Percolation thresholds of the duals of the face-centered-cubic, hexagonal-close-packed, and diamond lattices

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A calculation of percolation thresholds of the *dual lattices* of the face-centered-cubic (fcc) lattice, the hexagonal-close-packed (hcp) lattice, and the diamond lattice is presented. The results are used to investigate whether these thresholds can be related to the thresholds of the fcc, hcp, and diamond lattices themselves. In two dimensions there is such a relation, but the present results indicate that there is no such relation in three dimensions. Also, the site percolation threshold of the dual of the diamond lattice turns out to be high: Although the average coordination number q of this lattice is $6\frac{2}{3}$, its site percolation threshold is higher than for many lattices with $q=5$. [S1063-651X(97)00906-9]

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I. INTRODUCTION

Percolation processes are relevant to a variety of physical problems and have been treated by many authors (for reviews, see Refs. [1,2]). Most of the attention has been given to percolation on regular lattices because it is much easier to compute quantities for these lattices. Nevertheless, exact percolation thresholds are known for only few lattices. For some other lattices, rigorous bounds on the percolation thresholds have been derived (e.g., in Ref. [3]). For most lattices only numerical estimates are known.

Many investigators have sought some sort of regularity in the mostly numerical results. For instance, people have searched 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 use the dimension d and the coordination number q of the lattice. For instance, Galam and Mauger, who presented a brief review of the progress in this area, proposed a single formula that would apply to all lattices [4,5]:

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

The parameters a, b, and p_0 were 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 results of Eq. (1) for all lattices in Ref. [4] were very good.

However, in Refs. [6,7], percolation thresholds were calculated for many lattices that were not included in the Galam-Mauger study. Among these lattices were many that had equal d and q, but different percolation thresholds. The conclusion was therefore that d and q are *not* sufficient to predict percolation thresholds.

This raises the question of what is really known about the trends in the values of the percolation thresholds. In general, one can say that lattices with a higher coordination number have lower percolation thresholds. There is an exception to this rule in two dimensions (the Kagomé lattice [7]), but in three dimensions this rule holds for all known percolation thresholds. However, the rule is only an observation on the basis of (numerically) known threshold values; there is no theoretical proof.

In two dimensions, there is another rule that has been established, in this case theoretically. Sykes and Essam [8] conjectured that the bond percolation threshold of a two-dimensional lattice and the one of its dual lattice should add to one. Kesten later proved this rigorously for periodic two-dimensional lattices with at least one axis of symmetry [9]. In three dimensions, not much is known theoretically. Even numerically, the only example one had until recently was the percolation threshold of the simple cubic lattice, which is its own dual lattice. In this case the sum is $0.2488+0.2488=0.4976$. From the recent data in Ref. [7], one can check

TABLE I. Description of the dual of the face-centered-cubic lattice as a lattice with a three-point basis. Each of the points in the first row is connected to the points listed in its column.

1, **x**	2, **x**	3, **x**
2, **x**	1, **x**	1, **x**
2, **x**+(−1,0,0)	1, **x**+(1,0,0)	1, **x**+(1,0,0)
2, **x**+(−1,1,0)	1, **x**+(1,−1,0)	1, **x**+(0,1,0)
2, **x**+(−1,0,1)	1, **x**+(1,0,−1)	1, **x**+(0,0,1)
3, **x**		
3, **x**+(−1,0,0)		
3, **x**+(0,−1,0)		
3, **x**+(0,0,−1)		

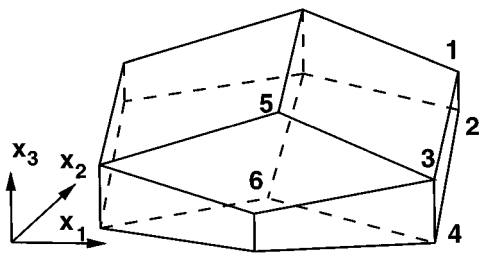

FIG. 1. Wigner-Seitz cell for the hexagonal-close-packed lattice. The basis points for the dual lattice are numbered; see also Table II.

