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COMMENT

Phenomenological renormalisation of Monte Carlo data for percolation

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Abstract. The accuracy of a phenomenological renormalisation which is based on Monte Carlo data is tested by investigating site percolation in a simple cubic lattice. The method appears to be very accurate and can yield precise estimates of the quantities of interest with small to moderate lattice sizes. The site percolation threshold of the lattice is predicted to be 0.3115 ± 0.0005. If ν is the exponent of correlation length, we find $\beta/\nu \simeq 0.48 \pm 0.01$ for the exponent of percolation probability and $\beta_B/\nu \simeq 1.1 \pm 0.03$ for the backbone exponent, in agreement with most accurate data currently available. An analysis of the data at the percolation threshold based on the standard finite-size scaling method also supports the results.

Presently, none of the critical exponents for the percolation problem (Essam 1980, Stauffer 1985) are known exactly for two- or three-dimensional systems. However, in two dimensions the conjectures of den Nijs (1979), Nienhuis *et al* (1980) and Pearson (1980) are strongly supported by a variety of precise estimates of the exponents or by (not entirely rigorous) theoretical arguments, and are widely believed to be exact. These have been summarised and reviewed by Sahimi (1983). In three dimensions, the situation is less satisfactory and there is no general consensus concerning the values of the critical exponents obtained from series expansions, Monte Carlo (MC) simulations, renormalisation group (RG) method or any other technique. Therefore there remains the need for an accurate method of estimating the quantities of interest.

Phenomenological renormalisation (PR) (Nightingale 1976, 1982) has proven to be a very powerful method of probing critical behaviour. In this approach, the correlation lengths $\xi_L(p)$ and $\xi_{L'}(p)$ of the system are computed for two different systems of linear dimensions L and L' at the fraction p of active sites or bonds. The systems are usually $L \times \infty$ strips. One infers a renormalisation transformation (RT) $p \to p'$ by setting

$$\xi_L(p)/L = \xi_{L'}(p')/L'. \tag{1}$$

The fixed point $p = p' = p^*(L, L')$ of the RT is an estimate of the percolation threshold p_c, while the exponent ν of the correlation length is estimated from

$$(\mathrm{d}p'/\mathrm{d}p)_{p=p^*} = (L/L')^{1/\nu}. \tag{2}$$

These estimates of p_c and ν depend upon L and L', but in practice the convergence to the asymptotic ($L \to \infty$) values is apparently very rapid as L and L' are increased, if the ratio L/L' is kept as close to unity as possible; see Derrida and de Seze (1982), Privman and Fisher (1983), Herrmann and Stauffer (1984) and Luck (1935) for a

discussion of the rate of convergence. For percolation and lattice animal problems in two dimensions this method has been employed by Derrida and co-workers with considerable success (Derrida and de Seze 1982, Derrida and Stauffer 1985, Derrida and Vannimenus 1980, Nadal *et al* 1982). By combining the PR method with MC calculations accurate estimates of the exponents of percolation conductivity have also been obtained (Derrida and Vannimenus 1982, Derrida *et al* 1983, Herrmann *et al* 1984, Zabolitzky 1984). A computer program which uses this method to calculate the conductivity of very large systems at any p has also been published (Derrida *et al* 1984). Kinzel and Yeomans (1981) employed the PR method for two-dimensional directed percolation. Many other statistical and quantum mechanical systems in two dimensions have been studied with this method (see Nightingale (1982) for a review). In such systems the temperature T plays the role of p (see Blöte *et al* 1981).

However, the application of the PR has been limited to two-dimensional systems and the efficiency of the method is less obvious in three dimensions. One needs a sequence of several systems of moderate to large sizes for the extrapolation methods to work, but the sheer numerical size of the problem forbids one from calculating exact eigenvalues (i.e. the left side of (2)) which are needed for calculating the critical properties of large systems. The largest system that we are aware of is a $L=5$ lattice (i.e. a $5\times5\times N$ lattice where N is large) that was used by Hamer (1983) to study a (2+1)D Ising model. Since the PR is a consequence of finite-size scaling (for a review see Barber 1983), it is natural to look for another RT using some other quantities that satisfy finite-size scaling but are also more accessible than the correlation length, particularly from the point of view of MC calculations. One also needs a method that can be used for three-dimensional systems.

