Percolation thresholds and universal formulas

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A calculation of percolation thresholds of 11 two-dimensional and 18 three-dimensional lattices is presented. Among the three-dimensional ones are a random lattice and its dual, plus a number of anisotropic regular lattices. The results are used to test universal formulas that relate the percolation thresholds of lattices to their dimension and coordination number. The evidence suggests that dimension and coordination number are *not* sufficient to predict percolation thresholds. [S1063-651X(97)13002-1]

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I. INTRODUCTION

The idea of percolation processes was introduced in 1957, to describe a fluid which spreads randomly through a porous medium [1]. Since then, percolation problems have been studied extensively, and a variety of applications has been reported (see, e.g., Ref. [2,3]). Most of the attention has been given to percolation on regular lattices, because it is much easier to compute quantities for these lattices. Nevertheless, an exact calculation of the percolation threshold has remained elusive for most lattices.

This has prompted the search for empirical formulas, which express the percolation threshold p_c of a lattice in terms of its more simple properties. The formulas that have been proposed all use the dimension d and the coordination number q of the lattice. For example Sahimi *et al.* proposed the relation $p_{c,s}=d/[(d-1)(q-1)]$ for site percolation [4]. Several other relations, which are applicable for different classes of lattices, have been proposed. Galam and Mauger, who presented a brief review of the progress in this area, recently proposed a single formula that is applicable to all lattices [5]:

$$p_c=p_0[(d-1)(q-1)]^{-a}d^b. \tag{1}$$

The parameters a, b, and p_0 are determined by fits to known values for a number of lattices. For site percolation thresholds one always has $b=0$, whereas for bond percolation thresholds $b=a$.

Galam and Mauger observed that there are only two classes of lattices (for $d<7$). The first class consists of all two-dimensional lattices except the kagomé lattice, and has $\{p_0=0.8889;\ a=0.3601\}$ for site percolation and $\{p_0=0.6558;\ a=0.6897\}$ for bond percolation. The rest of the lattices all have thresholds which are described by $\{p_0=1.2868;\ a=0.6160\}$ for site percolation and $\{p_0=0.7541;\ a=0.9346\}$ for bond percolation. Indeed, the results of Eq. (1) for all lattices in Ref. [5] are very good.

However, although Galam and Mauger considered many lattices, there are quite a few interesting ones which are not included in their study. This enables one to test the predictive power of their formula. In Ref. [6] the percolation thresholds of a ''stacked triangular'' lattice were calculated. As it turned out, this lattice has the same dimension and coordination number as the body centered cubic lattice, but markedly different percolation thresholds.

This difference could be caused by the anisotropy in this stacked triangular lattice. Since Galam and Mauger did not consider anisotropic lattices, this difference is not in contradiction with their result. Moreover, if one introduces an effective coordination number $q_e=7.65$, as was done in Ref. [7], both the site and the bond percolation threshold are described by Eq. (1). In other words, if one calculates q_e using Eq. (1) with a known value for the site percolation threshold, one can predict the bond percolation threshold, or the other way around.

The more fundamental question remains therefore whether the two parameters d and q are sufficient to predict percolation thresholds even for isotropic lattices. To address this issue I present here a calculation of percolation thresholds in many different lattices, both isotropic and anisotropic. The results lead to the conclusion that d and q are *not* sufficient to predict percolation thresholds.

II. METHOD AND RESULTS

A conventional way to calculate percolation thresholds is described by Stauffer and Aharony [2]. This method requires a three-dimensional array (in Fortran ARRAY(I,J,K)) for the simple cubic lattice, for instance. All the so-called ''Bravais lattices'' [8] can be coded using such an array. For the non-Bravais lattices, which I will call ''lattices with a basis'' here, the coding is more complicated. In general, the lattices with a basis have received less attention as a result. As an example of a lattice with a basis I have described the dual of the body-centered-cubic (bcc) lattice in Table I and Fig. 1 as a lattice with a six-point basis.

One could describe a lattice with a basis in computer code as an array with an additional dimension, i.e., ARRAY(B,I,J,K), where B loops over the basis points. This does not solve all the associated problems, however, because a site ARRAY(1,I,J,K) is not connected in the same way as, e.g., ARRAY(2,I,J,K). An alternative way to characterize the lattice is by making an explicit list of bonds that connect the sites. By numbering the sites from 1 to N_s, one can list for each bond the two sites it connects. Although this is somewhat elaborate for regular lattices, it has the advantage of maintaining full flexibility, allowing one to handle any desired topology. One can divide the calculation in two parts. First

TABLE I. The description of the dual of the body-centered-cubic lattice as a lattice with a six-point basis. Each of the points in the first row is connected to the four points listed in its column (i.e., the coordination number is 4).

