LETTER TO THE EDITOR

Percolation by position-space renormalisation group with large cells†§

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Abstract. We demonstrate that the critical properties of the percolation model can be obtained with a rather high degree of accuracy by extrapolating to $b = \infty$ a sequence of position-space renormalisation group calculations for finite cells of side b. For $b \le 5$ we calculate the recursion relations in closed form, while for $4 \le b \le 500$ we find the recursion relations by Monte Carlo methods. We then obtain a sequence of estimates for the critical concentration p_c and the scaling powers y_p and y_h at the various values of b. Finally, we introduce a transformation from a cell of side b to a cell of side b', which may be veiwed as an 'infinitesimal' transformation with a scale change of b/b'.

1. Introduction

In this Letter we consider the position-space renormalisation group (PSRG) for the percolation problem with a sequence of cells of ever increasing size. We show that we can *extrapolate* the results of finite-cell PSRG calculations to get reliable numbers for the critical concentration, p_c , the temperature-like scaling power, $y_p = v^{-1}$, and also the field-like scaling power y_b .

The idea of very large cells for PSRG was put forth for the Ising model by Friedman and Felsteiner (1977). However, it has never been tested for percolation. More importantly, Friedman and Felsteiner considered cells of maximum size 729 spins. Here we treat a sequence of cells up to size 250 000 sites. Clearly, if one is to extrapolate from the results of finite-cell PSRG, it is desirable to have cells as large as possible. In addition to its accuracy, this approach is further notable for the ease with which it may be modified to treat related models.

This work is based on a PSRG cluster formulation of the percolation problem (Reynolds et al 1977) in which a cell is renormalised to a site using a connectivity weight function. For other PSRG approaches to percolation see, for example, Harris et al (1975), Young and Stinchcombe (1975), Dasgupta (1976) and Kirkpatrick (1977). In this approach to the site percolation problem on the two-dimensional (d = 2) square lattice, a cell is occupied if a connected path of occupied sites exists which spans the cell either horizontally or vertically. We call this transformation R_0 . We have also treated other connectivity weight functions: the transformation R_1 requires spanning in a single direction, while R_2 requires spanning both ways. Only two of

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these three transformations are independent since $2R_1(p) = R_0(p) + R_2(p)$. Furthermore, R_0 and R_2 obey matching relations with each other, and R_1 is 'self-matching' (Reynolds, Stanley, and Klein, to be published). All three transformations behave qualitatively the same, so for this discussion we will treat only R_0 .

We consider here the single- or independent-cell approximation, in which one ignores the possible loss or gain of connecting paths between cells upon renormalisation (see figure 1(b) of Reynolds et al 1977). This appears to be a good approximation in the large cell limit, where the connectivity between cells (which is a surface effect) is negligible compared with the connectivity within a cell (which involves the cell volume). Thus we expect this approximation to become more accurate as b increases.

2. Renormalisation of the site occupation probability

Within the context of the independent-cell approximation, we have calculated exactly the closed-form recursion relations

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

for site percolation on the d=2 square lattice with rescaling factors of b=2,3,4 and 5. These recursion relations are polynomials of degree b^2 . Here p is the probability that a site on the original lattice is occupied, and p' is the renormalised probability. For each value of b, we have calculated both the fixed point, p^* —the point at which p'=p, corresponding to the critical point $p=p_c$ —and the scaling power $y_p=\nu^{-1}$ which may be calculated from

$$\lambda_{p} \equiv \mathrm{d}R(p)/\mathrm{d}p|_{p=p^{*}} = b^{\gamma_{p}} \tag{2}$$

(see Wilson and Kogut 1974 or Niemeyer and Van Leeuwen 1974, for example). As mentioned earlier, the larger cells should provide a better approximate PSRG transformation, and this is indeed borne out upon comparison with series results. The 5×5 cell (with its 2^{25} states) is larger than any cell used for closed-form PSRG calculations on the d=2 Ising model. However, using the PSRG to make a 'one-shot' approximation to the critical properties, even at this size, leads to values of p_c and ν (cf column 1 of table 1) which differ from series estimates by about 10%.