TABLE II. Description of the dual of the hexagonal-close-packed lattice as a lattice with a six-point basis. Each of the points in the first row is connected to the points listed in its column.

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

that in almost all cases the bond percolation thresholds of a three-dimensional lattice and its dual add up to 0.495 ± 0.002. The only exceptions are the body-centered-cubic lattice (0.583) and a random lattice (0.491). One could speculate that there is a general rule with only a few outliers. However, all the lattices for which the bond percolation thresholds add to 0.495 ± 0.002 are ''stacked lattices.'' That is, these lattices are constructed by stacking two-dimensional lattices directly on top of each other. These lattices are therefore almost all anisotropic.

The most important three-dimensional lattices are the ones that one encounters in nature. In solid state physics these are called the simple cubic, the bcc, the fcc, the hcp, and the diamond lattice [10]. The percolation thresholds of all these lattices have been calculated numerically [1]. For the *dual lattices* this has only been done for the bcc lattice [7] (and the simple cubic lattice, which is self-dual).

Therefore I calculated the percolation thresholds for the duals of the fcc, hcp, and diamond lattices. The results justify two conclusions. First, the sum of bond percolation thresholds of a lattice and its dual is different for all lattices. Second, the dual of the bcc lattice has a high coordination number ($\overline{q} = 6\frac{2}{3}$), but its site percolation threshold is higher than that of many lattices with $\overline{q} = 5$. In other words, the site percolation thresholds are *not* ordered with respect to the coordination number of the lattice.

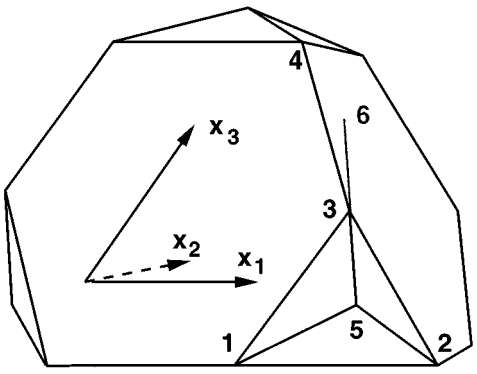

FIG. 2. Wigner-Seitz cell for the diamond lattice. The basis points for the dual lattice are numbered; see also Table III. Point 6 is indicated in gray because it is located in an adjacent Wigner-Seitz cell. Its position can be found by extending the line from point 5 to point 3.

II. DUAL LATTICES

The dual lattice of a given lattice can be constructed by use of the Wigner-Seitz cell (or Voronoi polyhedron [11]). The ''corners'' of the Wigner-Seitz cell are the sites of the dual lattice; the edges of the Wigner-Seitz cell are the bonds of the dual lattice. If one considers a number of spheres that are stacked to form a fcc lattice, the dual lattice can be used, e.g., to describe the empty space in between the spheres. This method has been used, among other things, for calculations of fluid flow [12] and electrical conductivity [13] in random bead packs.

A picture of the Wigner-Seitz cell for the fcc lattice can be found in Ref. [10]. The dual of the fcc lattice can be described as a lattice with a three-point basis; see Table I. One basis point has eight connected neighbors, the other two basis points have four. Therefore the average coordination number of this lattice is $5\frac{1}{3}$.

The dual of the hcp lattice is described in Table II as a lattice with a six-point basis. I have indicated my choice for these basis points in Fig. 1, where a picture of the Wigner-Seitz cell of the hcp lattice is shown. These Wigner-Seitz cells are stacked to fill the space. In the case of the hcp lattice, the cells that are displaced by one unit in the $\mathbf{x}_3$ direction are also rotated by π around $\mathbf{x}_3$. Two basis points of the dual lattice have eight connected neighbors, whereas the remaining four basis points have four. Therefore this lattice also has an average coordination number $5\frac{1}{3}$.

