## Comments

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## Correlation-length exponent in two-dimensional percolation and Potts model

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Following Reynolds *et al.* and Swendsen, Monte Carlo renormalization calculations were made for percolation on the triangular lattice for rescaling up to  $10\,000 \times 10\,000$ , and for the 4-state Potts model on square lattices up to  $64 \times 64$ . In contrast to earlier studies, our comparison with the den Nijs hypothesis gives good agreement with its prediction  $y = \frac{3}{4}$  for percolation but bad agreement with its prediction  $y = \frac{3}{2}$  for the 4-state Potts model.

Whereas critical exponents for the two-dimensional Ising model have been known exactly for decades, no exponent has thus far been calculated exactly in two dimensions for the more general q-state Potts model or the simpler percolation problem. den Nijs<sup>1</sup> suggested a formula for the correlation length exponent  $y = 1/\nu$  which is defined through  $\xi \propto e^{-\nu}$  ( $\xi$  = correlation length,  $\epsilon$  = distance from critical point):

$$(y-3)\left[\frac{2}{\pi}\arccos\left(\frac{\sqrt{q}}{2}\right)-2\right]=3$$
 (1)

This formula gives the exact y = 1 for the Ising model (q = 2) and predicts  $y = \frac{3}{4}$  for percolation (q=1) and  $y=\frac{3}{2}$  for the 4-state Potts model (q = 4). On the other hand, Klein *et al.*<sup>2</sup> suggested that the result  $y = \log(\frac{3}{2}) / \log(\sqrt{3}) = 0.738$ , which follows from a simple renormalization argument on the triangular lattice,<sup>3</sup> is exact; and Zittartz<sup>4</sup> suggested  $y \ge (4/\pi) \arccos(\sqrt{2}-1) = 1.456$  for the 4-state Potts model. As a step toward a future exact solution of the two-dimensional percolation and Potts model, one would like to know which of these competing formulas is wrong. Series expansions, analytic renormalization techniques, and early Monte Carlo renormalization methods<sup>5</sup> were not accurate or reliable enough to settle these problems. Recent Monte Carlo renormalization for percolation,<sup>6</sup> on the other hand, gave  $y = 0.738 \pm 0.008$  for square site percolation<sup>6</sup> and  $y = 0.733 \pm 0.008$  for square bond percolation,<sup>7</sup> in better agreement with Klein *et al.* than with den Nijs. The careful analysis of Reynolds et al.<sup>6</sup> did not yet rule out the den Nijs hypothesis.

The original intention of the present percolation work was to employ the same Monte Carlo renormalization method as Reynolds *et al.*<sup>6</sup> but to increase the accuracy enough to rule out Eq. (1). We hoped to increase our accuracy by:

(i) Throwing away those computer runs which gave a percolation threshold far away from the fixed point before much computer time was used for these runs.

(ii) Employing lattices larger than those used before in any Monte Carlo simulation known to us: Our maximum size is 10000 in length compared with 500 in Refs. 6 and 7 (presumably we established a new world record here).

(iii) Working with triangular site percolation  $(p_c = \frac{1}{2})$  which uses less computer memory and time than square site percolation. (To save memory only two consecutive rows of the lattice were stored, and for *b* above 1000 unused labels of finite clusters were discarded in regular intervals.<sup>6</sup>)

(iv) Last but not least by using two CDC Cyber 76 computers six times faster than the computer at Boston University<sup>6</sup> together with a much slower CDC Cyber 72 where more time was available.

The Reynolds method employed here determines for a fixed sequence of random numbers (which determine the occupation numbers) at what concentration p a  $b \times b$  lattice percolates from top to bottom. This is achieved by varying p in suitable steps until the threshold for that particular sequence of random numbers is determined with the desired accuracy. By repeating this procedure over and over for different random numbers one obtains a histogram L(p), where L(p)dp is the probability that the finite system has its percolation threshold at a concentration between p and p + dp. The integral<sup>6</sup>

$$R(p) = \int_0^p L(\tilde{p}) d\tilde{p}$$
<sup>(2)</sup>

is the probability that at concentration p the finite system percolates, i.e., that *at least* one path of occu-

