Surface-order parameter in three-dimensional percolation

1989 J. Phys. A: Math. Gen. 22 2635

(http://iopscience.iop.org/0305-4470/22/13/056)

J. Phys. A: Math. Gen. **22** (1989) 2635-2638. Printed in the UK

COMMENT

Surface-order parameter in three-dimensional percolation

A Hansen†‡, P M Lam§‖ and S Roux¶

† Institut for Theoretische Physik, Universität zu Köln, D-5000 Köln 41, Federal Republic of Germany

§ Fachberich Physik, Universität zu Essen, D-4300 Essen 1, Federal Republic of Germany

¶ Laboratoire de Physique des Milieux Hétérogènes, URA CNRS 857, Ecole Supérieure de Physique et Chimie Industrielles de Paris, 10 rue Vauquelin, F-75231 Paris Cedex 05, France

Received 18 January 1989

Abstract. We calculate numerically by a transfer-matrix algorithm the critical exponent of the surface order parameter, β_s, for the case of the ordinary transition. Our result, $\beta_s/\nu = 0.98 \pm 0.02$, agrees with recently published series expansion results, $\beta_s/\nu = 1.04 \pm 0.05$ and ε-expansion results with Padé approximants, $\beta_s/\nu = 1.01 \pm 0.06$.

Most studies of percolation deal with the bulk properties of (generally) infinite systems. However, real systems are finite. The study of the influence of boundaries on percolation problems has attracted much less attention than it deserves. We will not get into a precise description of the complex phase diagram appearing in connection with a bounded percolation problem. These different situations are examined in a recent review by Diehl [1]. We will only be concerned in this comment with the 'ordinary' transition in this classification.

We study the case where the probability of having a surface bond is the same as that of the bulk. In order to exhaustively describe this transition, only *one* extra critical exponent is necessary compared with the bulk critical properties. All other critical exponents can be obtained from those scaling relations [1]. We choose here to study the critical exponent of the surface order parameter, β_s. The surface order parameter is the probability that a surface bond belongs to the infinite cluster. This exponent has recently been determined to be $\frac{4}{9}$ in two-dimensional percolation, by methods based on conformal invariance [2]. This result has been confirmed numerically [3, 4].

In three dimensions, to our knowledge, only series expansions and small-scale renormalisation results have been published. More specifically, de'Bell and Essam [5] obtained

$$\beta_s/\nu = 1.04 \pm 0.05 \tag{1}$$

by series expansions methods. Christou and Stinchcombe [6] calculated the ratio β_s/β, where β is the bulk critical exponent, on a simple cubic lattice of size $2 \times 2 \times 2$ using a small-cell renormalisation group technique. Their results were

$$\beta_s/\beta = 1.659 \tag{2}$$

‡ Present address: IBM Bergen Scientific Center, Thormøhlensgate 55, N-5008 Bergen, Norway.

‖ Permanent address: Institute for Theoretical Physics, Chinese Academy of Science, Beijing, People's Republic of China.

0305-4470/89/132635+04$02.50

or

$$\beta_s/\nu = 0.84 \tag{3}$$

using $\beta = 0.45$ and $\nu = 0.89$. The most recent work is the one by Diehl and Lam [7]. They used Padé approximants on the ε-expansion results and obtained

$$\beta_s/\nu = 1.01 \pm 0.06. \tag{4}$$

We report here a numerical determination of this exponent. We use a transfer-matrix method very similar to the one used in [4]. Imagine a simple cubic lattice of dimension $w \times w \times L$, along the x, y and z axes respectively. The bonds between the nodes in the lattice are present with probability p or absent with probability $(1-p)$. At the bottom plane ($x = 0$), we set $p = 1$. In the y direction, the boundary conditions are periodic. The geometry is illustrated in figure 1. Surface sites are those whose first coordinate x is equal to w, whereas bottom sites are those for which x is zero.

The idea behind transfer-matrix algorithms is to 'knit' the network by adding layer after layer in the z direction. As each new layer is added, we keep track of and update all the necessary information on the connections between the sites, i.e. which sites belong to which clusters, in the recently added layer. The algorithm shares certain similarities with the Hoshen-Kopelman procedure [8] for identifying the clusters of connected sites. More specifically, we store an integer-valued matrix $A(x, y)$ which can contain two kinds of information. Each connected cluster which crosses the z plane can be labelled by a 'root', i.e. a unique site which is chosen to be the closest to the bottom plane. Therefore a site is either the root of a cluster, or it belongs to a