1, **x**	2, **x**	3, **x**	4, **x**	5, **x**	6, **x**
3, **x**	4, **x**	1, **x**	2, **x**	3, **x**	4, **x**
6, **x**+(−1,0,0)	5, **x**+(0,−1,0)	4, **x**	3, **x**	6, **x**	5, **x**
4, **x**+(−1,1,−1)	3, **x**+(0,0,−1)	5, **x**	6, **x**	1, **x**+(1,0,1)	2, **x**+(1,0,1)
5, **x**+(−1,0,−1)	6, **x**+(−1,0,−1)	2, **x**+(0,0,1)	1, **x**+(1,−1,1)	2, **x**+(0,1,0)	1, **x**+(1,0,0)

one can write a small program that generates lists of bonds for a specific lattice. Then one can use a generic program that calculates the percolation threshold for the specified lattice. This program typically contains separate arrays for the sites and for the bonds. The array of bonds would list the sites it connects (e.g., BONDS(2,NBONDS)), while the array of sites would list the bonds that are connected to it (SITES(QMAX,NSITES), with QMAX the maximum coordination number). To determine the percolation threshold for such a system, a cluster algorithm is needed. For this purpose the cluster algorithm by Hoshen and Kopelman [9] can be cast into a suitable form.

For each of the lattices listed in Table II I have calculated percolation thresholds $p_c(L)$ for various lattice sizes L. In two dimensions the largest lattice size was 512×512 (i.e., $L=512$), in three dimensions $64\times64\times64$. The results quoted in Table II are fits of p_c to the scaling relation

$$|p_c(L)-p_c|\sim L^{-1/\nu}, \tag{2}$$

where the critical exponent ν was kept fixed at 4/3 in two dimensions and at 0.88 in three dimensions.

All the two-dimensional lattices can be ''stacked'' to form three-dimensional lattices. For instance one can stack the layers of square lattices directly on top of one another to obtain the simple cubic lattice. Analogously one can stack the triangular lattice to form what is sometimes called the simple hexagonal lattice [8]. By stacking various two-dimensional lattices one obtains several anisotropic lattices. A calculation of percolation thresholds for these lattices should give some information on the validity of universal formulas for anisotropic lattices. Therefore these lattices have been included in Table II.

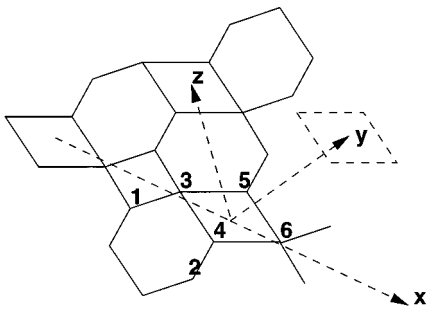

FIG. 1. The definition of the basis points for the dual of the body-centered-cubic lattice. The dashed arrows marked x, y, and z indicate the three directions in which this basis is repeated to build the lattice.

Table II also lists the results for an irregular lattice (''Finney'') and its dual. This lattice is defined on the basis of a real bead pack, which was constructed and measured by Finney [10]. One can define the beads of the packing as the sites of a lattice. The bonds of the network are given once one defines the neighbors of each site. I have used the Delaunay triangulation for this purpose, which is equivalent to, e.g., Bernal's definition of ''geometrical neighbors'' [11]. The dual of the lattice thus obtained is given by the Voronoi tessellation [12]. I have taken subsets of the Finney pack of increasing size, calculated the percolation thresholds for each size, and fitted the results to Eq. (2).