To proceed further, we have calculated the PSRG recursion relations of equation (1) by Monte Carlo methods for b=8, 16, 32, 64, 100, 150, 200 and 500†. (For the purpose of comparison, we have also calculated the recursion relations by Monte Carlo for b=4, 5, for which we have closed-form expressions, and the agreement is excellent.) Of course, b=500 still amounts to a one-shot approximation (albeit a very good one). However, we can do better by extrapolating these finite-cell results to the $b\to\infty$ limit. This limit essentially corresponds to an infinite cell comprising the entire lattice, and the results of this extrapolation should be the true values. Although the PSRG itself becomes singular at $b=\infty$, our PSRG calculations are always for finite b. It is the result of successive finite transformations which we then extrapolate to $b=\infty$, in order to obtain reliable estimates of the true values of p_c and ν .

[†] The algorithm we used both for the Monte Carlo calculations and the closed-form derivations was inspired by Hoshen and Kopelman (1976), and uses the concept of cluster multi-labelling with the equivalence of labels established by a rooted tree structure.

There are several ways in which extrapolation of p_c and ν may proceed. We will discuss certain of our methods here, some of which are analogous to series extrapolation, and others are more similar to the analysis of experimental data in the vicinity of a critical point (which in this case is $b \to \infty$).

In order to extrapolate y_p , first consider the eigenvalue, λ_p , calculated from the PSRG. We may write

$$\lambda_{p}^{\text{true}}(b) = A(b)\lambda_{p}^{\text{calc}}(b), \tag{3}$$

thereby defining A(b), a 'correction' whose magnitude (different from unity) is a measure of the accuracy of the approximation. Then (cf equations 2 and 3) $y_p^{\text{true}} = \ln A(b)/\ln b + y_p^{\text{calc}}$. Thus, if y_p^{calc} is to approach y_p^{true} as $b \to \infty$, we need only impose the relatively weak condition that A(b) must either not tend to zero or infinity, or do so no faster than logarithmically. If A does not diverge we assume $\ln A \to c$ or oscillates about c. Thus asymptotically,

$$y_{\rm p}^{\rm true} = y_{\rm p}^{\rm calc} + c/\ln b, \tag{4a}$$

or

$$\ln \lambda_{p}^{\text{calc}}(b) = y_{p}^{\text{true}} \ln b - c. \tag{4b}$$

Equation (4a) suggests that the sequence $y_p(b)$ should be extrapolated against the variable $1/\ln b$, and that in the asymptotic region where (4a) is valid, this should be a straight line with intercept of y_p^{true} . This procedure leads to $\nu = 1.358^{+0.020}_{-0.013}$, where the error bars represent confidence limits much like those obtained when extrapolating the results from series expansions. Furthermore, equation (4b) suggests that a plot of $\ln \lambda_p^{\text{calc}}(b)$ against $\ln b$ should also be a straight line asymptotically, and this line should have a slope of y_p^{true} . Figure 1 shows this plot, and the inverse slope is $\nu = 1.354 \pm 0.010$. Both these values are somewhat larger than the series estimate $\nu = 1.32^{+0.02}_{-0.07}$ (Cox and Essam 1976).

Extrapolation of the sequence $p^*(b)$ is somewhat different. We expect from finite-size-scaling considerations (Fisher 1971, Sur et al 1976) that

$$(p_c^{\text{true}} - p^*(b)) \sim b^{-1/\nu}.$$
 (5)

In figure 2 we plot $p^*(b)$ against b^{-1/ν_t} , with a trial value of $\nu_t = 1.356$. This leads to an extrapolation for p_c^{true} at the intercept $b^{-1/\nu} = 0$ (i.e. $b = \infty$). We find $p_c = 0.5936^{+0.0005}_{-0.0010}$ —slightly larger than, but consistent with, $p_c = 0.593 \pm 0.02$ predicted by series (Sykes *et al* 1976). Other trial values of ν do not fit the data as well, though the sensitivity for determining ν this way is not high. The predicted value of p_c is essentially unchanged for a range of reasonable choices of ν .