The Wigner-Seitz cell for the diamond lattice (Fig. 2) is

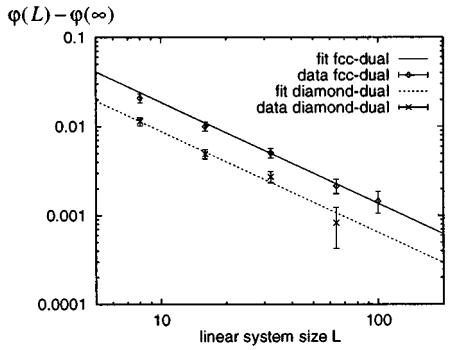

FIG. 3. Examples of the scaling of the site percolation threshold with the linear system size L: the duals of the fcc and diamond lattices. The lines are determined by fits to the data points for the three largest lattices, using a fixed value $\nu = 0.88$.

TABLE III. Description of the dual of the diamond lattice as a lattice with a six-point basis. Each of the points in the first row is connected to the points listed in its column.

1, $\mathbf{x}$	2, $\mathbf{x}$	3, $\mathbf{x}$	4, $\mathbf{x}$	5, $\mathbf{x}$	6, $\mathbf{x}$
2, $\mathbf{x}$	1, $\mathbf{x}$	1, $\mathbf{x}$	1, $\mathbf{x}+(0,0,1)$	1, $\mathbf{x}$	1, $\mathbf{x}+(0,0,1)$
2, $\mathbf{x}+(0,-1,0)$	1, $\mathbf{x}+(0,1,0)$	1, $\mathbf{x}+(0,0,1)$	1, $\mathbf{x}+(-1,0,1)$	2, $\mathbf{x}$	2, $\mathbf{x}+(0,-1,1)$
3, $\mathbf{x}$	3, $\mathbf{x}$	2, $\mathbf{x}$	2, $\mathbf{x}+(-1,0,1)$	3, $\mathbf{x}$	3, $\mathbf{x}$
3, $\mathbf{x}+(0,0,-1)$	3, $\mathbf{x}+(0,1,-1)$	2, $\mathbf{x}+(0,-1,1)$	2, $\mathbf{x}+(0,-1,1)$	4, $\mathbf{x}+(1,0,-1)$	4, $\mathbf{x}$
4, $\mathbf{x}+(0,0,-1)$	4, $\mathbf{x}+(1,0,-1)$	4, $\mathbf{x}$	3, $\mathbf{x}$		
4, $\mathbf{x}+(1,0,-1)$	4, $\mathbf{x}+(0,1,-1)$	4, $\mathbf{x}+(1,0,-1)$	3, $\mathbf{x}+(-1,0,1)$		
5, $\mathbf{x}$	5, $\mathbf{x}$	5, $\mathbf{x}$	5, $\mathbf{x}+(-1,0,1)$		
6, $\mathbf{x}+(0,0,-1)$	6, $\mathbf{x}+(0,1,-1)$	6, $\mathbf{x}$	6, $\mathbf{x}$		

rather difficult to depict. It is a sort of ''pyramid,'' built from four regular hexagons. On the four corners of the pyramid, an additional small tetrahedron (points {1,2,3,5} in Fig. 2) is placed. To stack the Wigner-Seitz cells of the diamond lattice, half the cells are rotated by π around $\mathbf{x}_1$. Moreover, half the cells are rotated by $\pi/3$ around $\mathbf{x}_1 \wedge \mathbf{x}_2$, where $\wedge$ is the outer product. The dual lattice is described in Table III as a lattice with a six-point basis. Four of the basis points have eight connected neighbors, while the other two basis points have four. The average coordination number is therefore $6\frac{2}{3}$.

