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Monte Carlo renormalisation group approach to critical percolation behaviour in three dimensions: simple cubic lattice

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Abstract. A Monte Carlo renormalisation group approach using a scaling transformation in real space is applied to the critical properties for the site percolation problem on the simple cubic lattice. We find a sequence of estimates for the critical concentration p_c and the eigenvalue λ at various values of the rescaling length b. Extrapolation of these sequences to the limit $b \to \infty$ yields the site percolation threshold $p_c = 0.3115^{+0.0004}_{-0.0003}$ and the connectedness length exponent $\nu = 0.88 \pm 0.04$.

1. Introduction

Percolation has been actively studied using both momentum-space and position-space renormalisation group approaches. A variety of position-space renormalisation group approaches have been developed recently, and some of them are highly promising for the study of the critical percolation phenomena.

In this paper we present the position-space renormalisation group approach for the three-dimensional site percolation problem on the simple cubic lattice with a sequence of cells of ever increasing size. Our renormalisation method is based on the block formulation used in the derivation of the exact critical percolation probability for the simple cubic lattice with simplest cell size (Yuge 1979). For other renormalisation group approaches to percolation, see Harris *et al* (1975), Young and Stinchcombe (1975), and Reynolds *et al* (1978, 1980).

The technique we use for determination of the fixed point p^* and the connectedness length exponent ν is the Monte Carlo renormalisation group approach (Reynolds *et al* 1980). For a two-dimensional lattice, Monte Carlo renormalisation studies has so far been performed by several investigators who have succeeded in obtaining a precise estimate of the percolation threshold (Reynolds *et al* 1980, Vicsek and Kertész 1981, Derrida and de Seze 1982, Djordjevic *et al* 1982). There has, however, been no attempt to apply this approach to the three-dimensional percolation system.

The layout of the paper is as follows. In § 2, we give some principles of the real space renormalisation group approach to percolation and demonstrate with an example using small cells. In § 3, we give a brief review of this Monte Carlo technique and the results obtained by the renormalisation group approach. Then we present sequences for the values of the critical percolation probability and the scaling power ν from

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which the critical exponent may be obtained. We also discuss how extrapolation of these sequences to the limit of infinite cell size leads to numerical results.

2. Renormalisation group approach to percolation

We start by partitioning a lattice into cells which cover the lattice and maintain its original symmetry. These cells will play the role of renormalised sites; given that the sites are independently occupied with probability p, then the occupation probability p' for the site of the new lattice may be derived from the renormalisation transformation

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

where $R(p; b)$ is the probability which connects the cell either horizontally or vertically and b is the change of scale of length. The simplest example is $b = 2$. The basic scaling procedure is defined by a simple renormalisation transformation on finite lattices. In figure 1, we show how the basic scaling lattice (full line) scales into the new lattice (broken line) with a scale factor $b = 2$; the cell with the black sites of the $2 \times 2 \times 2$ lattice scales into a single white site with probability p'. The sites in the original lattice are independently present (conducting) with probability $1 - p$. When an electric voltage is applied to the cell sandwiched between two electrodes A and B in figure 1(b), a conductive cell is defined as a graph in which a continuous conducting path from electrode A to electrode B exists. The transformed probability $R(p; b)$ is defined as the probability of the cell being conductive when the cell is sandwiched between two plane electrodes. We can obtain the transformed probability from the combinations of paths contributing to the connectivity according to the exclusion-inclusion principle:

$$\begin{aligned} R(p; b = 2) = {} & 4p^2(1-p)^6 + 24p^3(1-p)^5 + 54p^4(1-p)^4 \\ & + 56p^5(1-p)^3 + 28p^6(1-p)^2 + 8p^7(1-p) + p^8. \end{aligned} \tag{2}$$

The function $R(p; b)$ has been evaluated for b up to 50 by Monte Carlo methods. As b increases, $R(p; b)$ become sharper and approaches the step function.