3. Connection with finite-size scaling

Thus far we have presented the PSRG analysis. However, in the process of determining the recursion relations we generate ρ Monte Carlo realisations, where $b^2 \rho \ge 10^7$. Each lattice realisation is filled with random numbers in the interval (0, 1), and the Monte Carlo program asks the question: 'At what p does this array of numbers first span?' (where numbers below p are wetted, and the rest not). We thus generate a distribution, L(b:p), of p values at which spanning occurs, and this distribution appears to be roughly Gaussian. The function R(b:p) (cf equation (1)) is actually

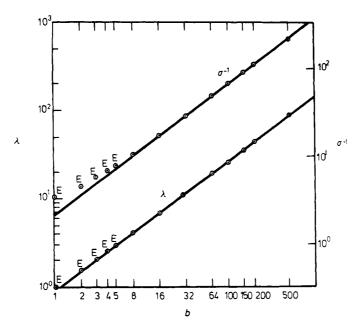


Figure 1. Dependence on $\log b$ of $\log \lambda_p$ and $\log \sigma^{-1}$. From PSRG, $\ln \lambda_p = \nu^{-1} \ln b$, while from finite-size scaling, $\ln \sigma^{-1} \sim \nu^{-1} \ln b$; the calculated slopes yield $\nu = 1.354 \pm 0.010$ and $\nu = 1.357 \pm 0.015$ respectively. The symbol E (for b = 1.5) denotes that the recursion relations for these cases are exact.

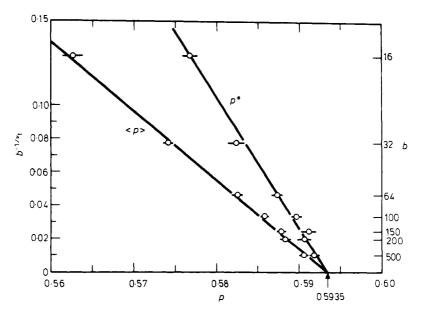


Figure 2. The fixed points, $p^*(b)$, as well as the means, $\langle p \rangle$, at which one spans $b \times b$ cells, are plotted against the variable $b^{-1/\nu}$. Both plots extrapolate to virtually the same value of $p_c = 0.5935^{+0.0005}_{-0.0010}$. We have chosen $\nu_{\text{trial}} = 1.356$ for this particular plot.

determined by integrating L(b:p). However L(b:p) may be treated in a purely statistical sense (Levinshtein et al 1976), as may R(b:p) (Roussenq et al 1976). In this case L(b:p) is called the probability density function, while R(b:p) is the cumulative distribution function. For each b, we have calculated the mean, $\langle p \rangle$, of L(b:p) and the standard deviation from the mean, $\sigma = [(p - \langle p \rangle)^2]^{1/2}$. The mean is an estimate of p_c ; for large b, both $[\langle p \rangle - p_c^{\text{true}}]$ and σ should scale as $b^{-1/\nu}$. Figure 1 shows a plot of $\ln \sigma^{-1}$ against $\ln b$. From its inverse slope we find $\nu = 1.357 \pm 0.015$, which is consistent with both PSRG and series analysis. We have also extrapolated $\langle p \rangle$ in a manner entirely analogous to our extrapolation of p^* , using trial values of ν in linear plots of $\langle p \rangle$ against $b^{-1/\nu}$ (see figure 2). To check self-consistency we plotted $\ln(p_c^{\text{trial}} - \langle p \rangle)$ against $\ln b$. From these plots we find $p_c = 0.5933 \pm 0.0008$ and $\nu = 1.34 - 0.08$ respectively.

We have also calculated the first nine moments and central moments of L(b:p), as well as its skewness, kurtosis, and fourth cumulant. We find that although L(b:p) is not Gaussian for any finite b, it becomes more Gaussian as b increases, and in the limit $b \to \infty$ it tends toward a delta-function. Furthermore, all 'p-like' quantities (e.g. nth roots of nth central moments) vanish as $b^{-1/\nu}$, to within the statistical errors inherent in determination of these higher moments.

