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Renormalisation-group approach for critical percolation behaviour in three dimensions

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Abstract. A renormalisation-group approach to three-dimensional site percolation systems on the diamond, simple cubic, body-centred cubic, face-centred cubic and hexagonal close-packed lattices is developed using a scaling transformation in real space.

1. Introduction

We present a renormalisation-group approach for calculating the critical behaviour of three-dimensional site percolation systems. The renormalisation-group approach has been studied by several authors (Harris *et al* 1975, Young and Stinchcombe 1975, Stinchcombe and Watson 1976, Kirkpatrick 1976, 1977, Rosman and Shapiro 1977, Reynolds *et al* 1977, 1978, Yuge and Murase 1978, Yuge 1978) for the percolation systems on the various lattices in two dimensions. There has been, however, no attempt to adapt this approach to three-dimensional percolation systems. We develop a simple approximate method for applying the renormalisation-group approach to the diamond, simple cubic, body-centred cubic, face-centred cubic and hexagonal close-packed site lattices for calculating the critical percolation probability p_c and the correlation length critical exponent ν. This simple cluster approximation has been formulated recently and applied to the study of critical behaviour in two-dimensional percolation systems (Yuge and Murase 1978, Yuge 1978).

If the sites in the original lattice are independently occupied with probability p, which will, in the case of the sites, scale into a transformed probability p' of a single site on the new lattice, then the scaling relationship of the transformation will be determined by

$$p' = R(p). \tag{1}$$

Then the fixed point p^* can be determined by

$$p^* = R(p^*). \tag{2}$$

The linearised form R^L of the renormalisation-group transformation near the fixed point has eigenvalues λ_i and $\lambda_1 > 1 > \lambda_2 \ldots$. The correlation length index ν is then given by $b^{1/\nu} = \lambda_1$, where b is the change in length scale.

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2. Cluster approximations

Our simple scaling procedure is defined by a renormalisation transformation on finite lattices sandwiched by two plane electrodes. Cluster approximations will be worked out for the diamond (D), simple cubic (SC), body-centred cubic (BCC), face-centred cubic (FCC), and hexagonal close-packed (HCP) lattices.

The illustration of the basic scaling procedure on the five lattices is provided in figures 1 to 5. The original lattice (full line) is scaled into the new lattice (broken line)

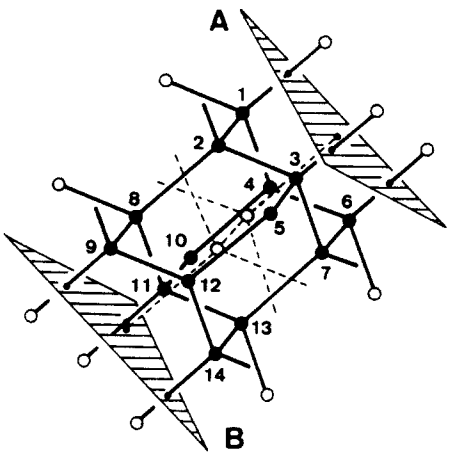

Figure 1. Transformation of the diamond site lattice: the full line is the original lattice; the broken line is the new lattice with the scale factor $b = 2$. Cluster group of sites 1–14 sandwiched between two plane electrodes A and B.

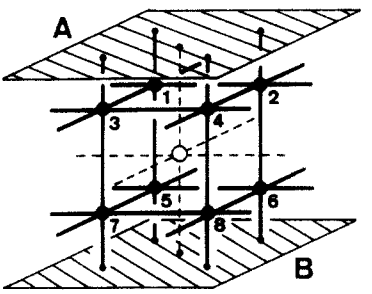

Figure 2. Transformation of the simple cubic site lattice by the scale factor $b = 2$, showing the cluster group of sites 1–8 sandwiched between two plane electrodes.

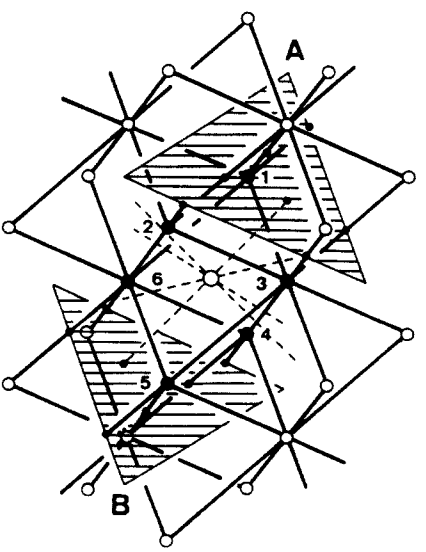

Figure 3. Transformation of the body-centred cubic site lattice by scale factor $b = 2\sqrt{2}/\sqrt{3}$, showing the cluster group of sites 1–6 sandwiched between two plane electrodes.

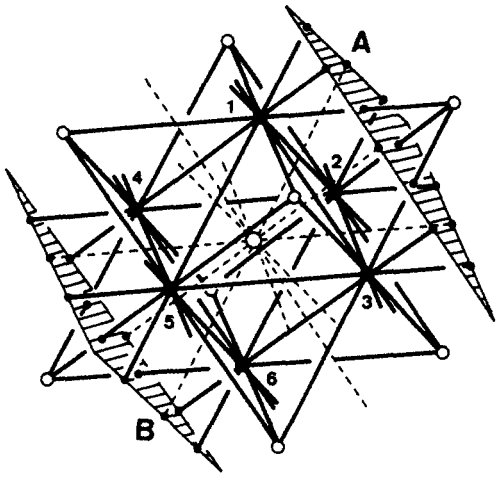

Figure 4. Transformation of the face-centred cubic site lattice by the scale factor $b = 2$, showing the cluster group of sites 1–6 sandwiched between two plane electrodes.