Equation (1) serves as the highly approximate renormalisation group transformation with fixed points given by

$$p^*(b) = R(p^*; b). \tag{3}$$

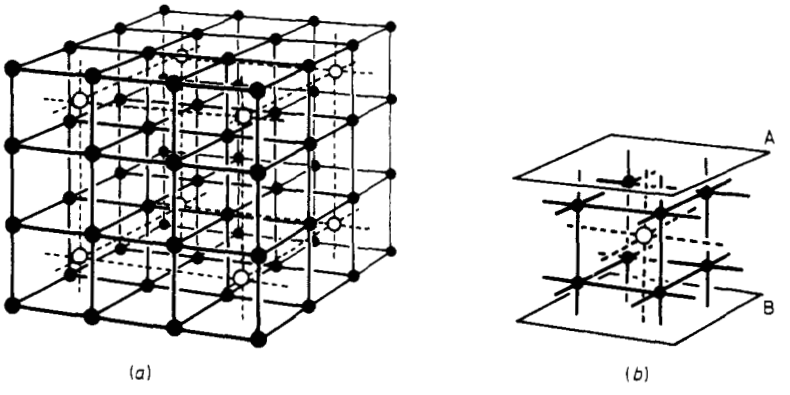

Figure 1. (a) Transformation of the simple cubic site lattice: the full line refers to the original lattice and the broken line expresses the new lattice with the scale factor $b = 2$. (b) Cell with eight sites sandwiched between two plane electrodes A and B.

A non-trivial fixed point gives the critical percolation probability p_c for the finite cell of size b. From equations (2) and (3), we find two trivial fixed points at $p^* = 0, 1$, and also a non-trivial fixed point at

$$p^*(b=2) = 0.2818. \tag{4}$$

From the fixed point p^* of equation (1), the eigenvalue λ is defined by

$$\lambda = \left.\frac{dR(p;b)}{dp}\right|_{p=p^*} \tag{5}$$

from which we determine the exponent ν through

$$\nu = \ln b / \ln \lambda. \tag{6}$$

For the simplest example $b = 2$, the eigenvalue and the connectedness length exponent are given from the scaling transformation (2) by

$$\lambda(b=2) = 1.7588 \qquad \nu(b=2) = 1.2276. \tag{7}$$

3. Monte Carlo renormalisation group and determination of $R(p;b)$

We consider here the Monte Carlo renormalisation group for the percolation problem with a sequence of cells up to a cell size of 125 000 sites. We first define $R(p;b)$ to be the connecting probability. Then we determine the underlying probability density function $L(p;b)$ from

$$R(p;b) = \int_0^p L(p';b)\,dp' \tag{8}$$

where $L(p;b)\,dp$ gives the probability that a $b \times b \times b$ cell first percolates when the occupation probability lies between p and $p+dp$. In other words, $R(p;b)$ is the cumulative distribution function corresponding to the probability density function $L(p;b)$. The eigenvalue is a value of the density function $L(p;b)$ at $p = p^*$:

$$\lambda = \left.\frac{dR(p;b)}{dp}\right|_{p=p^*} = L(p^*;b). \tag{9}$$

We present the results of our renormalisation group approach for various cell sizes on the simple cubic lattice in table 1. The error bars on all our Monte Carlo data are derived by comparing the values obtained using different subsets of the data and taking their mean-square errors.

We may extrapolate our results to the $b \to \infty$ limit from Monte Carlo results for a sequence of values of b. We expect from finite-size scaling arguments that

$$\lambda \sim b^{-1/\nu}. \tag{10}$$

In figure 2 we plot $\log \lambda(b)$ against $\log b$. The slope of $\log \lambda(b)$ against $\log b$ gives the estimated value of ν. This procedure leads to $\nu = 0.88 \pm 0.04$, where the error bars are obtained by comparing the results of least-square fits with successive data points sampled from the set. Our estimated value is somewhat larger than the Monte Carlo estimate $\nu = 0.8 \pm 0.1$ (Sur *et al* 1976). Heerman and Stauffer (1981) found $\nu = 0.89 \pm 0.01$ through Monte Carlo simulations. The connectedness length exponent for the Delaunay network is calculated as $\nu = 0.88 \pm 0.05$ from Monte Carlo simulations (Jerauld *et al* 1984). The best estimate of the exponent ν in three dimensions is $\nu = 0.88 \pm 0.02$ as found by Gaunt and Sykes (1983) using series expansions.