III. CALCULATION OF PERCOLATION THRESHOLDS

The method to calculate the percolation thresholds for these lattices with a basis is described in Ref. [7]. It boils down to writing a small computer program to make an explicit list of bonds for a specific lattice with a given size. Tables I–III can be used for this purpose. This list can be read by a program that uses two arrays, i.e., SITES(QMAX,NSITES) and BONDS(2,NBONDS) to handle any desired topology (QMAX is the maximum coordination number). This program uses the method given in Ref. [1] to calculate percolation thresholds. The results for several lattice sizes are given in Table IV.

The percolation threshold for finite lattices scales with the linear lattice size L as

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

Here ν is a critical exponent, which in three dimensions has the value 0.88 [1]. I have fitted the results in Table IV to this scaling relation, keeping ν fixed at 0.88. The results of the fits are also shown in the table.

I have checked the results in Table IV in the following way. I generated a set of, e.g., fcc lattice coordinates. Based on these coordinates, I explicitly constructed the dual lattice by means of the Voronoi tessellation. In Ref. [7] this was done for the body-centered-cubic lattice, which was relatively simple because the dual of the bcc lattice has coordination number 4. However, for the duals of the fcc, hcp, and diamond lattices the Voronoi tessellation is degenerate and therefore the tessellation had to be performed more carefully. In all these cases, results were obtained for several lattice sizes and the percolation threshold at infinite lattice size was determined by fitting these results to the scaling relation.

IV. DISCUSSION

The results for the percolation thresholds are listed in Table IV. The fit results on the last row were obtained by using the data points for the three largest lattice sizes only. Examples of the scaling behavior and the fit through the data points are shown in Fig. 3. In the figure, the fit goes through the data points for the smallest lattice sizes when taking into account their estimated error margins. (For the dual of the fcc lattice these are the points at $L=8,16$, whereas for the dual of the diamond lattice this is the point at $L=8$.) This implies that the used lattice sizes were comfortably within the scaling regime.

Galam and Mauger [4,5] noted that the fcc and hcp lattices have equal dimension ($d=3$) and coordination number ($q=12$) and have equal percolation thresholds too. This is a nontrivial result because topologically these lattices are not

TABLE IV. Percolation thresholds as a function of linear lattice size L. The values in the last row are results of a fit of the last three data points to the scaling relation. Error estimates concerning the last digit are indicated in parentheses.

	Sites			Bonds		
L	fcc dual	hcp dual	diamond dual	fcc dual	hcp dual	diamond dual
8	0.3550(24)	0.3391(10)	0.4018(12)	0.2802(16)	0.2735(10)	0.2392(10)
16	0.3442(12)	0.3233(6)	0.3953(6)	0.2760(8)	0.2644(4)	0.2376(4)
32	0.3392(6)	0.3163(4)	0.3931(4)	0.2729(4)	0.2606(4)	0.2362(4)
64	0.3363(4)	0.3128(4)	0.3912(4)	0.2714(2)	0.2588(2)	0.2355(2)
100	0.3356(4)			0.2710(2)		
∞	0.3341(5)	0.3101(5)	0.3904(5)	0.2703(3)	0.2573(3)	0.2350(5)

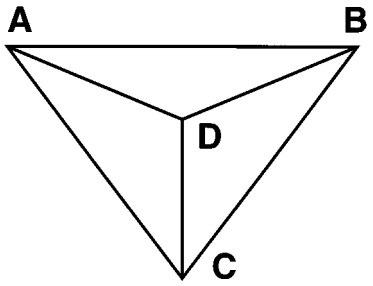

FIG. 4. Two-dimensional example of a situation where a point (D) is irrelevant for site percolation.

identical. An intriguing result from the present study is that their dual lattices also have equal d and q (3 and $5\frac{1}{3}$, respectively), but that for these dual lattices the percolation thresholds are *not* equal. This is another piece of evidence to prove that d and q are not enough to predict percolation thresholds.

