

Three-dimensional percolation with removed lines of sites

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The site percolation problem on a cubic lattice in which entire lines of sites are removed randomly is analyzed with use of both analytical and large-cell (up to 100^3) Monte Carlo renormalization-group techniques. Because of strong correlation effects, the behavior of small systems deviates appreciably from regular percolation, and the percolation threshold is lowered. However, it is shown that the asymptotic values of the critical exponents are consistent with those of regular percolation. The results suggest a practical way to generate macroscopic three-dimensional percolating samples, which can be used to measure various physical properties of percolating systems.

Certain physical properties of percolating systems can be conveniently investigated by performing "table-top experiments," in which one creates a macroscopic sample of material with a well-defined percolation geometry and then measures the dependence of physical properties of the sample on the volume fraction of remaining material. For example, the conductivity,^{1,2} Hall coefficient,² and elasticity³ of two-dimensional (2D) systems have been investigated by punching holes in a sheet of material and measuring its properties. Such experiments are not trivial analogues of computer Monte Carlo (MC) simulations, since in some cases there exists an ambiguity as to which discrete equations should be used to represent correctly the properties of the actual system: For example, different discretization schemes can lead to different predictions for the Hall coefficient;⁴ different discrete elastic Hamiltonians lead to different predictions for the elastic behavior of percolating solids.⁵ Unfortunately, table-top experiments are frequently limited to 2D. Attempts to create a three-dimensional (3D) percolating system by combining many 2D percolating sheets have not been successful because of problems created by the contacts between the sheets, and because the 3D percolation threshold is lower than the 2D percolation threshold, forcing the experimentalist to work with very fragmented sheets.²

A seemingly simple solution is obtained by randomly drilling holes in a cube of material: We take one of the orthogonal planes, say xy , and generate a 2D percolating pattern, namely, we determine at which points we would punch holes if this would be a 2D problem. Then we drill holes at those points through the entire sample in the z direction. The entire procedure is then repeated for the yz and xz planes.⁶ Such a process generates a random 3D structure, which differs from a regular percolation structure, since it introduces correlations between different parts of the object. In this work I analyze this problem using both analytical techniques and a large-cell MC renormalization group (RG) and present evidence that it belongs (or is very close) to the same universality class as the regular (uncorrelated) 3D percolation (R3DP).

I consider a 3D site percolation problem on a cubic lattice in which entire lines of sites (pointing in the x , y , or z direction) are selected at random and removed from the

lattice. Percolation with removed lines of sites (PRLS) is the lattice analogue of the 3D table-top problem defined above. If we removed only lines of sites pointing in, say, the z direction and the concentration of the removed lines was q , then in the xy plane we would have a regular 2D site percolation on a square lattice with a fraction $p = 1 - q$ of sites present, with a percolation threshold⁷ at $p_{c,2D} = 0.5928$. If we remove a fraction q of lines in each of the three orthogonal directions, then a site will be present only if none of the orthogonal lines passing through that site have been removed, i.e., it will be present with probability $P = p^3$. In subsequent discussions I will use both the 2D variable p , and the 3D variable P : Since the removed lines are the independent objects of PRLS, the probabilities of finite configurations will be polynomials in the variable p (or q), but will contain noninteger powers of P (or $Q \equiv 1 - P$) if expressed in terms of the 3D variables. However, we will see that it is more natural to use P in the RG transformations. Clearly, PRLS has long-range correlations: If a site (x_0, y_0, z_0) is present, then the probability that sites $(x_0 + n, y_0, z_0)$, $(x_0, y_0 + n, z_0)$, or $(x_0, y_0, z_0 + n)$, where $n = \pm 1, \pm 2, \dots$, are present is p^2 , which is greater than P . While such correlations do not even decrease with the distance between the sites, they are limited to particular directions in space, so that out of $\sim r^2$ sites located at distance r from a given present site, only six sites will be correlated. Since the directionally averaged correlations decay as $1/r^2$, application of the extended Harris criterion⁸ may lead to a conclusion that the critical exponents of PRLS differ from those of R3DP. (In particular, Ref. 8 predicts that the correlation-length exponent $\nu = 1$.) However, it is not clear whether this criterion can be used for such "deterministic" correlations as those of PRLS, since it can also be applied to the complementary problem (percolation of lines of sites) or to the 2D percolation with removed lines of sites, and the behavior of both these problems is not consistent with the predictions of the theory of percolation with long-range correlations.⁸

