determine $s^*_{b,b'}$ from equation (1). The eigenvalue $\lambda_{b,b'}$ can be obtained from

$$\lambda_{b,b'} = L(s, b)/L(s, b')|_{s=s^*_{b,b'}}.$$

We generated q Monte Carlo realisations such that $q \times b^2 \geqslant 5 \times 10^5$. Cells of $n = 4$, 6, 8, 11, 16, 22, 32, 64 were renormalised into a cell of $n' = 3$. (Hence b is in general not an integer since $b = (n \times n \times \alpha)^{1/2}$, where α is the mean number of discs in one subcell. For various sizes $1.8 \leqslant \alpha \leqslant 2.4$ was chosen depending on the size of the cell to be renormalised in a manner to minimise the number of sites within one cell, and at the

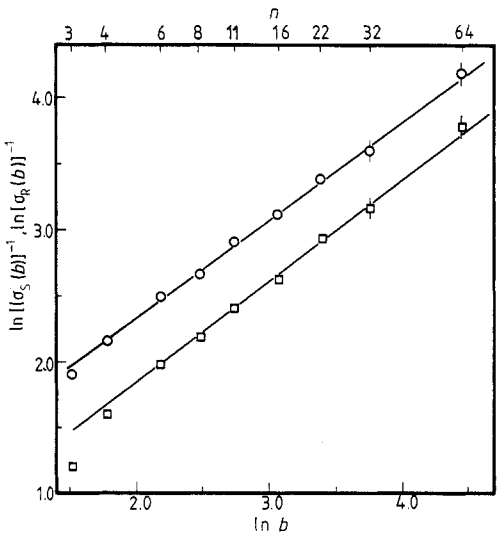

Figure 1. Determination of the correlation-length exponent ν from the finite-size scaling theory. From the slope of the plots $\ln[\sigma_s(b)]^{-1}$ (○) and $\ln[\sigma_R(b)]^{-1}$ (□) against $\ln(b)$ we obtain $\nu_s = 1.34 \pm 0.06$ and $\nu_R = 1.31 \pm 0.07$ respectively. For the definitions of $\sigma_s(b)$, $\sigma_R(b)$, n and b see the text. The typical uncertainties are represented for two pairs of experiments.

same time to avoid overlaps of discs of critical radius belonging to the next-nearest-neighbouring subcells.) In figure 1 we display the $\ln b$ dependence of $\ln[\sigma_s(b)^{-1}]$ and $\ln[\sigma_R(b)^{-1}]$, where $\sigma_s(b)$ is the standard deviation of the critical area fractions in the various runs and $\sigma_R(b)$ is the same quantity for the normalised critical radius $R_c = 2r_c(\pi\rho)^{1/2}$. $\sigma_s(b)$ and $\sigma_R(b)$ should scale as $b^{-1/\nu}$, and therefore from the inverse slope of these finite-size scaling plots we find $\nu_s = 1.34 \pm 0.06$ and $\nu_R = 1.31 \pm 0.07$. Next we plot (figure 2) $\ln \lambda_{b,b'}$ against $\ln(b/b')$ $(3b)$. The inverse slope is $\nu = 1.35 \pm 0.07$. We have also plotted $y_{b,b'} = \ln \lambda_{b,b'}/\ln(b/b')$ against $1/\ln(b/b')$. Eschbach *et al* (1980) found that a parabola fit in such a plot takes the results for small cells better into account than a straight line (Reynolds *et al* 1980). In this manner we obtain $y = 0.76 \pm 0.04$, which corresponds to $\nu = 1.316 \pm 0.07$.

