Percolative conduction in three dimensions

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(Received 22 March 1990)

We employ finite-size scaling to analyze the critical behavior of large [up to $(80)^3$] threedimensional random resistor lattices. The ratio of the conductivity exponent t to the correlation length exponent v is found to be $t/v=2.276\pm0.012$. Combining this with the accepted value $v=0.88\pm0.02$ gives $t=2.003\pm0.047$, very close to the upper bound t=2 recently proposed by Golden. Studying the connectivity of lattices up to $(200)^3$, we estimate that the bond percolation threshold $p_c=0.24883\pm0.00005$, slightly smaller than some recent estimates, and have also confirmed the accepted value of v.

I. INTRODUCTION

Consider a simple cubic lattice of resistors, where a fraction p of the resistors have conductance 1, while the remaining fraction (1-p) have conductance $0.^1$ For $p < p_c$, only finite clusters of resistors are present, so that a very large sample will have a bulk conductance G=0. For p equal to, or slightly greater than, the percolation threshold p_c , the bulk conductance of a large cube measured from one face to the opposite face is known to vary as

$$G \sim \frac{L}{l} (p - p_c)^t , \qquad (1)$$

where L is the length of the cube and l is the length of a single resistor, and t is the conduction critical exponent. (The factor of L/l reflects the fact that a cube's conductance increases linearly with size.)

A second quantity of interest is the correlation length ξ . Near the percolation threshold, the probability of finding two resistors a distance r apart on the same finite connected cluster varies as $\exp(-r/\xi)$, where ξ varies as

$$\xi \sim l |p - p_c|^{-\nu} \tag{2}$$

and v is the correlation-length exponent.

Fogelholm developed an algorithm that applies successive transformations to an arbitrary two-terminal resistor network until the conductance between the two terminals is obtained.² Fogelhom applied his algorithm to two-dimensional percolation. We have used his method on *d*-dimensional cubic lattices, and found that it is computationally very efficient. For example, our program will find the conductance of an $(80)^3$ lattice at $p = p_c$ in 36 CPU seconds on a Sun 4/280.

The Fogelholm algorithm makes an improved determination of t possible in three dimensions. We discuss our simulations in detail in Sec. II. We first describe how simulations of finite lattices can be extrapolated to the infinite-sample limit where (1) is expected to hold, and then give our data on lattices up to size $(80)^3$, and our analysis of the data, to determine t. In Sec. III, a description of our determination of p_c using lattices up to $(200)^3$ is given. Our results are summarized in Sec. IV.

II. THE EXPONENT t

Two finite random resistor lattices with the same size Land the same bond probability p will not, in general, have the same conductance G. For lattices where $L \gg \xi$, the spread in the conductances is small, but as p approaches p_c , fluctuations become large for any finite lattice. This makes the use of (1) for determining t problematic.

An alternative is to determine the average conductance, $\langle G \rangle$, which is well-defined in finite lattices. Finite-size scaling arguments³ suggest that

$$\langle G \rangle \sim \frac{L}{l} (p - p_c)^l f \left[\frac{L}{\xi(p)} \right],$$
 (3)

which is correct if $\xi(p)$ is the only relevant length scale in the problem. For (3) to agree with (1), $f(\infty)$ must be a constant because $\langle G \rangle = G$ when $L/\xi(p) \rightarrow \infty$. Similarly, in order for $\langle G \rangle \neq 0$ when $p = p_c$, which will be true for finite lattices,

$$f(L/\xi(p)) = f(L/l(p-p_c)^{-\nu}) \sim [L/l(p-p_c)^{-\nu}]^{-t/\nu}$$

in order to cancel the $(p - p_c)^t$ dependence of (3). This gives, for $p = p_c$,

$$\langle G \rangle \sim \left[\frac{L}{l} \right]^{1 - t/\nu}$$
 (4)

The prescription we follow, then, is to determine $\langle G \rangle$ by calculating the conductances of a large number of lattices at various sizes with $p = p_c$, and to fit the resulting data to (4) to determine t/v.