The method of construction relates PRLS to the usual 2D percolation: If two sites of the 3D problem belong to the same cluster, then if we consider only the removed lines pointing in, say, the z direction and disregard all the

others, the projections of these points on the xy plane belong to the same 2D cluster. This means that the percolation threshold p_c ($\equiv P_c^{1/3}$) of PRLS satisfies $p_c \geq p_{c2D}$. The converse, however, is not true, since there are configurations in which two points of the 3D problem do not belong to the same cluster, while in some of the “projected” 2D problems they do belong to the same cluster. For these reasons, we expect a sharp inequality $p_c > p_{c2D}$. Note also that the number of different configurations in a cubic cell of linear size L in PRLS is 2^{3L^2} , in contrast to 2^{L^3} configurations of a R3DP. Moreover, for finite L , several different configurations of removed lines may produce an identical site configuration. Thus, for large L , the configurations of PRLS are a negligible subset of the possible configurations of the R3DP.

The connectivity correlation length ξ of a percolation problem diverges as $(P - P_c)^{-\nu}$, while the volume fraction of the infinite cluster vanishes as $(P - P_c)^\beta \sim \xi^{-\beta/\nu} \equiv \xi^{-A}$, where A is the fractal codimension⁹ of the infinite cluster. The pair of exponents ν and A determine all the other “thermodynamic” exponents, and in that sense they suffice to establish the universality class of a problem. Nevertheless, there exist additional exponents, both geometrical and dynamical, which are not directly related to the above pair of exponents, and may differ in two problems having the same “thermodynamic” exponents. Therefore, in addition to ν and A , I also calculate the exponent Z , which determines the scaling of the shortest

path between two points on length scales shorter than ξ . Following Reynolds *et al.*,^{10,11} I will treat the probability $R(P, L)$ that a given cubic cell of size L percolates in one (predetermined) direction as the renormalized probability of a site to be present after the original problem has been rescaled by a factor L . The fixed point $P^*(L)$ of this RG transformation is determined from the equation $R(P^*, L) = P^*$. [The trivial (stable) fixed points, $P^* = 0$ and 1, are excluded from the discussion.] The effective correlation-length exponent $\nu(L)$ will be given by the ratio $\ln L / \ln \lambda$, where $\lambda \equiv dR/dP_{P=P^*}$. For $L \rightarrow \infty$, we expect $P^* \rightarrow P_c$ and $\nu(L) \rightarrow \nu$. For $L = 2$, the polynomial R can be found rather easily, while for $L = 3$, I resorted to computer enumeration of the $2^{27} \cong 10^8$ possible configurations in order to determine R . The resulting polynomials, as well as the values of the fixed point and the effective exponent $\nu(L)$, are presented in Table I. For comparison, I also calculated the analogous quantities for the R3DP. These results, as well as the results for a regular 2D problem,¹¹ are also shown in Table I. Note that for such small cells, both the fixed point and the effective exponent of our problem are closer to the corresponding values of the regular 2D problem than to those of the 3D problem. This is not very surprising, since small cells correspond to a large distance from the percolation threshold in an infinite system, where such resemblance to a 2D system can be expected because of the way in which our system has been constructed.

TABLE I. Percolation probability, fixed points, and $\nu(L)$ for PRLS and regular percolation problems (see text for definitions).

System	L	R	p^*	P^*	$\nu(L)$
PRLS	2	$p^{12} + 12p^{11}q + 58p^{10}q^2 + 124p^9q^3 + 136p^8q^4 + 84p^7q^5 + 28p^6q^6 + 4p^5q^7$	0.5743	0.1707	1.782
	3	$p^{27} + 27p^{26}q + 351p^{25}q^2 + 2891p^{24}q^3 + 16804p^{23}q^4 + 72185p^{22}q^5 + 233716p^{21}q^6 + 576220p^{20}q^7 + 1092077p^{19}q^8 + 1611607p^{18}q^9 + 1879971p^{17}q^{10} + 1755591p^{16}q^{11} + 1322238p^{15}q^{12} + 804494p^{14}q^{13} + 393704p^{13}q^{14} + 153252p^{12}q^{15} + 46511p^{11}q^{16} + 10644p^{10}q^{17} + 1734p^9q^{18} + 180p^8q^{19} + 9p^7q^{20}$	0.5893	0.2046	1.679
Regular	2	$P^{16} + 8P^{15}Q + 28P^{14}Q^2 + 56P^{13}Q^3 + 54P^{12}Q^4 + 24P^{11}Q^5 + 4P^{10}Q^6$		0.2818	1.227
3D site					
Percolation	3	$P^{27} + 27P^{26}Q + 351P^{25}Q^2 + 2925P^{24}Q^3 + 17550P^{23}Q^4 + 80730P^{22}Q^5 + 296010P^{21}Q^6 + 888030P^{20}Q^7 + 222075P^{19}Q^8 + 4684804P^{18}Q^9 + 8410022P^{17}Q^{10} + 12878876P^{16}Q^{11} + 16788468P^{15}Q^{12} + 18515346P^{14}Q^{13} + 17122490P^{13}Q^{14} + 13136990P^{12}Q^{15} + 8264191P^{11}Q^{16} + 4208062P^{10}Q^{17} + 1709418P^9Q^{18} + 544436P^8Q^{19} + 132850P^7Q^{20} + 24000P^6Q^{21} + 3032P^5Q^{22} + 240P^4Q^{23} + 9P^3Q^{24}$		0.2978	1.161
Regular	2	$p^4 + 4p^3q + 2p^2q^2$	0.6180		1.635
2D site					
Percolation	3	$p^9 + 9p^8q + 36p^7q^2 + 67p^6q^3 + 59p^5q^4 + 22p^4q^5 + 3p^3q^6$	0.6193		1.624