Table 1. Exact and Monte Carlo results on the simple cubic lattice. The quantities p_m^+ and p_t^+ refer to the median and the value at which the cumulative distribution function $R(p; b)$ is $\frac{1}{3}$, respectively.

b	No of realisations	p^*	$p_m^+(c=\frac{1}{2})$	$p_t^+(c=\frac{1}{3})$	λ	λ_m	ν	ν_m
2	Exact	0.2818	0.3989	0.3100	1.7588	1.8974	1.2276	1.0822
5	100 000	0.3072 ± 0.0003	0.3486 ± 0.0003	0.3131 ± 0.0003	4.36 ± 0.07	4.8	1.093 ± 0.012	1.026
7	102 677	0.3099 ± 0.0003	0.3389 ± 0.0002	0.3138 ± 0.0002	6.20 ± 0.15	7.6	1.067 ± 0.014	0.959
9	74 712	0.3105 ± 0.0003	0.3323 ± 0.0002	0.3133 ± 0.0002	8.14 ± 0.14	9.1	1.048 ± 0.009	0.995
10	48 460	0.3111 ± 0.0003	0.3307 ± 0.0003	0.3136 ± 0.0003	9.1 ± 0.3	10.4	1.043 ± 0.015	0.983
11	38 426	0.3112 ± 0.0003	0.3288 ± 0.0003	0.3134 ± 0.0003	10.1 ± 0.1	11.1	1.037 ± 0.005	0.996
12	40 490	0.3112 ± 0.0002	0.3273 ± 0.0002	0.3131 ± 0.0002	11.3 ± 0.2	12.4	1.025 ± 0.007	0.987
15	18 526	0.3111 ± 0.0002	0.3239 ± 0.0002	0.3127 ± 0.0002	14.1 ± 0.8	15.8	1.023 ± 0.021	0.981
16	16 368	0.3116 ± 0.0003	0.3236 ± 0.0002	0.3131 ± 0.0003	14.2 ± 0.6	17.6	1.045 ± 0.016	0.967
17	16 994	0.3108 ± 0.0003	0.3219 ± 0.0003	0.3123 ± 0.0003	16.1 ± 0.5	18.9	1.020 ± 0.012	0.964
18	14 577	0.3112 ± 0.0002	0.3218 ± 0.0003	0.3125 ± 0.0002	17.7 ± 0.6	19.9	1.006 ± 0.012	0.966
20	8 905	0.3115 ± 0.0003	0.3207 ± 0.0003	0.3127 ± 0.0002	19.7 ± 1.0	24.4	1.005 ± 0.016	0.938
25	5 555	0.3113 ± 0.0004	0.3183 ± 0.0003	0.3122 ± 0.0003	25.2 ± 0.9	28.8	0.998 ± 0.011	0.958
30	2 726	0.3114 ± 0.0004	0.3172 ± 0.0003	0.3122 ± 0.0004	31.7 ± 3.5	36.8	0.984 ± 0.029	0.943
34	5 550	0.3113 ± 0.0003	0.3165 ± 0.0002	0.3121 ± 0.0002	31.3 ± 4.3	40.2	1.024 ± 0.037	0.955
40	1 974	0.3115 ± 0.0002	0.3154 ± 0.0002	0.3120 ± 0.0002	42.8 ± 3.1	48.6	0.982 ± 0.018	0.950
50	2 273	0.3109 ± 0.0005	0.3142 ± 0.0004	0.3112 ± 0.0004	56.3 ± 2.2	65.9	0.971 ± 0.010	0.935
∞		$0.3115^{+0.0004}_{-0.0003}$	0.3094 ± 0.0005	$0.3115^{+0.0002}_{-0.0004}$			0.88 ± 0.04	0.87

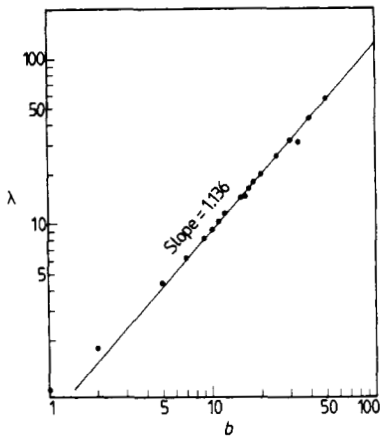

Figure 2. Determination of the critical exponent ν from the log-log plot of the eigenvalue λ against the scale factor b. From the slope of this line we obtain the exponent estimate $\nu = 0.88 \pm 0.04$.