We see here a rather intimate relationship between finite-size scaling and the renormalisation group (see also Suzuki 1977). The eigenvalue of the PSRG is the value, $L(b:p^*)$, of the distribution function at $p=p^*$. This approaches a constant times the value, $L(b:p_{max})$, of the distribution at its peak. The limiting value of $L(b:p^*)/L(b:p_{max})$ appears to be very close to one. Because the integral over the entire distribution function is unity, $L(b:p_{\text{max}}) \rightarrow 1/(\sqrt{2\pi}\sigma)$ if the distribution approaches a Gaussian, and in general $\lambda_p \rightarrow \text{constant}/\sigma$. Then, the renormalisation group statement that $\nu = \ln b / \ln \lambda_p$ implies finite-size scaling: asymptotically, $-\nu \ln \sigma = \ln b + \text{constant}$. From a log-log plot, with at least two values of b, this constant may be eliminated, and ν determined. Our two values of b must, of course, both be in the asymptotic region, or we will not eliminate the constant properly. The renormalisation group chooses $\lambda_{\rm p}$ (its ' σ -like' parameter) in such a way that if σ is replaced by λ_p^{-1} , the constant is zero, and we need not be in any asymptotic region. This is because $\lambda_{\rm p}(b=1)=1$, since the eigenvalue of the identity transformation is unity. One might say that the renormalisation group 'knows' a priori its eigenvalue at one other value of b, b = 1. However, since our λ_p^{calc} is only an approximation to λ_p^{true} , asymptotically the intercept need not be zero with the renormalisation group either (cf equation (4b)), and only asymptotically need the slope of $\ln \lambda_p$ against $\ln b$ actually become ν^{-1} .

4. Renormalisation of the ghost bond

In order to obtain the remaining percolation exponents we need to find the 'magnetic' scaling power y_h . To this end we introduce 'ghost-bonds' from every site in the lattice to the single 'ghost-site' (figure 3(a))†, and these are independently occupied with

[†] The ghost-site was originally introduced by Griffiths (1967) as a formal way of introducing a magnetic field in an Ising model. Later Kasteleyn and Fortuin (1969) applied the idea to percolation. In a PSRG context, the ghost was used by Reynolds et al (1977), and later by Marland and Stinchcome (1977).

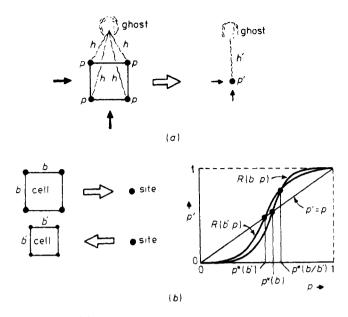


Figure 3. In (a) we show an example of the PSRG transformation for the case b=2. On the original lattice, sites are occupied with probability p, and ghost-bonds with probability h. If we can traverse the cell either horizontally or vertically, the renormalised site is occupied, and this happens with probability p'. Thus, $p' = p^4 + 4p^3(1-p) +$ $4p^2(1-p)^2+2p^2(1-p)^2h^2$, where the last term comes from traversing the cell diagonally through the ghost-site (which cannot be done by nearest-neighbour bonds alone). Likewise, the probability of getting to the ghost site—which necessitates getting into the cell in the first place—occurs with probability $p'h' = p^4[1 - (1 - h)^4] + 4p^3(1 - p)[1 - (1 - h)^3] +$ $5p^2(1-p)^2[1-(1-h)^2]+p^2(1-p)^2h+3p(1-p)^3h$. This is readily brought into the form of equation (6). Evaluated at either $p = p' = p^*$ or $p = p' = p_c$, the eigenvalue, λ_h , is calculated at the fixed point h = 0. Part (b) shows, schematically, a cell-to-cell transformation. The usual cell-to-site transformation, R(b:p), has an inverse, as may be seen from its shape, above. Thus, we may follow a cell-to-site transformation, by the inverse of another cell-to-site transformation, thereby achieving a cell-to-cell transformation with rescaling length b/b'. Just as the fixed point of the cell-to-site transformation occurs when p = R(b:p), so the fixed point value of p in the cell-to-cell transformation occurs at the solution to R(b:p) = R(b':p).

probability h. The recursion relation analogous to equation (1) is then

$$h' = hR_h(b:p,h), \tag{6}$$

where we renormalise the probability of reaching the ghost, again by a horizontal or vertical path through the cell. Since one ghost-bond is always necessary to reach the ghost, we have factored out an h in equation (6).