For larger cells, PRLS can be analyzed using MC methods. I performed such an analysis for cell sizes $L=2,3,\dots,68,80,100$. In addition to $P^*(L)$ and $\nu(L)$, I also calculated the effective exponents $A(L)\equiv 3 - \ln M / \ln L$ and $Z(L)\equiv \ln L_s / \ln L$, where M is the average mass of the spanning cluster, and L_s is the average shortest distance between opposite faces of the cell through that cluster at P^* . For $L\rightarrow\infty$, we expect $A(L)\rightarrow A (= \beta/\nu)$ and $Z(L)\rightarrow Z$. Note, that these definitions of the effective exponents, which have been made in the spirit of the position space RG approach,¹¹ may differ by terms of order $1/\ln L$ from other definitions.

For each L and p , I calculated the function R by checking what fraction of 10 000 computer-generated random configurations actually spanned the cell. The value of p was changed in steps of 0.0025. The crossing point of the R curve with the line $R=P (=p^3)$ defined the fixed point $P^*(L)$. (The value of P^* was further refined by repeating the calculations with even larger samples close to P^* .) The values of $P^*(L)$ converge very fast (they almost do not change for $L > 20$) to $P_c = 0.2554 \pm 0.0004$ (or $p_c = 0.6345 \pm 0.0003$). Values of p^* ($\equiv P^{*1/3}$) are depicted in Fig. 1 versus the inverse cell size. Values of p for which $R=0.2$ and 0.3 are indicated as well. Clearly, they also converge to p_c . Our choice of P as the variable of the RG was somewhat arbitrary, since p could have been used as well. However, a fixed point determined from $R=p$ converges extremely slowly to p_c (almost all the points would be outside the scale of Fig. 1), and therefore we can expect to obtain more rapidly converging results using the variable P in the RG transformation.

Once the values for P^* were known, we turned to an accurate determination of dR/dP at P^* . This was done by calculating the values of R at two concentrations close

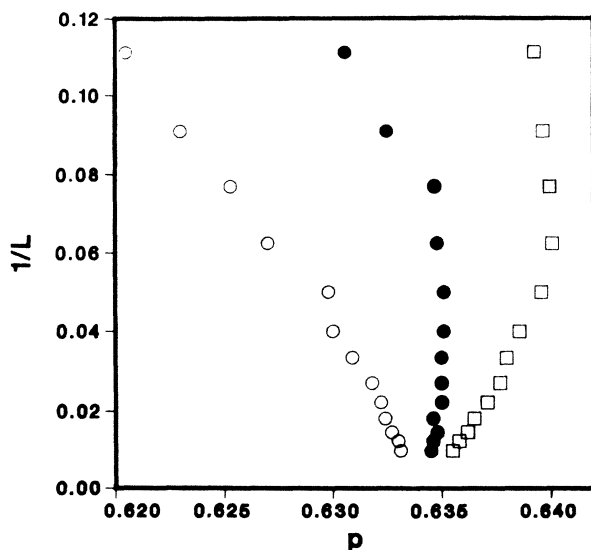


FIG. 1. Estimates of the percolation threshold (in terms of the 2D variable p) vs the inverse cell size. The estimates are obtained from the equations $R=P=p^3$ (●), $R=0.2$ (○), and $R=0.3$ (□). The error bars (of p) are ± 0.0001 (3 times smaller than the symbol size).