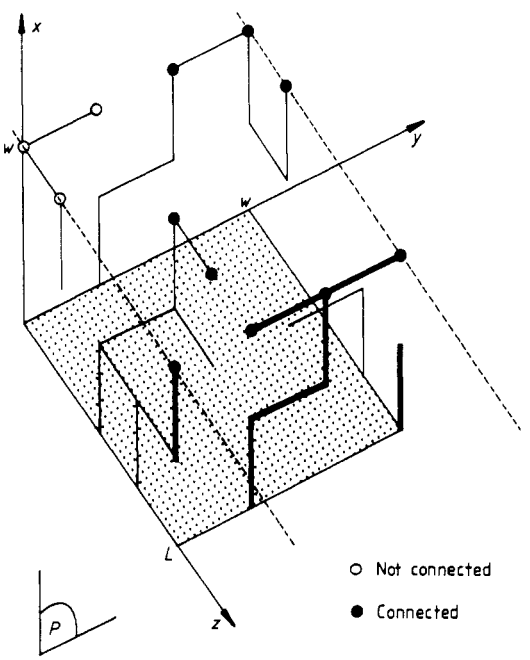

Figure 1. A schematic representation of the lattice used to calculate P_s. The surface sites are shown as circles, filled when they are connected to the bottom plane (grey), or empty if not. The transfer matrix method allows one to keep track of all necessary information about connectedness, in a single plane, P, cut through the bar. The bonds within such a plane (constant z) are shown as bold lines.

cluster whose root is another site. If a site (x, y) is the root of such a cluster, then the value of $A(x, y)$ will be the number of surface sites of the cluster. If the site (x, y) is not the root of a cluster, then it belongs to a cluster whose root is (x', y'). We record this information in storing the address of the root in $A(x, y)$, for instance as $[1+x'+(w+1)y']$ in order to get a single integer. Now, in order to distinguish between the two possible kinds of information stored (either the address of the root, or the number of surface sites connected to the site), we choose by convention to record as negative numbers the values of A which are roots. Changing z to $(z+1)$, implies that all connections between the two planes, and within the $(z+1)$ plane have to be taken into account in order to correctly update the A matrix. The proportion of surface sites that are connected to the bottom plane is finally the value of $A(0, 0)$ divided by the area of the surface wL, since all sites of the bottom plane are connected together.

This proportion, $P_s(w, L)$, is estimated at the percolation threshold $p = p_c = 0.2488$. The width w is a small number, varying in our case from $w = 2$ to 32, whereas the length L is chosen to be large in order to average out the fluctuations, $L = 10^6$ for $w = 2$ to 20 000 for $w = 32$. $P_s(w, L)$ is thus considered, for these L, to be a function of w alone, i.e. $P_s(w)$. In order to minimise spurious edge effects, the initial part of the 'bar' (on a length of 1000) is first omitted. Then the value of $A(0, 0)$ is recorded every tenth of the final length, in order to get an estimate of the statistical errors involved. The computation has been carried out on a Cyber 76. The data are shown in figure 2.

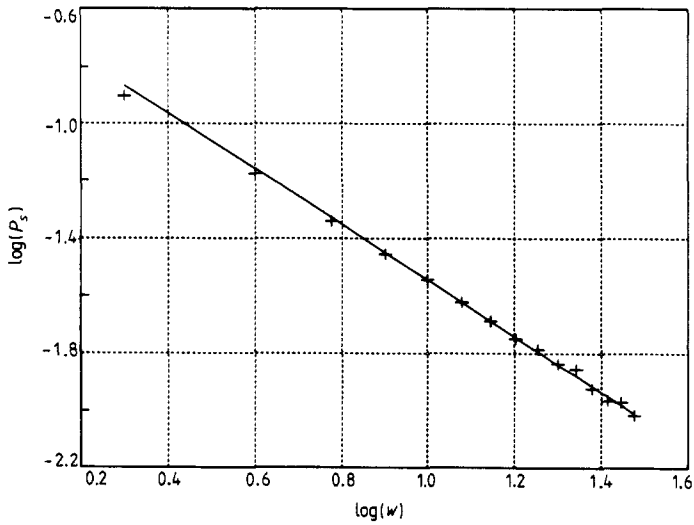

Figure 2. The probability that a bond at the top surface is connected to the bottom surface, P_s, plotted against the width of the lattice, w, in a log-log scale. A straight line of slope 0.98 is shown for reference.

Usual finite-size scaling arguments lead to the following dependence of $P_s(w)$ on w at the percolation threshold:

$$P_s(w) \propto w^{-\beta_s/\nu}. \tag{5}$$

A χ^2 fit gave the estimate

$$\beta_s/\nu = 0.98 \pm 0.02. \tag{6}$$

This result agrees well with the results previously cited (equations (1) and (4)).

Acknowledgments

We acknowledge useful discussions with E Guyon. AH thanks SFB 125, PML thanks the SFB 237 and SR thanks the Ecole Nationale des Ponts et Chaussées for financial support.

References

[1] Diehl H W 1986 *Phase Transitions and Critical Phenomena* vol 10, ed C Domb and J L Leibowitz (New York: Academic) p 76
[2] Cardy J L 1984 *Nucl. Phys.* B **240** 514
Vanderzande C and Stella A C 1987 *J. Phys. A: Math. Gen.* **20** 3001
[3] Vanderzande C 1988 *J. Phys. A: Math. Gen.* **21** 833
[4] Roux S and Hansen A 1988 *Phys. Rev.* B **38** 5170
[5] de'Bell K and Essam J W 1980 *J. Phys. C: Solid State Phys.* **13** 4811
[6] Christou A and Stinchcombe R B 1986 *J. Phys. A: Math. Gen.* **19** 757
[7] Diehl H W and Lam P M 1989 *Preprint*
[8] Hoshen J and Kopelman R 1976 *Phys. Rev.* B **14** 3438