In order to obtain equation (6), we calculate p'h' = f(p, h) for each cell size b (figure 3). Just as equation (1) is already calculated at h = 0, the fixed point of equation (6), so (6) is calculated at p^* , the fixed point of (1). Thus $R_h(p^*, h) = f(p^*, h)/p^*h$. We have also calculated equation (6) by choosing $p = p' = p_c^{\text{true}}$. In analogy with equation (2), the scaling power y_h is obtained from the eigenvalue of the linear part of equation (6),

$$\lambda_h \equiv dh'/dh|_{\substack{h=0 \ p=p^*}} = R_h(p^*, h=0) = b^{y_h}.$$
 (7)

We have calculated equations (6) and (7) in closed form for b = 2, 3 and 4 (cf table 1). For $b \ge 4$ we have used Monte Carlo methods to find $R_h(p, 0)$. Extrapolation of y_h follows precisely the same arguments as for y_p (see equations (3) and (4)), leading to $1/\ln b$ as the appropriate extrapolation variable.

Table 1. The results of a cell-to-cell transformation in the cases where we have closed-form recursion relations. These transformations are from cells of side b to cells of side b', corresponding to a length rescaling of b/b'. The case b'=1 is the usual cell-to-site transformation, with a rescaling length b. The fixed point p^* , the correlation length exponent $\nu = y_p^{-1}$ and the field-like scaling power, y_h (obtained by evaluating equation (7) both at $p = p^*$ and at $p = p_c$) are displayed. Series estimates for these quantities are $p_c = 0.593 \pm 0.002$, $\nu = 1.32^{+0.07}_{-0.07}$ and $y_h = 1.895 \pm 0.004$.

From b =		To $b'=1$	2	3	4
2	p*	0.382		_	_
	ν	1.64	_	_	
	y_h at p^*	1.86	_	_	_
	y_h at p_c	1.94	_	_	
3	p*	0.473	0.560		
	ν	1.51	1.28		_
	y_h at p^*	1.86	1.87		_
	y_h at p_c	1.93	1.91	_	-
4	p*	0.509	0.574	0.591	
	ν	1.49	1.32	1.38	
	y_h at p^*	1.87	1.88	1.89	
	y_h at p_c	1.92	1.91	1.90	_
5	p*	0.529	0.581	0.594	0.598
	ν	1.47	1.34	1.39	1.40

5. Cell-to-cell transformation

Thus far all our transformations have been from cells of ever increasing size, b^2 , to a single site. One would also like to be able to go in the other direction, toward an 'infinitesimal transformation' in which $b \rightarrow 1$ (Wilson and Kogut 1974). In principle, our large cells enable one to achieve this goal.

By rescaling from a cell of side b to a site, we obtain a transformation p'(b) = R(b:p) (cf equation (1)). Another cell with side b' only slightly smaller than b has an analogous transformation. Both transformations are analytic and, in the range (0, 1), have inverses[†]. Hence, one can find a recursion relation

$$p'(b) = R[b:R^{-1}(b':p'(b'))] = R(b/b':p'(b')), \tag{8}$$

which gives the probability of having an occupied cell of side b as a function of having an occupied cell of side b' (see figure 3(b)). The value of p at which p'(b) = p'(b'), or equivalently at which R(b:p) = R(b':p), corresponds to p_c . The exponent ν is

[†] This is because p'(p)—the probability of getting across a cell at a given site probability p—is an increasing function of p, and the transformation $R: p \to p'$ is one-to-one and onto.

obtained from

$$\nu = \frac{\ln(\text{scale change})}{\ln(\text{eigenvalue})} = \frac{\ln b/b'}{\ln dp'(b)/dp'(b')} = \frac{\ln b - \ln b'}{[\ln dR(b:p)/dp - \ln dR(b':p)/dp]|_{p=p^*}}, \quad (9)$$

where p^* is the fixed point value of p in the cell-to-cell transformation. The scaling power y_h is calculated analogously.