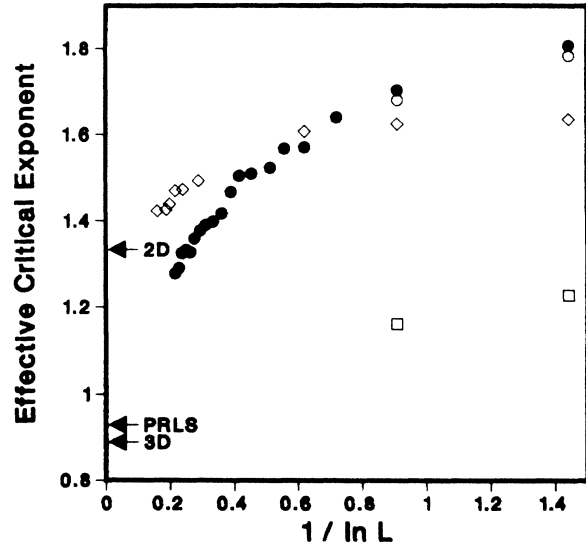


FIG. 2. Effective exponent $\nu(L)$ of PRLS from Table I (○) and from MC simulation (●). The error bars (of ν) are ± 0.015 (the symbol size). For comparison, the results of the regular 2D problem (Ref. 11) (◇) and of a regular 3D problem (Table I) (□) are also shown. The arrows indicate the known values of ν for regular 2D and 3D problems (Refs. 12 and 13) and the extrapolated value for PRLS.

to P^* and finding the ratio of the finite differences $\Delta R/\Delta P$. Values of R were obtained by averaging over 50 000 configurations (for $L \leq 16$, more than 100 000 configurations), and for each L , a sufficiently small spacing ΔP was chosen so that the replacement of the derivative by a ratio of finite differences introduced a systematic er-

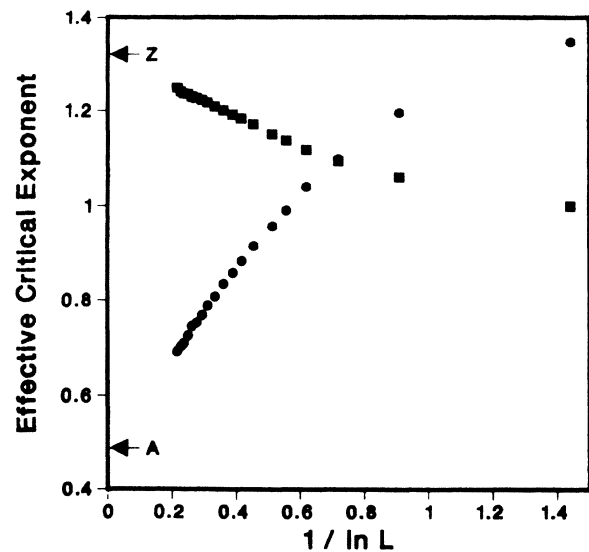


FIG. 3. Effective exponents $A(L)$ (●) and $Z(L)$ (■) for PRLS from MC simulation. The error bars of both A and Z are ± 0.002 ($\frac{1}{5}$ of the symbol size). The arrows indicate the extrapolated values of the exponents.

ror [overestimated $\nu(L)$] which did not exceed the statistical error of the simulation. The resulting values of $\nu(L)$ are depicted in Fig. 2. For comparison, I also show $\nu(L)$ of a regular 2D problem¹¹ and the results of R3DP from Table I. [There are no R3DP results for $L > 3$ using the same definition of $\nu(L)$.] Note that for small L , the values of $\nu(L)$ of the PRLS are very large. They are even larger than the values of $\nu(L)$ in a 2D problem. However, for $L \geq 7$, they become smaller than the 2D values and continue to decrease very fast with increasing L . The considerable curvature of the line and rather large scatter of the data points restricts the accuracy of the extrapolation to $1/\ln L = 0$. We estimate the asymptotic value $\nu = 0.93 \pm 0.06$, where the error bars represent the variability of the results due to different methods of extrapolation. The asymptotic value of ν is consistent with the best estimate¹² 0.89 for the R3DP, but we cannot exclude the $\nu = 1$ value predicted in Ref. 8.

The fractal codimension $A(L)$ and the exponent of the shortest path $Z(L)$ are depicted in Fig. 3. Each point of those graphs was obtained from averages over 50 000 con-

figurations. The smoothness of the graphs (compared with Fig. 2) is a consequence of the fact that both M and L , change very slowly near P^* , while dR/dP has a sharp maximum at (or near) P^* . The extrapolated values $A = 0.49 \pm 0.03$ and $Z = 1.32 \pm 0.03$ agree very well with known values of the fractal codimension¹³ and the exponent of the shortest path.¹⁴

I have presented numerical evidence that PRLS belongs to the same universality class as the R3DP. The results, however, do not exclude the possibility that the problem has slightly different exponents, and more accurate simulations would be useful. It would be interesting to see measurements of various physical quantities in percolating systems generated using this method.

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