Figure 1 shows a finite lattice with b=2, where $b \equiv L/l$. We chose to calculate the conductance of finite samples with the shape shown in Fig. 1 because the twodimensional analog of this type of sample is known to converge quickly to the infinite-sample limit.⁴ Each sample was generated using a random-number generator to determine which resistors were present and which were absent. The Fogelholm method was used to determine the conductance of each realization. Equipotential boundary conditions were applied to opposite faces of the sample, so that, for example, the b=2 sample shown in Fig. 1 has 12 bonds which carry current. Arithmetic,

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FIG. 1. Cell used for finite sample of size b=2. Bonds are randomly assigned conductances of 0 or 1, and the cell conductance G is calculated by imposing equipotentials on two opposite faces.

geometric, and harmonic means were calculated, where means were taken over the connected realizations. All three means are different, but all should fit to the same value of t/v, as in (4).

originally used Wilke's value⁵ We of p_c =0.2492(± 0.0002) because it was based on a very careful analysis of lattices up to b=200. We found, however, that our samples for b > 20 or so had a rapidly increasing fraction of realizations which conducted as b was increased. We concluded that Wilke's value of p_c was slightly high, and that our sample shape was more sensitive to slight errors in p_c than the shapes used by Wilke. Another possibility was that our random number generator had subtle correlations in it, which shifted p_c slightly. We concluded, after extensive testing of different random number generators, that this was not the case. Using a "maze-solving" program on lattices up to b=200, we concluded that $p_c = 0.24883 \pm 0.00005$, which is very close to Wilke's value. These results will be described in detail in the next section. We note that short-range correlations can shift p_c , but are not believed to affect the values of t or v.

The data generated with p = 0.24883 are shown in Table I. Equation (4) can be rewritten as

$$\frac{\ln(\langle G \rangle^{-I})}{\ln(b)} = \left(\frac{t}{\nu} - 1\right) + \frac{\text{const}}{\ln(b)} + \cdots \qquad (5)$$

Thus, to fit the data we plotted $\ln(\langle G \rangle^{-1})/\ln b$ against $1/\ln(b)$. The data thus plotted should fall on a straight line, with a y intercept of (t/v)-1.

The data for b=2 do not fall on a straight line with the other data. Eliminating the point at b=2 yields remarkably straight lines, as shown in Fig. 2. Fitting the data from b=4 through b=80, we obtain t/v=2.277, 2.279, and 2.280 for the arithmetic, geometric, and harmonic means, a spread of only 0.13%. Fitting the points from b=6 through b=80 gives 2.277, 2.278, and 2.278 for the three means, a spread of only 0.044%.

If the data were free of statistical fluctuations, eliminating still more of the small-b data points could give a better estimate of t/v. We found that doing this just increased the normalized χ^2 of the fits without systematically changing the value obtained for t/v.

We have also estimated t/v from a second independent set of data. Letting p'(p,b) be the probability that a lattice of size b with bond occupation probability p conducts, the fixed point $p^*(b)$ is implicitly defined by $p'(p^*,b)=p^*$. When $p > p^*$, the lattice is more likely to be connected than an individual bond in it, and when $p < p^*$, it is less likely to be connected. Thus, for example, $p^*(\infty)=p_c$. Rather than setting $p=0.248\,83$ for all b, as was done above, we determine the fixed point $p^*(b)$, and did our calculations for $p=p^*(b)$. Our determination of $p^*(b)$ is discussed in Sec. III.

Table II gives the second set of data. These data also fit (5) well when the data at b=2 were omitted, giving t/v=2.272, 2.276, and 2.279 for the arithmetic, geometric, and harmonic means, respectively. When the points at b=2 and b=4 were omitted, the values obtained from the three means were 2.270, 2.272, and 2.273. We note that, once again, omitting the two smallest-*b* data gives less spread than omitting only the smallest-*b* data.

As a further check, fits were done to the second data set with the b=60 and b=80 data points removed. This was done because the statistics on these last two points were not as good as on the other points. This did not

TABLE I. Average conductances at p = 0.24883 as a function of lattice size b. N is the total number of realizations simulated, N_c is the number which conducted, and the subscripts a, g, and h refer to arithmetic, geometric and harmonic means.

b	N	N _c	$\langle G \rangle_a$	$\langle G \rangle_{g}$	$\langle G \rangle_h$
2	200 000	58 317	0.52774 ±0.00077	$0.50296\ \pm 0.00065$	$0.478\ 18\ \pm 0.000\ 61$
4	200 000	60 7 37	$0.22947\ \pm 0.00040$	$0.21236\ \pm 0.00033$	$0.19788\ \pm 0.00030$
6	100 000	30 197	0.136 52 ±0.000 34	0.12600 ± 0.00028	$0.11718\ \pm 0.00025$
8	40 000	12034	$0.09488\ \pm 0.00038$	$0.08751\ \pm 0.00031$	$0.08135\ \pm 0.00028$
10	20 000	5 924	$0.07135\ \pm 0.00041$	0.06577 ± 0.00034	$0.06112\ \pm 0.00030$
15	20 000	5 927	$0.04266\ \pm 0.00024$	$0.03931\ \pm 0.00020$	$0.03649\ \pm 0.00018$
20	20 000	5 806	0.02923 ± 0.00017	0.02699 ±0.00014	$0.02512\ \pm 0.00012$
30	20 000	5 739	$0.01740\ \pm 0.00010$	$0.016036{\pm}0.000083$	$0.014913{\pm}0.000073$
40	24 000	6933	0.012210 ± 0.000065	$0.011245{\pm}0.000053$	$0.010442{\pm}0.000047$
60	11 000	3215	0.007261 ± 0.000057	$0.006683{\pm}0.000047$	$0.006205{\pm}0.000041$
80	11 000	3 096	$0.004955{\pm}0.000039$	0.004571 ± 0.000032	$0.004253{\pm}0.000028$