While the Monte Carlo accuracy is not yet sufficient for reliable cell-to-cell estimates, our closed-form results for $b, b' \le 5$ lead to estimates of p_c , ν , and y_h (table 1) whose discrepancy with series results is comparable to the single-shot cell-to-site transformation for $b \approx 100$.

6. Conclusion

In summary, we have demonstrated that critical properties for the percolation threshold can be obtained with a rather high degree of accuracy by extrapolation to $b=\infty$ of a sequence of PSRG calculations for finite cells of side b. We find that the critical properties are essentially the same regardless of the method used. Our best estimates for the two scaling powers are $y_p = 0.7375^{+0.0072}_{-0.0081}$ and $y_h = 1.898 \pm 0.003$ from which we obtain

$$\alpha = -0.712 \pm 0.030, \qquad \beta = 0.138^{+0.006}_{-0.005}, \qquad \gamma = 2.435 \pm 0.035, \qquad \delta = 18.6 \pm 0.6,$$

$$\nu = 1.356 \pm 0.015 \quad \text{and} \quad 2 - \eta = 1.796 \pm 0.006, \tag{10}$$

which compare well with estimates obtained by other methods (see, e.g., table 1 of Stanley 1977). The site percolation threshold is found to occur at $p_c = 0.5935^{+0.0005}_{-0.0010}$ on the square lattice. We have recently learned that Kirkpatrick (private communication) is applying our method of studying R(b:p) to the bond problem. His results thus far confirm our contention that this method produces highly accurate estimates for the critical properties of the percolation problem. In addition, Klein, Stanley, Reynolds and Coniglio (to be published) have provided detailed renormalisation group analysis to support the validity of the closed-form expression $\nu = \ln \sqrt{3}/\ln \frac{3}{2} = 1.3547...$ obtained for the triangular lattice in Reynolds et al (1977). This value of ν is in excellent agreement with the value $\nu = 1.356$ reported above.

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References

Dasgupta C 1976 Phys. Rev. B 14 1221-4

Dunn A G. Essam J W and Ritchie D S 1975 J. Phys. C: Solid St. Phys. 8 4219-35

Fisher M E 1971 Critical Phenomena: Enrico Fermi Summer School, Varenna, Italy, Course 51 ed. M S Green (New York: Academic)

Friedman Z and Felsteiner J 1977 Phys. Rev. B 15 5317-9

Griffiths R B 1967 J. Math. Phys. 8 484-9

Harris A B, Lubensky T C, Holcomb W K and Dasgupta C 1975 Phys. Rev. Lett. 35 327-30

Hoshen J and Kopelman R 1976 Phys. Rev. B 14 3438-45

Kasteleyn P W and Fortuin C M 1969 J. Phys. Soc. Japan Suppl. 26 11-14

Kirkpatrick S 1977 Phys. Rev. B 15 1533-8

Levinshtein M E, Shklovskii B I, Shur M S and Efros A L 1976 Sov. Phys.-JETP 42 197-200

Marland L G and Stinchcombe R B 1977 J. Phys. C: Solid St. Phys. 10 2223-32

Niemeyer Th and Van Leeuwen J M J 1974 Physica 71 17-40

Reynolds P J, Klein W and Stanley H E 1977 J. Phys. C: Solid St. Phys. 10 L167-72

Roussenq J, Clerc J, Giraud G, Guyon E and Ottavi H 1976 J. Physique 37 L99-101

Stanley H E 1977 J. Phys. A: Math. Gen. 10 L211-20

Sur A, Lebowitz J L, Marro J, Kalos M L and Kirkpatrick S 1976 J. Statist. Phys. 15 345-53

Suzuki M 1977 Prog. Theor. Phys. 58 1142-1150

Sykes MF, Gaunt DS and Glen M 1976 J. Phys. A: Math. Gen. 9 97-103

Wilson K G and Kogut J 1974 Phys. Rep. 12 75-199

Young A P and Stinchcombe R B 1975 J. Phys. C: Solid St. Phys. 8 L535-40