In this comment we test the accuracy of a method (Barber and Selke 1982, see also Binder 1981), phenomenological renormalisation of Monte Carlo data, by applying it to site percolation in three dimensions. This method is based on calculating a quantity $P_L(p)$ and consequently determining the quantity $\zeta_{L,L'}(p)$ defined by

$$\zeta_{L,L'}(p)=\ln(P_L/P_{L'})/\ln(L/L'). \tag{3}$$

If $P_L(p)$ scales with L as

$$P_L(p)\sim L^{-\omega}F(L^{\theta}\varepsilon) \tag{4}$$

as in finite-size scaling theory, where $\varepsilon=(p-p_c)/p_c$, $\theta=\nu^{-1}$, $\omega=x/\nu$, and x is the critical exponent of $P_L(p)$ as $L\to\infty$, i.e.

$$P_\infty(p)\sim\varepsilon^x, \tag{5}$$

then from (3), the intersection of $\zeta_{L,L'}(p)$ and $\zeta_{L',L''}(p)$ from *three* lattice sizes as a function of p is (p_c, ω). The exponent of correlation length ν can still be estimated from (2). An alternative method, using data from *four* lattice sizes, is to let

$$R_{L,L'}(p)=P_L(p)/P_{L'}(p). \tag{6}$$

Then R_{L_1,L_2} and R_{L_3,L_4} should intersect at (p_c, b^ω) provided that

$$L_1/L_2=L_3/L_4=b. \tag{7}$$

Barber and Selke (1982) employed this method to analyse the structure factor of the $d=2$ axial next-nearest-neighbour Ising model. In this comment we calculate $X_L^A(p)$, the fraction of active sites in the infinite percolation cluster and $X_L^B(p)$, the fraction of sites in the *backbone* of the infinite cluster, which is its current-carrying part in the

conduction problem, for lattices of various sizes L. Our goal is to obtain accurate estimates of β, the critical exponent of Z^A and β_B, the critical exponent of X^B. Both β and β_B have been estimated in the past by a variety of methods and their estimates vary widely (see below), especially in the case of β_B.

We first carried out some MC simulations with small lattices. To calculate X^A and X^B we made 4×10^5 MC runs of site percolation on a simple cubic lattice with $L=4$ and $L'=6$ and 2×10^5 runs with $L''=9$ at different values of p ranging from 0.26 to 0.34. We then calculated $\zeta_{L,L'}$ and $\zeta_{L',L''}$ from which we obtained $\beta/\nu\simeq0.505$, $\beta_B/\nu\simeq0.66$ and $p_c\simeq0.305$. Given the very small sizes of the lattice the estimates of β/ν and p_c were very encouraging while that of β_B/ν was low (see below); therefore we carried out MC simulations with larger lattices. (Periodic boundary conditions were used in this work.)

We made 5×10^4 MC runs of $L'=12$ lattice and 8×10^3 runs of $L''=24$ lattice. The results (with $L=6$) for $X^A(p)$ and $X^B(p)$ are presented in figures 1 and 2 respectively. In both figures p_c is found to be about 0.311. This is in very good agreement with $p_c\simeq0.3117\pm0.0003$ (Heermann and Stauffer 1981, Gaunt and Sykes 1983) and with $p_c\simeq0.3116\pm0.0006$ (Wilkinson and Barsony 1984). The consistency of the two figures in estimating p_c is remarkable. From figure 1 one finds $\beta/\nu\simeq0.485$. (In all cases discussed here the third digit (in the case of an exponent) or the fourth digit (in the case of p_c) is included if the location of the arrow is between two consecutive values that can be read on the figure.) This compares well with the best estimates of β/ν (see below). β_B/ν is found to be about 0.88, a significant increase from the value obtained from smaller lattices; therefore, we did simulations with larger lattices.

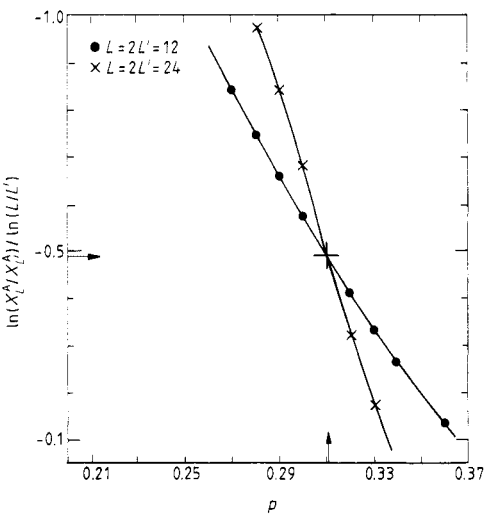

Figure 1. Plot of the function $\zeta_{L,L'}=\ln(X^A_L/X^A_{L'})/\ln(L/L')$ against p. X^A is the fraction of active sites in the infinite cluster and arrows indicate the location of p_c and β/ν.