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pied sites connects the top row of the lattice with the bottom row. This renormalization transformation R(p) has a fixed point at some  $p^*$ :  $R(p^*) = p^*$ . If the length b of the lattice is increased,  $p^*$  approaches the percolation threshold of the infinite lattice. Standard renormalization arguments give the critical exponent y as

$$y = \log(\lambda) / \log(b), \quad (b \to \infty)$$
, (3a)

where<sup>6</sup>

$$\lambda = L\left(p^*\right) \quad , \tag{3b}$$

such that  $R(p) = p^* + \lambda(p - p^*) + \cdots$  close to the fixed point. Within the accuracy of our data one may identify, as pointed out by Reynolds *et al.*,<sup>6</sup> the fixed point  $p^*$  with the average  $\langle p \rangle$  or with the position  $p_{\text{max}}$  of the maximum in L(p), but not with  $p_c$ . (For small lattices  $p^*$  is smaller than  $\langle p \rangle$ .) The resulting  $\lambda = L(p_{\text{max}})$  increases asymptotically as  $b^y$ ; if the ratio  $y_b = \log(\lambda)/\log(b)$  is plotted versus  $1/\ln(b)$ then<sup>6</sup> the intercept gives this asymptotic y. (Time was saved by a factor of 3 by stopping the iterative search for p if it was outside the interval  $p_c - \Delta with <math>\Delta = \frac{1}{4}L^{-0.75}$ .)

Figure 1 shows a histogram for L(p) at b = 1000, based on 570 runs away from the maximum (crosses) and on 6000 runs close to the maximum (full circles). The error bar at the maximum gives the error bar for  $y_b$  and has to be regarded as a typical error, not as a maximum error. Table I gives details for all lattice sizes b used here. There  $y_G$  refers to the Gaussian approximation: If

$$L(p) = (2\pi\sigma^2)^{-1/2} \exp[-\frac{1}{2}(p - p_{\max})^2/\sigma^2]$$

near the maximum, then  $\lambda_G = (2\pi\sigma^2)^{1/2}$  is this maximum, and  $y_G = \log(\lambda_G)/\log(b)$  is the Gaussian



FIG. 1. Histogram of L(p) vs p for b = 1000. The error bars on the wings are much larger than the error bar at the maximum, which is based on many more runs. The solid line gives the Gaussian approximation for L(p).



FIG. 2. Variation of the exponent estimates versus  $1/\ln(b)$ . The solid line is a parabola fitted through all points with the constraint y = 0.75 for  $b = \infty$ . The sum of weighted squared deviations from such parabolas, fitted with the intercept constrained to be y, has a minimum near y = 0.75 and is about twice as large at y = 0.738 (see inset).

approximation<sup>6</sup> for  $y_b$ . Figure 2 summarizes the data and shows that a parabola fitted on all data with the constraint  $y = \frac{3}{4}$  at the intercept gives an excellent fit over the three decades of b studied here. (In that analysis we combined the four less accurate points for b > 1000 into a single average:  $y_b = 0.720 \pm 0.010$  for b = 5900.)

The averages  $\langle p \rangle = \int pL(p)dp$  lie between 0.48 and 0.50 even for very small lattices; we did not employ periodic boundary conditions where  $\langle p \rangle$  is lower.<sup>8,9</sup> Finite size scaling asserts  $p_c - \langle p \rangle \propto b^{-y}$ ; and with y = 0.75, b > 100 we find  $p_c = 0.49997$ , confirming excellently the not yet rigorously<sup>10</sup> proven result  $p_c = \frac{1}{2}$ . More details are given elsewhere.<sup>9</sup>

With the different Swendsen Monte Carlo renormalization group (RG) technique<sup>11</sup> we studied the 4state Potts model.<sup>12</sup> We employed mainly two kinds of RG procedures with b = 2 as the scaling factor: the common "tie breaker" method, and a symmetric procedure with one cell influenced by 17 surrounding sites. We took into account up to eight different interactions and performed four RG steps. A run starting with a  $64 \times 64$  lattice was observed for 90 000 Monte Carlo steps per spin. Attempting to quantify our Monte Carlo RG results we calculated the average of the best values of y for different runs. They are plotted with their statistical error bars in Fig. 3 for the two renormalization procedures. The different RG steps in Fig. 3 are plotted as if they approach the fixed point at the origin with a scaling factor of 0.5—the irrelevant eigenvalue of the scaling field which alters y most. (This was the approximate mean value of all the irrelevant eigenvalues considered.) As our values for the fourth RG step are not very accurate we plotted only some examples for that step. The extrapolations sketched in Fig. 3 have different curvature for the two different procedures, and the extrapolated value of  $y \simeq 1.34$  does not agree