The renormalisation group approach has an advantage in that one can systematically consider finite-size cells with different b. We find that the sequence $p^*(b)$ varies smoothly and predictably with b, following the relation

$$p^*(b) - p_c(b = \infty) \sim b^{-1/\nu} \tag{11}$$

suggested by finite-size scaling considerations. In figure 3 we plot $p^*(b)$ against $b^{-1/\nu}$, with a trial value of $\nu = 0.88$. Extrapolating a sequence of estimate for $p^*(b)$ for a range of b from 2 to 50, we find the estimate

$$p^*(b = \infty) = 0.3115^{+0.0004}_{-0.0003} \tag{12}$$

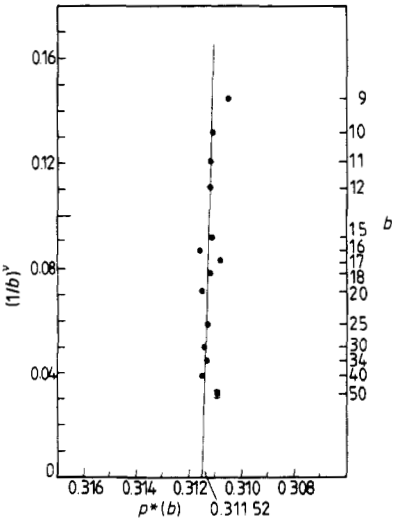

Figure 3. Extrapolation of the sequence of fixed points $p^*(b)$. This curve approaches an estimate of $p_c = 0.311\,52$ as $b \to \infty$. We have chosen the trial value of $\nu = 0.88$ for this plot.

where the error bars are obtained by comparing the results of least-square fits with successive data points sampled from the set, and also with the values of the individual data points varying within their own error bars. Our estimate is in good agreement with the most accurate previous estimates, $p_c = 0.3115 \pm 0.0005$ obtained by Monte Carlo experiments (Sur *et al* 1976), and 0.3117 ± 0.0003 obtained by the series expansion method (Gaunt and Sykes 1983).

In the renormalisation group analysis presented thus far, we have seen that the non-trivial fixed point for finite b gives a good estimate of the critical probability. As an alternate approximation we consider the $100c$-percentile $p^+(b; c)$ of the renormalisation function, defined by

$$\int_0^p L(p'; b)\, dp' = R(p^+; b) = c \tag{13}$$

where $0 < c < 1$. When c is equal to $\frac{1}{2}$, $p^+(b; c)$ expresses the median of the distribution function $R(p; b)$. As the cell size approaches infinity, $p^+(b; c)$ converges to p_c and therefore serves as an approximation for the critical percolation probability. Since the rate of convergence of $p^+(b; c)$ depends on c, the problem for us is to determine the best choice for c.

In the two-dimensional case, the exact relation

$$R(p_c; b) = \tfrac{1}{2} \tag{14}$$

holds for several types of lattices with finite size. In fact, (14) reduces to a known expression

$$R(\tfrac{1}{2}; b) = \tfrac{1}{2} \tag{15}$$

for the site percolation on self-matching lattices as well as for the bond percolation on self-dual lattices. Furthermore, formula (14) applies to the bond problem on the triangular and the honeycomb lattices. The existence of (14) suggests that the value of c should be chosen to be $\frac{1}{2}$ in two dimensions. In the three-dimensional case, we have at present no criterion for the determination of c, but we conjecture that $c = \frac{1}{3}$ is more suitable than $c = \frac{1}{2}$.

Let us take some values of c near $\frac{1}{3}$. The estimates $p^+(b; c)$ for $c = 0.28$, 0.29, 0.30, 0.31, 0.32, 0.33, 0.34, 0.35, 0.40, 0.45 and 0.50 are presented in table 2. In addition, for large b, $(p^+(b; c) - p_c(b; c))$ should scale as $b^{-1/\nu}$. Thus in figure 4 we have plotted $p^+(b; c)$ against $b^{-1/\nu}$, with $\nu = 0.88$, in complete analogy with the plot for p^* in figure 3. These estimated $p^+(b; c)$ essentially agree, giving an extrapolated value of $p_c = 0.3115$.