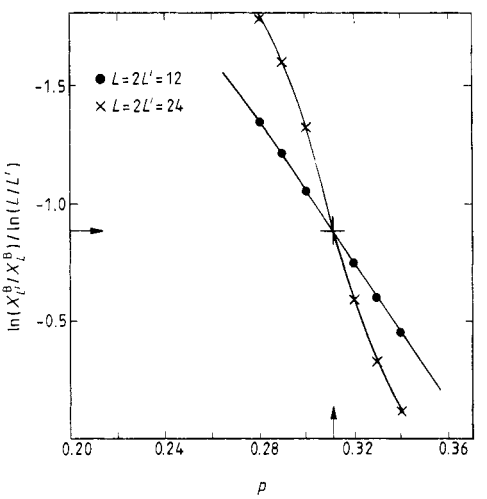

Figure 2. The same as in figure 1 but for the fraction X^B of active sites in the backbone of the infinite cluster.

We made 1.5×10^4 MC runs of the $L=18$ lattice and 5000 runs of the $L=36$ one. The result for X^A with $L=9$, $L'=18$ and $L''=36$ was $\beta/\nu\simeq0.48$, an insignificant change from the previous value obtained with smaller lattices. However, the same lattices yielded $\beta_B/\nu\simeq1$. Therefore, 1500 MC runs of the $L=48$ lattice were made.

The results for X^B with $L=12$, $L'=24$ and $L''=48$ are shown in figure 3. This figure shows that $p_c \simeq 0.3115$ and $\beta_B/\nu \simeq 1.08$. The results for X^A were $p_c \simeq 0.3115$ and $\beta/\nu \simeq 0.48$. The value of β_B/ν is still larger than the one obtained from smaller lattices, but the *rate* of increase in its value has considerably decreased.

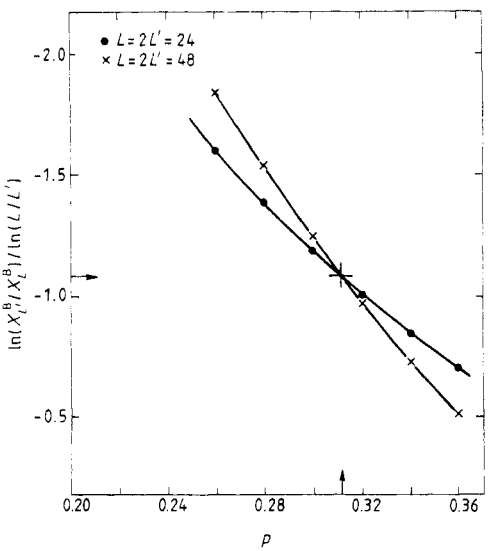

Figure 3. The same as in figure 2 but for larger lattices.

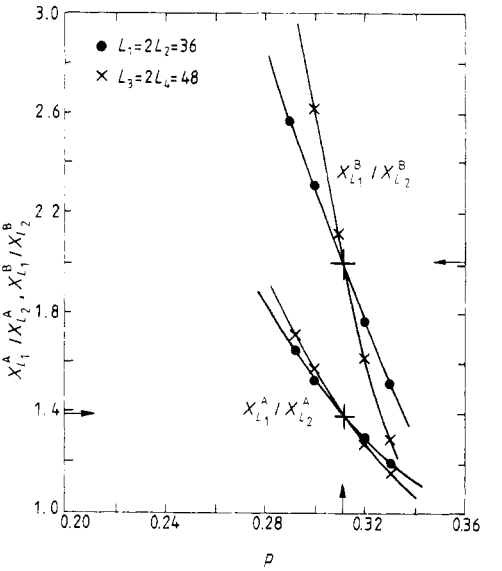

Figure 4. Plot of the function $R_{L,L'} = X_L^A/X_{L'}^A$ and $X_L^B/X_{L'}^B$ against p. Arrows indicate the locations of p_c and b^ω, where $b = L/L'$ and $\omega = \beta/\nu$ and β_B/ν.

Barber and Selke (1982) stated that they found $\zeta_{L,L'}$ to be susceptible to fluctuations in the data whereas $R_{L,L'}$ was much less so. To test this we first took our data with $L_1=6$, $L_2=12$, $L_3=9$ and $L_4=18$ and calculated R_{L_1,L_2} and R_{L_3,L_4}. The results were $\beta/\nu \simeq 0.48$ and $\beta_B/\nu \simeq 0.9$. p_c was found to be about 0.311. The results with $L_1=18$, $L_2=36$, $L_3=24$ and $L_4=48$ are presented in figure 4, where one finds $\beta/\nu \simeq 0.48$, $\beta_B/\nu \simeq 1.05$ and $p_c \simeq 0.3115$. Therefore, it appears that PR treatment of MC data from four lattice sizes results in much more stable results. Hence, allowing for some increase in the value of β_B/ν (by studying its *rate* of increase), we may list our best estimates as follows:

$$p_c \simeq 0.3115 \pm 0.0005 \tag{8}$$

$$\beta/\nu \simeq 0.48 \pm 0.01 \tag{9}$$

$$\beta_B/\nu \simeq 1.1 \pm 0.03. \tag{10}$$

The statistical errors of the individual points of figures 1-4 are very small (no more than 1% of the average values) because large numbers of MC runs were used. Since in the present method we use the logarithm of the ratio of the quantities of interest to construct the PR transformation, their effect is negligible. Therefore, to obtain estimates for the statistical errors for (8)-(10), we divided our MC data for each L into smaller groups of fewer MC runs and analysed them to obtain estimates of the quantities of interest. The variations of p_c, β/ν and β_B/ν among different groups yielded error

estimates quoted above. The estimated errors of p_c and β/ν are quite reasonable as they agree with the values obtained from smaller lattices, which also indicate that with the present PR method the errors in p_c and β/ν due to sample size are very small. However, in the case of β_B/ν the errors due to sample size might be quite large and we cannot rule out completely the possibility of larger values of β_B/ν with larger L. This strong L dependence of β_B/ν may be related to the structure of the backbone as discussed below.

To test (10) we also used the standard finite-size scaling analysis of X^B at $p = p_c$. One thousand MC runs with various values of L at $p = p_c$ were made. The results are presented in table 1. If we fit X^B to an expression like

$$X^B = L^{-\omega}(a + bL^{-\Omega}) \tag{11}$$

we obtain $\omega = \beta_B/\nu \simeq 1.1 \pm 0.05$ and $\Omega \simeq 1$. This is in agreement with (10).

Table 1. Values of the backbone fraction X^B at the percolation threshold $p_c = 0.3115$ of the simple cubic lattice. L is the linear dimension of the lattice and numbers in parentheses indicate the statistical errors of X^B in the last digit.

L	X^B
50	0.0084 (3)
60	0.0069 (4)
70	0.0056 (3)
80	0.0049 (5)
90	0.0043 (3)

At present, it is generally agreed that in three dimensions $\nu \simeq 0.88$ (Heermann and Stauffer 1981, Gaunt and Sykes 1983). The exponent β has been estimated by many authors, a list of which is too long to be given here (see Gaunt and Sykes (1983) and references therein). The most accurate estimate of β/ν appears to be that of Margolina *et al* (1982) who obtained $\beta/\nu \simeq 0.47 \pm 0.015$. More recently, Adler (1984) found $\beta/\nu \simeq 0.494 \pm 0.040$. These authors took into account the effect of correction-to-scaling. Heermann and Stauffer (1981) and Gaunt and Sykes (1983) ignored correction-to-scaling effects and obtained $\beta/\nu \simeq 0.515$. Even the smallest lattices used here yielded an estimate of $\beta/\nu (\simeq 0.505)$ which appears to exclude their estimate. Our estimate of β/ν fits nicely between those of Margolina *et al* (1982) and Adler (1984). It also predicts that the exponent $\eta = 2\beta/\nu - 1$ which describes the critical behaviour of the pair correlation function at p_c to be about -0.4.

As mentioned above, β_B/ν was found to be sensitive to the lattice size. We do not have a definite explanation of this. However, we note that Herrmann and Stanley (1984), in their study of the structure of the backbone, found that the backbone can be described as a randomly constructed 'necklace' (i.e. clusters of multiply connected bonds) whose building blocks are *volatile fractals*. This means that their structure is not stable under a change of length scale and changes identity. This may offer a plausible explanation for the sensitive dependence of β_B/ν on L.

The exponent β_B has also been estimated by many authors (see Sahimi 1984, Sarychev *et al* 1985 and references therein). Almost all of these estimates yield a value of β_B/ν in the range 1.02–1.15. The only exception is that of Herrmann and Stanley (1984) who obtained $\beta_B/\nu \simeq 1.26 \pm 0.04$, which appears to us to be too large. The

scaling law (Sahimi 1984)

$$\beta_B = \tfrac{1}{2}(\nu d + 3\beta) - 1 \tag{12}$$

yields $\beta_B/\nu \simeq 1.08$, consistent with our estimate and with most of the previous estimates.

In summary, we have tested the accuracy of the phenomenological renormalisation of Monte Carlo data method for percolation by estimating the site percolation threshold of the simple cubic lattice and the exponents β and β_B. The results agree with the most accurate available data. One reason for the accuracy of this method is perhaps the fact that one uses the *ratio* of the quantities of interest (and the logarithm of this ratio is one variant of the method). It is plausible that this causes some error cancellations. An interesting question is whether this method or any other PR method can be used to evaluate the scaling function of the cluster size distribution.

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Note added in proof. Recently, Saleur and Derrida (1985) have combined the transfer matrix and Monte Carlo methods with the fourth-moment method of Binder (1981) to study site percolation and the Ising model in two and three dimensions. For site percolation in three dimensions, they have obtained $p_c \simeq 0.3118 \pm 0.0004$ amd $\beta/\nu \simeq 0.05 \pm 0.06$.

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