## COMMENTS

b	$\langle p \rangle$	p*	Уь	y <sub>G</sub>	N
10.000	0.4998			$0.701 \pm 0.012$	39
9 000	0.4999			$0.745 \pm 0.015$	28
5 000	0.4998			$0.708 \pm 0.025$	30
3 000	0.4999		· · · · · ·	$0.725 \pm 0.017$	36
1 000	0.4995	0.4993	$0.713 \pm 0.002$	$0.707 \pm 0.002$	6 1 5 0
630	0.4991		$0.712 \pm 0.006$	$0.715 \pm 0.004$	800
430	0.4988		$0.698 \pm 0.010$	$0.703 \pm 0.006$	1 000
300	0.4985		$0.702 \pm 0.004$	$0.693 \pm 0.002$	1 950
215	0.4984		$0.697 \pm 0.004$	$0.703 \pm 0.006$	4 200
160	0.1975		$0.702 \pm 0.004$	$0.693 \pm 0.002$	6 500
110	0.4971	0.4969	$0.695 \pm 0.004$	$0.685 \pm 0.001$	16 000
80	0.4961		$0.693 \pm 0.003$	$0.681 \pm 0.002$	38 000
57	0.4957		$0.688 \pm 0.002$	$0.680 \pm 0.001$	30 500
40	0.4943	0.4931	$0.679 \pm 0.004$	$0.674 \pm 0.003$	30 000
27	0.4924		$0.671 \pm 0.003$	$0.667 \pm 0.001$	110 000
20	0.4896	0.4848	$0.668 \pm 0.003$	$0.665 \pm 0.003$	200 000
17	0.4906	0.4868	$0.660 \pm 0.003$	$0.660 \pm 0.001$	120 000
14	0.4899		$0.658 \pm 0.003$	$0.658 \pm 0.001$	120 000
12	0.4890	0.4790	$0.653 \pm 0.003$	$0.655 \pm 0.001$	130 000
10	0.4874		$0.649 \pm 0.002$	$0.652 \pm 0.003$	220 000
9	0.4879		$0.645 \pm 0.005$	$0.654 \pm 0.002$	130 000
8	0.4877		$0.640 \pm 0.003$	$0.653 \pm 0.002$	130 000
7	0.4880		$0.637 \pm 0.003$	$0.650 \pm 0.002$	130 000
6	0.4877	0.4770	$0.628 \pm 0.003$	$0.652 \pm 0.002$	130 000
5	0.4880		$0.621 \pm 0.002$	$0.659 \pm 0.002$	130 000
4	0.4896	0.4702	$0.614 \pm 0.003$	$0.671 \pm 0.002$	280 000
3	0.4921	0.4814	0.60515	0.702 59	exac
2	0.5000	0.5000	0.58496	0.835 21	exac

TABLE I. Details of statistics and results for our percolation study. Only the total number N of runs is given, not the fraction which ended close to  $p_{\text{max}}$ . For  $\langle p \rangle$  our errors are  $10^{-4}$  to  $10^{-3}$ , for  $p^*$  they are about 0.001. One run for  $b = 10\,000$  needed about one hour on the CDC Cyber 76.



FIG. 3. Values for the 4-state Potts model y, obtained by the tie breaker procedure (crosses) and the symmetric procedure (circles) at different RG steps.

with den Nijs's conjecture  $y = \frac{3}{2}$ . But since the asymptotic behavior is not known we cannot estimate y reliably. No eigenvalue of any of our interactions seems to tend to unity with growing number of RG steps, and thus we do not think that marginality effects or logarithmic correction factors<sup>13</sup> are important. We did not take into account vacancies. More details are given separately.<sup>14</sup>

In conclusion, our value  $y \approx 0.75$  for percolation agrees well with den Nijs (y = 0.75) but not with Klein *et al.* y = 0.738), whereas our  $y \approx 1.34$  (4-state Potts model) does not agree with den Nijs (y = 1.50) and only slightly better with Zittartz ( $y \ge 1.46$ ). Our Fig. 2 suggests y = 0.738 is wrong for percolation *unless* the extrapolated curve has zero slope at the interface or changes drastically its curvature. Similarly Fig. 3 suggests y = 1.50 to be wrong *unless* the curve has infinite slope at the intercept or changes drastically its curvature due to marginal behavior (as expected from the picture of Ref. 13). Whether these possible exceptions actually do occur is a question beyond the scope of our numerical study. Monte Carlo results alone can never rigorously invalidate a theory.