We investigate again the relationship between finite-size scaling and the renormalisation group approach. The eigenvalue of the renormalisation group transformation is given by the value of the density function $L(p; b)$ at $p = p^*$. As the cell size becomes infinite, $L(p; b)$ and $R(p; b)$ approach a delta function and a step function, respectively. Both $L(p^*; b)$ and $L(p^+; b)$ approach the eigenvalue λ. Provided the cell size b is reasonably large, we can approximate the fixed point by $L(p^+; b)$. Therefore we approximate the fixed point by $p^* = p^+$, the concentration at which the cumulative distribution function $R(p; b)$ equal c. The 'eigenvalue' may be expressed as

$$\lambda(p^+) = \left.\frac{dR(p; b)}{dp}\right|_{p=p^+} \tag{16}$$

Table 2. Exact and Monte Carlo results on the simple cubic lattice with various values of c.

b	No. of realisations	0.30			0.31	0.32	0.33	0.34	0.35			0.40			0.45		
		p^+	$\lambda^{(p^+)}$	$\nu^{(p^+)}$	p^+	p^+	p^+	p^+	p^+	$\lambda^{(p^+)}$	$\nu^{(p^+)}$	p^+	$\lambda^{(p^+)}$	$\nu^{(p^+)}$	p^+	$\lambda^{(p^+)}$	$\nu^{(p^+)}$
2	Exact	0.2921	1.788	1.193	0.2976	0.3132	0.3187	0.3141	0.3195	1.851	1.126	0.3409	1.888	1.090	0.3726	1.904	1.076
5	100 000	0.3056	4.4	1.086	0.3079	0.3102	0.3124	0.3146	0.3168	4.5	1.070	0.3258	4.7	1.040	0.3383	4.9	1.013
7	102 677	0.3081	5.6	1.130	0.3099	0.3116	0.3116	0.3149	0.3165	6.0	1.086	0.3227	7.0	1.000	0.3315	6.8	1.015
9	74 717	0.3098	7.6	1.083	0.3104	0.3116	0.3128	0.3141	0.3152	7.8	1.070	0.3200	8.7	0.961	0.3268	8.5	1.027
10	48 460	0.3099	8.4	1.082	0.3111	0.3122	0.3133	0.3144	0.3154	8.4	1.082	0.3195	9.4	1.028	0.3259	9.9	1.004
11	38 426	0.3101	9.9	1.046	0.3112	0.3122	0.3131	0.3141	0.3152	9.7	1.055	0.3190	10.7	1.012	0.3243	11.0	1.000
12	40 490	0.3102	10.6	1.053	0.3110	0.3119	0.3128	0.3138	0.3147	11.4	1.021	0.3183	11.3	1.025	0.3233	12.6	0.981
15	18 526	0.3104	14.7	1.008	0.3110	0.3118	0.3125	0.3131	0.3137	14.8	1.005	0.3166	14.8	1.005	0.3205	15.3	0.993
16	16 368	0.3106	13.7	1.059	0.3115	0.3122	0.3129	0.3136	0.3143	14.1	1.048	0.3168	16.1	0.998	0.3206	17.3	0.973
17	16 994	0.3101	16.1	1.020	0.3107	0.3114	0.3120	0.3126	0.3132	16.4	1.013	0.3158	16.0	1.022	0.3192	17.9	0.982
18	14 577	0.3105	16.4	1.033	0.3112	0.3117	0.3122	0.3128	0.3134	16.3	1.036	0.3160	17.2	1.016	0.3192	19.5	0.973
20	8 905	0.3110	17.7	1.043	0.3114	0.3120	0.3125	0.3129	0.3135	19.1	1.016	0.3159	20.3	0.995	0.3185	23.2	0.953
25	5 555	0.3108	24.2	1.010	0.3112	0.3116	0.3120	0.3124	0.3128	25.6	0.993	0.3145	26.0	0.988	0.3166	30.3	0.944
30	2 726	0.3110	25.7	1.048	0.3114	0.3117	0.3121	0.3124	0.3127	31.4	0.987	0.3139	33.6	0.968	0.3158	32.9	0.974
34	5 550	0.3109	35.4	0.989	0.3112	0.3116	0.3120	0.3123	0.3125	40.6	0.952	0.3135	40.5	0.953	0.3151	44.5	0.929
40	1 974	0.3112	39.0	1.007	0.3114	0.3117	0.3119	0.3121	0.3124	42.0	0.987	0.3134	48.0	0.953	0.3144	55.1	0.920
50	2 273	0.3106	54.0	0.980	0.3108	0.3110	0.3111	0.3113	0.3115	55.3	0.975	0.3122	58.7	0.961	0.3132	62.7	0.945
∞		0.3116		0.89	0.3115	0.3115	0.3114	0.3114	0.3114		0.87	0.3108		0.87	0.3101		0.84