The sequence $s^*_{b,b'}$ is extrapolated on the basis of finite-size scaling considerations (Fisher 1971, Sur *et al* 1976). In figure 3 we plotted $s^*_{b,b'}$ against $b^{-1/\nu}$ with trial value $\nu = 1.33$ (b' is in all cases equal to the value of b corresponding to the cell of $n = 3$). We find $s_c = 0.688 \pm 0.005$, which is somewhat larger than the value 0.68 predicted by the Monte Carlo experiments of Pike and Seager (1974) and the value 0.67 calculated by

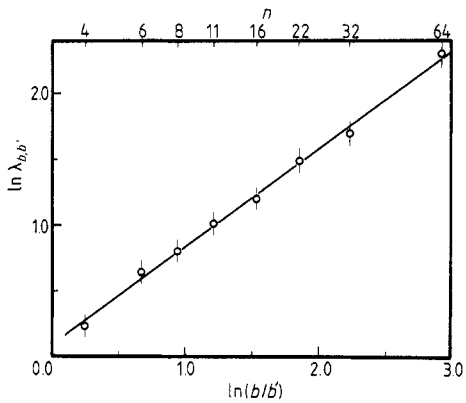

Figure 2. Dependence on $\ln(b/b')$ of $\ln \lambda_{b,b'}$ where b' characterises the size of the cell into which the larger cells are renormalised. The slope is $\nu = 1.35 \pm 0.07$. n characterises the size of the cell renormalised into a smaller cell of $n' = 3$.

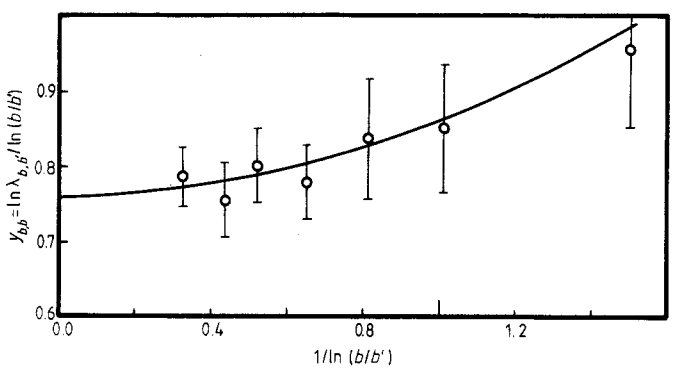

Figure 3. Extrapolation of $y_{b,b'} = \ln \lambda_{b,b'}/\ln(b/b')$. By fitting a parabola to our data we find $y = 0.76 \pm 0.04$, i.e. $\nu = 1.316 \pm 0.07$.

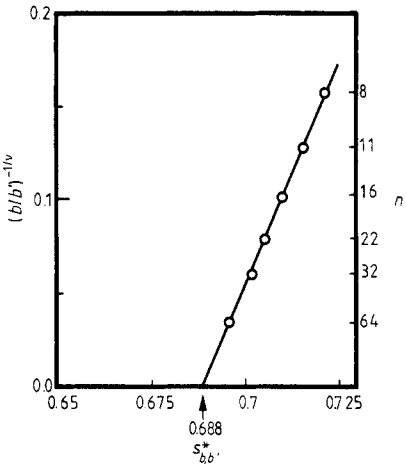

Figure 4. Sequence of fixed points $s^*_{b,b'}$ is plotted against $(b/b')^{-y}$. The straight line extrapolates to the value $P_c = 0.688 \bullet 0.005$.

Fremlin (1976). In an earlier work of Roberts (1967) the value 0.62 was obtained, while Domb (1972), from the study of percolation on regular lattices with long-range interaction, gave an estimation $s_c \sim 0.675$.

4. Conclusions

We have demonstrated that a real-space renormalisation-group technique originally developed for regular lattices can be used for the investigation of scaling properties of the random lattices.

Since the study of regular lattices is motivated by the assumption of the regular–irregular lattice universality, we decided to test this hypothesis. Besides, the system of overlapping discs can be modelled on a regular lattice with long-range interaction (Domb 1972), where sites are connected if they are nearer than l, where l is much greater than the lattice constant; therefore at the same time we check universality for this particular regular system too. For the latter system Stauffer and Coniglio (1980) argue that it should have the same critical exponents as the system with nearest-neighbour interaction. Hoshen *et al* (1978) also could not find any remarkable change in the exponent β and γ as the interaction range was increased up to $l = 7$.