Several checks have been performed to confirm the validity of the computer programs and their numerical results. First of all, a number of percolation thresholds in two dimensions are known exactly. For ''self-matching'' lattices [13], the site percolation threshold is $\frac{1}{2}$. Examples are the triangular lattice and the octagonal lattice (see Fig. 2). As a consequence the bond percolation threshold of the square lattice has been shown to be $\frac{1}{2}$ too. The bond percolation threshold of the triangular lattice is given by $p_\triangle=2\sin(\pi/18)=0.347296\ldots$, and for its dual lattice, the honeycomb lattice, it is therefore $1-p_\triangle$. Moreover, it was shown that the site percolation threshold of the Kagomé lattice is equal to the bond percolation threshold of the honeycomb lattice, i.e., $1-p_\triangle$. All these results have been reported by Sykes and Essam [13]. Wierman [14] proved that the bond percolation threshold of the bowtie lattice is given by $p_{\bowtie}=0.404518\ldots$ ($p_{\bowtie}$ actually is the root of $1-p-6p^2+6p^3-p^5=0$). The bond percolation threshold of the dual lattice of the bowtie lattice is $1-p_{\bowtie}$.

I have checked that the numerical results for these thresholds coincided with the exact results, within estimated error margins of 0.0005 at maximum. Furthermore, the statement that in two dimensions the bond percolation thresholds of a lattice and its dual should add to unity (for most lattices [13]), can be used to test some of the results in Table II.

Some of the lattices in Table II are Bravais lattices, viz. the simple cubic, the face-centered-cubic (fcc), the bcc, and the stacked triangular lattice. I have verified with a separate computer program, that, when coded as ARRAY(I,J,K), the results for the percolation thresholds are the same, within the estimated error margins. The largest system size used for this type of calculation was higher, $L=128$.

Finally I have checked the results for the dual of the bcc lattice. This could be done by using the Voronoi tessellation to generate an explicit dual lattice, based on the positions of

TABLE II. Site ($p_{c,s}$) and bond ($p_{c,b}$) percolation thresholds for various lattices and their dual lattices. The average coordination of the networks is listed under $\overline{q}$. In the references given in the column titled Ref., pictures of the lattices are given. In the top half of the table the two-dimensional lattices are listed, in the bottom half the three-dimensional ones. The thresholds marked with * are exact (see text). The lattices marked with √ were included in the Galam and Mauger study [5,7]. The result for the site percolation threshold of the square lattice is taken from Ref. [2]. The abbreviation ''hcp'' stands for hexagonal close packed. Between brackets are error estimates concerning the last digit.

Name lattice	$\overline{q}$	Ref.	$p_{c,s}$	$p_{c,b}$	Name dual	$\overline{q}$	Ref.	$p_{c,s}$	$p_{c,b}$
√ kagomé	4	[3]	0.6527 . . . *	0.5243(4)	dice	4		0.5848(2)	0.4755(4)
√ square	4		0.592746	0.5*	√ square	4		0.592746	0.5*
	5		0.5502(8)	0.4196(6)	pentagonal	$3\frac{1}{3}$	[15]	0.6471(6)	0.5800(6)
bowtie	5	[14]	0.5475(8)	0.4045 . . . *		$3\frac{1}{3}$	[14]	0.6653(6)	0.5954 . . . *
√ triangular	6	[2]	0.5*	0.3472 . . . *	√ honeycomb	3	[3]	0.6971(4)	0.6527 . . . *
octagonal	6	Fig. 2	0.5*	0.3237(6)		3	Fig. 2	0.7297(4)	0.6771(6)
kagomé stack	6		0.3346(4)	0.2563(2)	dice stack	6		0.2998(4)	0.2378(4)
√ (simple) cubic	6		0.3114(4)	0.2487(2)	√ (simple) cubic	6		0.3114(4)	0.2487(2)
	7		0.2872(4)	0.2142(4)	pentagonal stack	$5\frac{1}{3}$		0.3394(4)	0.2793(4)
bowtie stack	7		0.2822(6)	0.2092(4)		$5\frac{1}{3}$		0.3480(4)	0.2853(4)
triangular stack	8	[8]	0.2623(2)	0.1859(2)	honeycomb stack	5		0.3701(2)	0.3093(2)
octagonal stack	8		0.2524(6)	0.1752(2)		5		0.3840(4)	0.3168(4)
√ bcc	8	[8]	0.2458(2)	0.1802(2)		4	Fig. 1	0.4560(6)	0.4031(6)
					√ diamond	4	[8]	0.4286(4)	0.3888(2)
√ fcc	12	[8]	0.1994(2)	0.1200(2)					
√ hcp	12	[8]	0.1990(2)	0.1199(2)					
Finney pack [10]	14.3		0.1623(8)	0.0925(9)		4		0.4495(9)	0.3987(8)

a number of bcc lattice sites. Since the coordination number of the dual of the bcc lattice is four, the Voronoi tessellation is nondegenerate in this case, and therefore easy to use. Also in this case several lattice sizes were used and the results were fitted to Eq. (2).