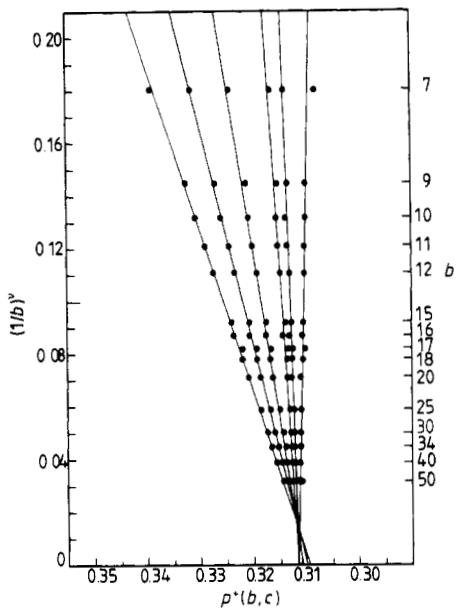

Figure 4. Finite-size scaling extrapolation of the sequence of $p^{+}(b; c)$. We have chosen the trial value of $\nu = 0.88$. The plot is similar to figure 3 where $p^{*}(b)$ is extrapolated.

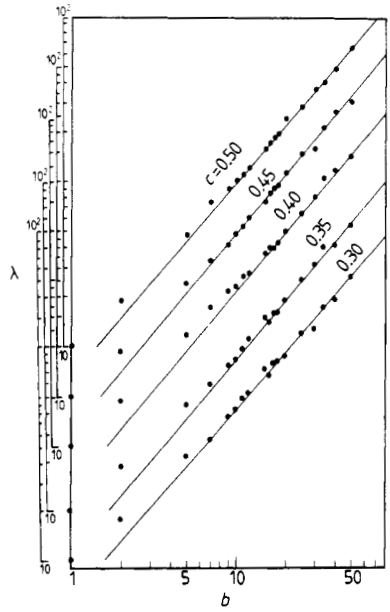

Figure 5. Dependence on log b of $\lambda^{(p^{+})}(b; c)$, for $c = 0.30$, 0.35, 0.40, 0.45 and 0.50. These plots have the same slope. The plots are similar to figure 3.

which is also expected to follow the relation

$$\lambda(p^+) \sim b^{-1/\nu}. \tag{17}$$

In figure 5 we have plotted $\lambda^{(p^+)}(b; c)$ against $b^{-1/\nu}$ for $c = 0.30$, 0.35, 0.40, 0.45 and 0.50, in complete analogy with the plot in figure 2. The slope of $\log \lambda^{(p^+)}(b; c)$ against $\log b$ essentially agrees with an extrapolated value of $\nu = 0.88$.

4. Conclusion

We have shown that critical properties for the site percolation problem on the simple cubic lattice can be obtained by extrapolating a sequence of Monte Carlo renormalisation group calculations to $b \to \infty$ for finite cells of size b. To obtain the percolation threshold p_c and the connectedness length exponent ν, we calculate $p^*(b)$, $\lambda(b)$, $p^+(b; c)$ and $\lambda^{(p^+)}(b; c)$ for finite cells by the renormalisation group technique. Then we find sequences for the critical percolation concentration $p_c(b)$ and the eigenvalue $\lambda(b)$ of a finite size. Furthermore, we find that sequences for the estimates $p^+(b; c)$ and $\lambda^{(p^+)}(b; c)$ also obey a power law. For the two-dimensional site percolation problem the best choice of c is found to be $\frac{1}{2}$, but $c = \frac{1}{3}$ seems to be more adequate in three dimensions.

Our best estimates for the critical percolation probability p_c and the connectedness length exponent ν obtained by these scaling laws are, for the simple cubic site lattice,

$$\begin{aligned} p_c &= 0.3115^{+0.0004}_{-0.0003} \\ \nu &= 0.88 \pm 0.04. \end{aligned} \tag{18}$$

Our estimate ν agrees with the estimate $\nu = 0.88 \pm 0.02$ of Gaunt and Sykes (1983) obtained by using series expansions.

Although the above arguments have been perforce limited to the simple cubic lattice, the basic idea is easily incorporated into common approximation methods for any lattice and we expect that it be applied advantageously to a wide variety of problems. Extension of the present renormalisation analysis to more complicated lattices will be presented in the near future.

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