FIG. 2. Dependence of mean conductance $\langle G \rangle$ on lattice size b at p = 0.24883. Harmonic mean is represented by \blacksquare , geometric mean by \Box , and arithmetic by \bullet . Data for $4 \le b \le 80$ are shown.

alter the results very much: fitting from b=4 through b=40 gave 2.273, 2.278, and 2.281, and fitting from b=6 through b=40 gave 2.271, 2.273, and 2.275.

All of these different estimates of t/v fall between 2.270 and 2.282. We take the midpoint as our estimate for t/v, and double the range as a subjective estimate of uncertainty, thus

$$\frac{t}{v} = 2.276 \pm 0.012$$
, (6)

which is the central result of this paper.

Equation (4) is asymptotically true when (L/l) is large. A more complete form for (4), which allows data from smaller lattices to be fit, is⁴

$$\langle G \rangle = \left[\frac{L}{l} \right]^{1-t/\nu} \left[c_1 + c_2 \left[\frac{L}{l} \right]^{-\Delta/\nu} + \cdots \right],$$
 (7)

where c_1 and c_2 are constants. This equation reduces to (4) when (L/l) is large, as long as Δ is positive. We found that corrections to scaling were too small to be determined from our data; c_2/c_1 was between 10^{-2} and 10^{-3} for $\Delta/v < 3$ when the data at b=2 were omitted.

Based on a number of values^{6,7,1} reported in the literature, it is probably safe to conclude that $\nu = 0.88 \pm 0.02$. (Our value, discussed in Sec. III, is toward the high end of this range, but is probably less accurate than other reported values.) Combining this with (6) gives

$$t = 2.003 \pm 0.047$$
 . (8)

Using the more recently determined⁷ value $v=0.875 \pm 0.008$ gives $t=1.992\pm0.021$. Although we believe that the more recent determination of v is probably accurate, we will emphasize the more conservative evaluation of t (8) in this paper.

III. THE THRESHOLD p_c AND EXPONENT v

It is easier to calculate whether or not lattices conduct than to calculate their conductances, so that we were able to estimate p_c and v on much larger lattices, up to $(200)^3$ in size. As mentioned above, we define p'(p,b) to be the probability that a lattice of size b with bond occupation probability p conducts. The fixed point p^* is implicitly defined by $p'(p^*,b)=p^*$. Knowing $p^*(b)$ and $(dp'/dp)_{p=p^*}$ will allow us to estimate p_c and v.

For each value of p and b, our program generated a large number N of different lattices and determined the number N_c of the lattices which conducted. Thus, $p'=N_c/N$, and the uncertainty in p' was taken to be $[p'(1-p')/N]^{1/2}$. For b=3, for example, 500 000 lattices were studied for each $p=0.223, 0.224, 0.225, \ldots 0.229$. A straight line of the form $p'=c_1p+c_2$ was fit to this data, and the intercept of this straight line with the line p'=p was used to estimate p^* . The data thus obtained are given in Table III, as well as the slope $(dp'/dp)_{p=p}^*$.

The uncertainties listed in Table III are derived from the statistical uncertainties in the data and the resulting uncertainties in c_1 and c_2 . Additional error may occur if the range over which p' varies linearly with p is exceeded in the fit. We decreased the range as b got larger, from $0.223 \le p \le 0.229$ for b=3 to $0.2485 \le p \le 0.2489$ for b=200. Although the curves appear to be straight in the ranges chosen, it should be noted that fitting over too

TABLE II. Average conductances at $p = p^*$ as a function of lattice size b. N is the total number of realizations simulated, N_c is the number which conducted, and the subscripts a, g, and h refer to arithmetic, geometric and harmonic means.