In Ref. [7] I concluded from a large collection of percolation thresholds that, as a general rule, the percolation thresholds decrease when the coordination number increases. There was 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). In the present study we encounter another exception, viz., the dual of the diamond lattice. The average coordination number of this lattice is $6\frac{2}{3}$ and the bond percolation threshold lies between the thresholds of lattices with $q=6$ and $q=7$ (see Ref. [7]). The exception is the site percolation threshold, which lies between thresholds of lattices with $q=4$ and $q=5$. This rather surprising result was confirmed by the independent calculation based on the Voronoi tessellation, as explained in Sec. III.

It is possible to understand roughly why the dual of the diamond lattice has a high site percolation threshold. Let us consider the basis points 5 and 6 of the lattice. From Fig. 2 it is clear that, e.g., points 1 and 3 are connected via point 5. However, they are also directly connected. In fact, *all* the ''neighbors'' of point 5 are also direct neighbors of each other. The same is true for point 6. So, in a manner of speaking, when one traverses the lattice from one side to the other, points 5 and 6 are always a ''detour.'' Therefore one can argue that for site percolation these points are completely irrelevant. This is illustrated in a two-dimensional example in Fig. 4. When one considers clusters of occupied sites, it does not matter whether the points of type D are occupied or not. For bond percolation, however, it does make a difference whether or not the bonds connecting, e.g., A with D are occupied.

I have studied the lattice that is obtained by omitting the basis points 5 and 6. One can take basis points 1–4 in Table III and use only the first six lines in the table. This defines a lattice with a four-point basis and $q=6$. I have calculated the percolation threshold for this ''reduced'' lattice to be 0.3898 ± 0.0008 for site percolation and 0.2709 ± 0.0006 for bond percolation. These results are as expected according to the above arguments. The bond percolation threshold is higher than for the dual of the diamond lattice. This is reasonable because the coordination number of the reduced lattice is lower. However, the site percolation threshold is the same as for the dual of the diamond lattice, despite the lower coordination number. It follows that the exceptional value for the site percolation threshold of the dual of the diamond lattice is in part due to the peculiar role of the basis points 5 and 6 in the lattice. The presence of these points makes no difference to the site percolation threshold, but does make the coordination number q higher.

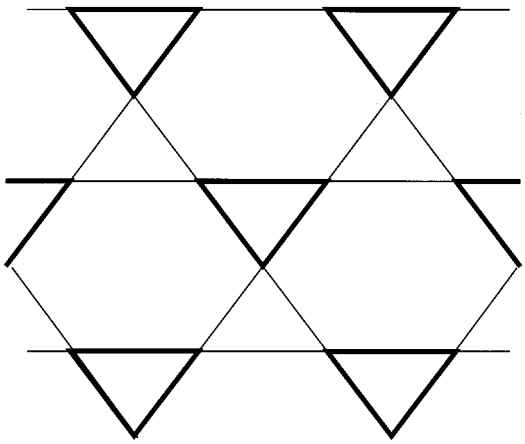

FIG. 5. Description of the Kagomé lattice as a lattice with a three-point basis. The basis points form a (regular) triangle.

The reduced lattice still has a high site percolation threshold compared to other lattices with $q=6$. Although this is not understood at present, it has an analog in two dimensions. The reduced lattice is a lattice with a four-point basis and the basis can be chosen such that the basis points form a regular tetrahedron. [For instance, one can choose the basis $\{(1,\mathbf{x}),(2,\mathbf{x}),(3,\mathbf{x}),(4,\mathbf{x}+(1,0,-1))\}$.] A two-dimensional analog of this lattice is a lattice with a three-point basis, where the three basis points form a regular triangle. This is the Kagomé lattice; see Fig. 5. The two-dimensional Kagomé lattice was noticed in [7] to have an exceptionally high site percolation threshold as well.

Finally, based on the results of Table IV, one can add the bond percolation thresholds for the fcc lattice and its dual (and likewise for the hcp and diamond lattice). The results are 0.390, 0.377, and 0.624, respectively, compared to 0.498 for the simple cubic lattice and 0.583 for the bcc lattice. I conclude that there is no obvious regularity in the sum of bond percolation thresholds in three dimensions.

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