III. DISCUSSION

There are several observations one can make when one looks carefully at Table II. For instance, there are many lattices with equal dimension and coordination number, but with different percolation thresholds. In particular it is interesting to compare the triangular and octagonal lattices, which both have $d=2$ and $q=6$. Their site percolation threshold is equal ($\frac{1}{2}$, exact result), but their bond percolation threshold is different: 0.347 296 . . . vs 0.3237 ± 0.0006. This means that d and q are not enough to predict percolation thresholds. For this case it is not even possible to define an ''effective'' coordination number q_e, as Galam and Mauger [7] suggest, that will allow such a prediction. Based on the site percolation thresholds one would infer that q_e is equal for these two lattices. This would lead one to predict that the bond percolation thresholds are equal too, which is not the case.

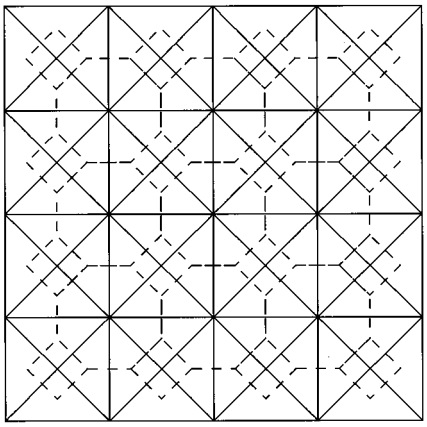

FIG. 2. The octagonal lattice (solid lines) and its dual (dashed lines).

The comparison of the diamond lattice with the dual of the bcc lattice is worth mentioning. Both lattices have $d=3$ and $q=4$, and are isotropic. That the dual of the bcc lattice is isotropic is not apparent from Fig. 1, but follows from the fact that the bcc lattice itself is isotropic. Both the site and bond percolation thresholds are distinctly different for the two lattices: 0.4286 ± 0.0004 vs 0.4560 ± 0.0006 (sites) and 0.3888 ± 0.0002 vs 0.4031 ± 0.0006 (bonds) for the diamond and bcc-dual lattice, respectively. So even for isotropic lattices one needs more than d and q to predict percolation thresholds.

In general one can conclude from the table that if a lattice has a higher coordination number q, its percolation thresholds are lower. There is only one exception to this rule: the site percolation threshold of the pentagonal lattice (0.6471) is lower than that of the Kagomé lattice (0.6527 . . .), although its average coordination number is lower ($3\frac{1}{3}$ vs 4). This does not contradict the results of Galam and Mauger [5], because the Kagomé lattice is in a different class than all the other two-dimensional lattices. Nevertheless, it is amazing in its own right that the ordering of the bond percolation thresholds is different from that of the site percolation thresholds. This occurs in the case of the bcc and the octagonal stacked lattice too. However, in this case the lattices have

equal d and q, so it might be considered less striking here .

The results for the irregular lattices are reasonably well described by Eq. (1). The site percolation threshold for the Finney pack is 0.1623 ± 0.0008 vs a prediction of 0.1705, while the bond percolation threshold is 0.0925 ± 0.0008 vs a prediction of 0.0981. Since the average coordination number of this lattice is 14.3, higher than any of the regular lattices, this is an extra test of Eq. (1). The results for the dual of the Finney pack, coordination number 4, lie between those of the diamond lattice and the dual of the bcc lattice. The bond percolation threshold (0.3987 ± 0.0008) is close to the predicted value (0.3945), but the site percolation threshold shows a deviation: 0.4495 ± 0.0009 vs 0.4267.

Finally, if d and q are not enough to predict percolation thresholds, are there alternatives? For the anisotropic lattices, one could try to quantify the anisotropy and add this quantity to the fit parameters. The results of Table II can be used to do this. For the isotropic lattices one could distinguish between lattices with only one coordination number, and lattices with a spread (e.g., the octagonal lattice has sites with four connected bonds, and sites with eight). However, these quantities do not separate the diamond lattice from the dual of the bcc lattice (or even from the dual of the Finney pack), so one will have to become more sophisticated.

In summary, I calculated site and bond percolation thresholds of many two- and three-dimensional lattices. The results indicate that one cannot predict percolation thresholds on the basis of dimension and coordination number only, not even for isotropic lattices.

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