b	р	N	N_c	$\langle G \rangle_a$	$\langle G \rangle_g$	$\langle G \rangle_h$
2	0.2085	200 000	41 664	$0.508\ 82\ \pm 0.000\ 78$	0.488 30 ±0.000 67	0.469 82 ±0.000 65
4	0.2331	200 000	46 708	$0.21962\ \pm 0.00040$	$0.205\ 37\ \pm 0.000\ 34$	$0.19305\ \pm 0.00031$
6	0.2400	100 000	24 013	0.13100 ± 0.00035	0.12185 ± 0.00029	$0.11409\ \pm 0.00026$
8	0.2430	40 000	9615	$0.09021\ \pm 0.00038$	$0.08396\ \pm 0.00032$	$0.07870\ \pm 0.00028$
10	0.2446	20 000	4 787	$0.06802\ \pm 0.00041$	$0.06318\ \pm 0.00034$	$0.05913\ \pm 0.00031$
15	0.2464	20 000	4 900	$0.04066\ \pm 0.00024$	$0.037~79~\pm 0.000~20$	$0.03538\ \pm 0.00018$
20	0.2472	20 000	4 880	$0.02832\ \pm 0.00017$	$0.02623\ \pm 0.00014$	0.02449 ± 0.00013
30	0.2479	20 000	5 082	0.01696 ± 0.00010	$0.015743{\pm}0.000083$	$0.014711{\pm}0.000075$
40	0.2482	8 000	1 935	$0.01176\ \pm 0.00012$	$0.010859{\pm}0.000095$	$0.010122{\pm}0.000084$
60	0.2484	5 500	1 168	$0.006923{\pm}0.000081$	$0.006465{\pm}0.000068$	0.006076 ± 0.000061
80	0.2485	4 500	988	$0.004971{\pm}0.000067$	$0.004598{\pm}0.000057$	$0.004281\!\pm\!0.000051$

TABLE III. Fixed point p^* and derivative $(dp'/dp)_{p^*}$ of the probability p' that a lattice is connected, as a function of lattice size b.

b	p*	$(dp'/dp)_{p*}$
3	$0.225317\ \pm 0.000075$	3.15±0.11
4	$0.233116\ \pm 0.000054$	4.19±0.11
5	$0.237281\ \pm 0.000052$	5.42±0.23
6	$0.239996 \ \pm 0.000047$	$6.99{\pm}0.30$
8	$0.242951\ \pm 0.000053$	9.71±0.51
10	$0.244551\ \pm 0.000047$	$10.87 {\pm} 0.51$
15	$0.246400\ \pm 0.000026$	$19.6 \ \pm 1.3$
20	$0.247182\ \pm 0.000028$	$26.3 \hspace{0.1in} \pm 1.8 \hspace{0.1in}$
30	$0.247870\ \pm 0.000032$	38.6 ± 5.8
40	$0.248173\ \pm 0.000019$	54.3 ±3.9
50	$0.248303\ \pm 0.000019$	77.5 ± 5.6
60	$0.248401\ \pm 0.000018$	$81.9\ \pm 5.6$
80	$0.248516\ \pm 0.000013$	122.2 ± 8.1
100	$0.2485977{\pm}0.0000081$	164.4 ±6.6
150	$0.2486848{\pm}0.0000078$	240 ±14
200	0.248 719 9±0.000 008 7	349 ±27

wide a range will cause us to underestimate $(dp'/dp)_{p=p}^*$.

We estimate p_c by extrapolating $p^*(b)$ to the infinitesample $(b \rightarrow \infty)$ limit. A finite-size scaling argument gives⁸

$$p^{*}(b) - p_{c} \sim b^{-1/\nu}$$
 (9)

Thus, when $p^*(b)$ is plotted against $b^{-1/\nu}$, the extrapolated y intercept gives p_c .

We did a number of different fits to our data, which had $3 \le b \le 200$. We found that the data points for $40 \le b \le 200$, which are shown in Fig. 3, gave excellent and nearly indistinguishable linear fits for trial values of



FIG. 3. Plot of fixed point $p^{*}(b)$ against $b^{-1/\nu}$ for $\nu = 0.88$. Data runs over the range $40 \le b \le 200$. The y intercept of this curve, 0.248 83, is an estimate for p_c .

v=0.86, 0.87, 0.88, 0.89, and 0.90, with intercepts of 0.24882, 0.24882, 0.24883, 0.24883, and 0.24883, respectively. When data for $10 \le b \le 200$ were plotted, curvature was apparent, so quadratic and cubic fits were done. The quadratic fits gave the same intercepts as the linear fits for the same values of v, while the cubic fits all gave an intercept of 0.24881. Finally, when all of the data points, for $3 \le b \le 200$, were fit, intercepts between 0.24885 and 0.24902 were obtained using quadratic and cubic fits. Our choice for p_c ,

$$p_c = 0.248\,83 \pm 0.000\,05 \tag{10}$$

is a subjective estimate chosen to encompass the results of the various fits. This is in excellent agreement with Grassberger's⁹ Monte-Carlo result, $p_c = 0.24875 \pm 0.00013$, and with Ziff and Stell's⁷ Monte-Carlo result, $p_c = 0.248812 \pm 0.000002$.