Lobb and Karasek<sup>15</sup> found that for bond percolation on the square lattice  $y_b$  is nearly independent of lattice size b, in contrast to the site percolation results of our Fig. 3. But their extrapolation y = 0.745 $\pm 0.009$ , based on rather small b, is not accurate enough to distinguish between y = 0.738 and y = 0.750. We find from 1700 runs for 1000 × 1001 square bond percolation:  $y_G = 0.745 \pm 0.003$ . For smaller sizes we confirm the exponents of Lobb and Karasek and also within  $10^{-4}$  the relation  $p^* = 0.5$  already for small b. Combining these exponents for 10 < b < 100 with our value for b = 1000 we extrapolate  $b = 0.75 \pm 0.01$  for infinite lattices, just as we found it for triangular site percolation.

Note added in proof. For percolation, Reynolds (private communication) reanalyzed the data of Ref. 6 and agrees with our conclusion  $y \approx \frac{3}{4}$ ; and Nightingale and Blöte [in Proceedings of the Statistical Physics Conference, Edmonton, Canada, August

- <sup>1</sup>M. P. M. den Nijs, J. Phys. A 12, 1857 (1979).
- <sup>2</sup>W. Klein, H. E. Stanley, P. J. Reynolds, and A. Coniglio, Phys. Rev. Lett. <u>41</u>, 1145 (1978).
- <sup>3</sup>P. J. Reynolds, W. Klein, and H. E. Stanley, J. Phys. C <u>10</u>, L167 (1977).
- <sup>4</sup>J. Zittartz (private communication).
- <sup>5</sup>M. E. Levinshtein, B. I. Shklovskii, M. S. Sur, and A. L. Efros, Zh. Eksp. Teor. Fiz. <u>69</u>, 386 (1975) [Sov. Phys. JETP <u>42</u>, 197 (1976)]. For Potts models see K. Binder, J. Stat. Phys. (in press) and Swendsen, Ref. 11.
- <sup>6</sup>P. J. Reynolds, H. E. Stanley, and W. Klein, J. Phys. A <u>11</u>, L199 (1978), and Phys. Rev. B <u>21</u>, 1223 (1980). For computational technique see J. Hoshen and R. Kopelman, Phys. Rev. B <u>14</u>, 3438 (1976).
- <sup>7</sup>S. Kirkpatrick, in *Ill Condensed Matter*, edited by R. Balian, R. Maynard, and G. Toulouse (North-Holland, Amsterdam, 1979), p. 340.
- <sup>8</sup>D. W. Heermann and D. Stauffer, Z. Phys. B (in press).
- <sup>9</sup>P. D. Eschbach, Staatsexamensarbeit (Universität zu Köln,

1980 (unpublished)] confirmed it with even greater accuracy: y = 0.7497. The latter paper also agrees with our y for the 4-state Potts model, but we agree with them that these deviations from the den Nijs formula presumably are numerical effects due to marginality.

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June, 1980) (unpublished).

- <sup>10</sup>P. D. Seymour and D. J. Welsh, in Advances in Graph Theory, Annals of Discrete Mathematics No. 3, edited by B. Bollobas (North-Holland, Amsterdam, 1979); H. Kesten, Commun. Math. Phys. <u>74</u>, 41 (1980); J. C. Wiermann (unpublished).
- <sup>11</sup>R. H. Swendsen, Phys. Rev. Lett. <u>42</u>, 859 (1979); and Phys. Rev. B <u>20</u>, 2080 (1979).
- <sup>12</sup>C. Rebbi and R. H. Swendsen, Phys. Rev. B <u>21</u>, 4094 (1980).
- <sup>13</sup>B. Nienhuis, A. N. Berker, E. K. Riedel, and M. Schick, Phys. Rev. Lett. <u>43</u>, 737 (1979); B. Nienhuis, E. K. Riedel, and M. Schick, J. Phys. A <u>13</u>, L31 (1980); T. W. Burkhardt (unpublished); see also M. Nauenberg and D. Scalapino, Phys. Rev. Lett. <u>44</u>, 837 (1980), and L. P. Kadanoff, Phys. Rev. B <u>22</u>, 1405 (1980). For a short review see M. N. Barber, Phys. Rep. <u>59</u>, 375, 406 (1980).
- <sup>14</sup>H. J. Herrmann (unpublished).
- <sup>15</sup>C. J. Lobb and K. A. Karasek, J. Phys. C <u>13</u>, L245 (1980).