For the correlation-length critical exponent of the system of overlapping discs, averaging ν's calculated by various ways, we obtained $\nu = 1.33 \pm 0.07$. This value is consistent with the literature estimates for site percolation on triangular and square lattices: $\nu = 1.32^{+0.02}_{-0.07}$ (Cox and Essam 1976), $\nu = 1.354 \pm 0.015$ (Reynolds *et al* 1978), $\nu = \frac{4}{3}$ (den Nijs 1979), $\nu = 1.33 \pm 0.01$ (Eschbach *et al* 1980) and $\nu = 1.334 \pm 0.002$ (M P Nightingale and H W J Blöte 1980, talk presented at STATPHYS 14, Edmonton, Canada). Hence we conclude that there is no evidence to suggest that the random lattice problem would be in a different universality class from the regular one.

Finally, we remark that a model from overlapping discs of various radii has some relation to the correlated percolation model on a two-dimensional regular lattice with strong attractive interaction, because in this case one expects circle-shaped clusters to

grow. Since Kirkpatrick (1980) obtained for a correlated-site percolation model non-universal connectivity properties, the investigation of scaling properties of the system of variable-size discs could also be of interest.

We are aware that the Boston group (Stanley 1980, private communication) is carrying out a finite-size scaling study of the same system.

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Note added in proof. After acceptance of this paper we learned of closely related work by Haan and Zwanzig (1977) studying the continuum percolation problem by series expansions. Their result concerning the mean cluster size exponent also indicates the lattice–off-lattice universality.

Reference

Haan S W and Zwanzig R 1977 *J. Phys. A: Math Gen.* **10** 1547–55

References

Blease J 1977 *J. Phys. C: Solid State Phys.* **10** 917–24
Cox M A A and Essam J W 1976 *J. Phys. C: Solid State Phys.* **9** 3985–91
Domb C 1972 *Biometrika* **59** 209–10
Eschbach P D, Stauffer D and Herrmann H J 1980 *Preprint*
Essam J W 1980 *Rep. Prog. Phys.* **43** 834–912
Fisher M E 1971 *Critical Phenomena: Enrico Fermi Summer School Varenna, Italy* (New York: Academic)
Fremlin D H 1976 *J. Physique* **37** 813–7
Hoshen J and Kopelman R 1976 *Phys. Rev.* B **14** 3438–45
Hoshen J, Kopelman R and Monberg E M 1978 *J. Statist. Phys.* **19** 219–42
Kertész J and Vicsek T 1980 *J. Phys. C: Solid State Phys.* **13** L343–8
Kirkpatrick S 1980 *AIP Conf. Proc.* **H58** 79–86
Kurkijärvi J 1974 *Phys. Rev.* B **9** 770–4
Levinshtein M E, Shklovskii B I, Shur and Efros A L 1975 *Zh. Exp. Theor. Fis.* **69** 386–92
den Nijs M P M 1979 *J. Phys. A: Math. Gen.* **12** 1857–68
Pike G E and Seager C H 1974 *Phys. Rev.* B **10** 1421–34
Reynolds P E, Stanley H E and Klein W 1978 *J. Phys. A: Math. Gen.* **11** L199–207
—— 1980 *Phys. Rev.* B **21** 1223–45
Roberts F D K 1967 *Biometrika* **54** 625–8
Shklovskii B I and Efros A L 1979 *Electronic Properties of Doped Semiconductors* (Moscow: Nauka)
Stauffer D and Coniglio A 1980 *Z. Phys.* B **38** 267–70
Sur A, Lebowitz J L, Kalos M L and Kirkpatrick S 1976 *J. Statist. Phys.* **15** 343–53
Webman I, Jortner J and Cohen M H 1977 *Phys. Rev.* B **16** 2593–6