In addition to providing an estimate for p_c for use in determining Table I, these calculations provided the fixed points $p^*(b)$ used in determining Table II. For $3 \le b \le 30$, the numerically determined fixed points of Table III were used to do the calculations for Table II. For $40 \le b \le 200$, the linear fit shown in Fig. 3 was used to determine the fixed points used in Table II, as a way of smoothing out statistical fluctuations. Significant differences would not have occurred in Table II if the numerically-determined fixed points had been used for all b.

Empirically, fits to (9) were much more sensitive to the choice of p_c than to the choice of v, so that fitting data to (9) is not an effective way to determine v. Another scaling result,⁸

$$\left[\frac{dp'}{dp}\right]_{p*} \sim b^{-1/\nu} \tag{11}$$

was used to attempt to extract an accurate value for v. This was fit using the same method as was used on (4) to extract a value for t/v. Large statistical uncertainties in dp'/dp prevented us from getting a highly accurate value of v. On the basis of our data alone, we would estimate $v=0.90\pm0.03$. Our result is in agreement with the accepted value for v, but is probably not as accurate.

IV. SUMMARY AND CONCLUSIONS

The central result of this paper is (6), which leads to (8)—that the critical exponent for conductivity in threedimensional percolation is very close to 2. In spite of two decades of work on this problem, a considerable spread exists in quoted values. Sahimi¹⁰ plotted a frequency distribution of reported values in 1984 ranging from 1.5 to 2.4, with 2 indicated as the "currently accepted value." Mitescu and Musolf¹¹ obtained $t/v=2.47\pm0.12$ using finite-size scaling on lattices with $b \le 20$. This would lead to a higher value of t if the presently-accepted value of $v=0.88\pm0.02$ were used. When their value of $v=0.83\pm0.05$, also obtained from small lattices, was used, they obtained $t=2.06\pm0.06$, in agreement with this work. Clerc *et al.*¹² favored a value of 1.9 ± 0.1 in 1989, giving preference to the transfer-matrix value.¹³ Adler's series analysis^{14,15} gives $t = 2.02 \pm 0.05$, in excellent agreement with this work.

Roman¹⁶ has very recently studied diffusion using the ant-in-the-labyrinth method. His two independent calculations can be analyzed to give $t/v=2.505\pm0.072$ and $t/v=2.465\pm0.054$.¹⁷ These values are clearly in conflict with the results presented here; note that they correspond to the v intercept of Fig. 2 being either 1.505 or 1.465. We point out that the analysis of data for Roman's method is much less straightforward than for our method. Random walks involve calculating slopes of rms displacement versus time on log-log plots, which is inherently less reliable than obtaining average conductances, as is done here.¹⁸ Note that our estimated uncertainty in (8) would have to be more than doubled to encompass the values 1.9 and 2.1, and the uncertainty in (6) would have to be multiplied by a factor of 19 to enclose Roman's value.

Of three recent calculations, then, the series method and this work favor a value for t near 2, while the ant-inthe labyrinth is 10% higher. A consensus on the values of the static critical exponents, in particular v and β/v in three dimensions, would greatly simplify comparison of values obtained by different methods. This, plus an extension of the present work to larger lattices, could narrow the error bars in (8) by a factor of 5 or more.

Golden¹⁹ has recently proposed the bound $t \le 2$ in three dimensions, with additional arguments for the value t=2. Series calculations and this work, coupled with Golden's bound, suggest that the value t=2 may indeed be *exact* in three dimensions. Further theoretical and numerical work are needed to check the bound, and the conjectured exact value.

Finally, three independent methods applied to large lattices now agree that the bond percolation threshold in three dimensions is $p_c = 0.2488$, with disagreement in the fifth digit to the right of the decimal point.

ACKNOWLEDGMENTS

K. Golden, R. Ziff, M. Sahimi, and M. Octavio made useful comments and suggestions in the course of this work. The work was supported in part by National Science Foundation Grant No. DMR86-14003. The final stages of this work were supported in part by the state of Maryland through the Center for Superconductivity Research.

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