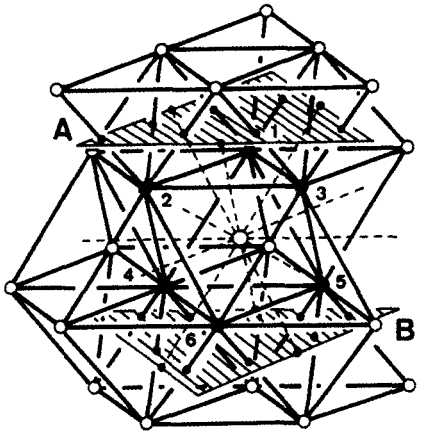

Figure 5. Transformation of the hexagonal close-packed site lattice by the scale factor $b = 2$, showing the cluster group of sites 1–6 sandwiched between two plane electrodes.

with a scale factor b indicated in the figures: the original cluster group of sites scales into the one or two sites with transformed probability p'. The probability p' of a single site on the new lattice is defined as the probability that the cluster group is conductive when the cluster is sandwiched between two plane electrodes A and B made of perfect conductors. Considering the possible connections and combining their probabilities using the exclusion–inclusion principle, we can obtain the transformed probability of the single site on the new lattice for the five lattices as, respectively,

D
$$p' = (12p^4 - 10p^5 - 3p^6 - 6p^7 - 39p^8 + 212p^9 - 408p^{10} + 432p^{11} - 262p^{12} + 84p^{13} - 11p^{14})^{1/2}, \tag{3}$$

SC
$$p' = 4p^2 - 6p^4 + 6p^6 - 4p^7 + p^8, \tag{4}$$

BCC
$$p' = 4p^2 - 2p^3 - 4p^4 + 4p^5 - p^6, \tag{5}$$

FCC $$p' = 6p^2 - 6p^3 - 3p^4 + 6p^5 - 2p^6, \tag{6}$$

HCP $$p' = 6p^2 - 6p^3 - 3p^4 + 6p^5 - 2p^6. \tag{7}$$

For the diamond site lattice, the original cluster group is scaled into the two sites on the new lattice, for which the probability of being conductive between two plane electrodes on the new lattice is p'^2. Therefore the renormalisation transformation can be given by $p' = \sqrt{R(p)}$.

From these scaling transformations, the fixed point p^* and the correlation length critical index ν for each lattice are given by

D	$p^* = 0{\cdot}3591$,	$\nu = 1{\cdot}329$,	
SC	$p^* = 0{\cdot}2812$,	$\nu = 1{\cdot}218$,	
BCC	$p^* = 0{\cdot}3289$,	$\nu = 1{\cdot}012$,	(8)
FCC	$p^* = 0{\cdot}2166$,	$\nu = 1{\cdot}316$,	
HCP	$p^* = 0{\cdot}2166$,	$\nu = 1{\cdot}316$.	

3. Discussion

We have treated the three-dimensional site percolation problem by the renormalisation-group approach in real space. The results for the fixed point p^*, the eigenvalue λ_1 and the correlation length exponent ν for the five lattices are summarised in table 1. The correlation length exponent for the three-dimensional systems is known to be $0{\cdot}82 \pm 0{\cdot}05$ from the Monte-Carlo experiment (Dunn *et al* 1975) and $0{\cdot}88 \pm 0{\cdot}05$ from the scaling relation (Kirkpatrick 1976, 1977).

The critical percolation probabilities of five lattices obtained from Monte-Carlo experiments (Frisch *et al* 1961, Kirkpatrick 1976) and the series expansions (Sykes *et al* 1976) are listed in table 1. For the simple cubic, face-centred cubic and hexagonal close-packed lattices, our results are in good agreement with them. The diamond lattice and the body-centred cubic lattice really fail to fit our results. The poor agreement may come from the fact that the cluster group is small. Although we calculated another type of renormalisation transformation, this destroyed the symmetry of the lattice and gave bad results for the fixed point and the correlation length exponent.

Table 1. Results of cluster approximations.

Lattice	No of sites	Scale factor	Eigenvalue	Correlation length index	Fixed point	Critical percolation probability
D	14	2	1·685	1·329	0·3591	$0{\cdot}428 \pm 0{\cdot}004$†
SC	8	2	1·768	1·218	0·2812	$0{\cdot}310 \sim 0{\cdot}312$‡
BCC	6	$2\sqrt{2}/\sqrt{3}$	1·624	1·012	0·3289	$0{\cdot}245 \pm 0{\cdot}004$†
FCC	6	2	1·693	1·316	0·2166	$0{\cdot}198 \pm 0{\cdot}003$†
HCP	6	2	1·693	1·316	0·2166	$0{\cdot}204 \pm 0{\cdot}008$§

† Sykes *et al* 1976.
‡ Kirkpatrick 1976, Sykes *et al* 1976.
§ Frisch *et al* 1961.

In a previous paper (Yuge 1978) a general method for applying the renormalisation-group approach to two-dimensional percolation systems was presented, in which the method for constructing an adequate cluster and preserving the symmetry of the lattice was described. For the three-dimensional renormalisation transformation, it must be mentioned that all the sites of the original lattices must be scaled into the new lattice, for which the sites should be, as shown in the figures, constructed in a convex polyhedron with the side length equal to the scale factor. The renormalisation-group approach for two-dimensional percolation systems has been tackled by other authors, but their methods are more complex than ours. We feel that our procedure for the renormalisation-group approach is a very simple but good method for estimating the critical percolation behaviour.

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