Universal formulas for percolation thresholds. II. Extension to anisotropic and aperiodic lattices

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In a recent paper, we reported a universal power law for both site and bond percolation thresholds in any Bravais lattice with q equivalent nearest neighbors in dimension d. We now extend it to three different classes of lattices which are, respectively, anisotropic lattices without equivalent nearest neighbors, non-Bravais lattices with two atom unit cells, and quasicrystals. The investigation is focused on $d=2$ and 3, due to the lack of experimental data at higher dimensions. The extension to these lattices requires the substitution of q by an effective (non integer) value q_{eff} in the universal law. For each of the 17 lattices which constitute our sample, we argue for the existence of one q_{eff} which reproduces both the site and the percolation threshold, with a deviation with respect to numerical estimates which does not exceed ∓ 0.01. [S1063-651X(97)10207-0]

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I. INTRODUCTION

Very recently we postulated a universal power law for both site and bond percolation thresholds [1]. The formula yields thresholds for any Bravais lattice, at any dimension with an impressive accuracy. It is written

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

with d the space dimension and q the coordination number. While $b=a$ for bond dilution, $b=0$ for site dilution. Three different classes were found with three distinct parameter sets $\{p_0;a\}$. The first class includes two-dimensional triangle, square, and honeycomb lattices. It is characterized by $\{p_0=0.8889;a=0.3601\}$ for site dilution and by $\{p_0=0.6558;a=0.6897\}$ for bond dilution. Two-dimensional Kagomé and all other lattices of cubic symmetry (for $3\leqslant d\leqslant 6$) constitute the second class, which is characterized by $\{p_0=1.2868;a=0.6160\}$ and $\{p_0=0.7541;a=0.9346\}$ for sites and bonds, respectively. A third class has been found at high dimensions ($d>6$), which recovers the infinite Cayley tree limit, but is not relevant to the present investigation, which deals with lattices only at $d=2$ and 3.

In addition to the dimension d, percolation thresholds within a class depend only on q. This is understood in lattices where the q nearest neighbors of any site are equivalent, which is indeed the case for all lattices mentioned above. However, this is a drastic restriction, since many percolation problems in physics deal with lattices which do not have this property. It is the purpose of the present work to investigate the extension of Eq. (1) to other lattices, via the substitution of q by an effective parameter q_{eff}.

We checked on a sample of 17 lattices, for each of which there exists one value of q_{eff} which reproduces both the site and the bond percolation thresholds. The error is within ± 0.006 for all the lattices, except for two of them (the dual Penrose lattice, and the dodecagonal lattice with ferromagnetic links), where the error reaches 0.01 for reasons we also discuss in this paper. We believe this sample is large enough to be representative of a general trend, and then conclude upon the existence of such a q_{eff} in any lattice. For a lattice which does not belong to our sample, this parameter could be used as an intermediate quantity to predict bonds from site percolation thresholds, or vice versa, with the same accuracy.

The paper is organized as follows. Section II discusses a series of lattices with nonequivalent neighbors. The introduction of an effective number of nearest neighbors in our universal formula for percolation is argued in Sec. III. The results are shown and discussed in Sec. III. Section V contains some remarks for future work.

II. NONEQUIVALENT NEIGHBORS

Some periodic Bravais lattices are anisotropic, for instance, the hexagonal lattice at $d=3$. In this case, any lattice site has six equivalent nearest neighbors in the a, b plane (the bonding angle is 60°) and two nonequivalent sites along the c axis (the bonding angle is 90°). Actually, the anisotropic lattice percolation threshold should depend on the degree of anisotropy. For the hexagonal lattice, this means that p_c should be different from that of the corresponding isotropic lattice with the same set $d=3,q=8$, i.e., the bcc lattice. This difference has indeed been observed recently [2] in the particular case of the stacked triangular lattice, which becomes the hexagonal lattice when $a=b=c$.

There also exist non-Bravais lattices which are periodic, such as fcc and bcc. Another case is the hexagonal-close-packed (hcp) lattice which, from a topologic viewpoint, is a simple hexagonal lattice with two atoms per unit cell. Percolation thresholds for the hcp lattice were obtained long ago [3].

Some lattices are not even periodic. This is the case for quasicrystals which are aperiodic lattices with long-range order. In addition to being interesting in their own right, such structures can serve as models for alloylike materials, causing a growing interest in the determination of the quasicrystalline lattice percolation thresholds. First, determinations of percolation thresholds on two-dimensional quasilattices have been made on the Penrose tiling and its dual [4–6]. Recently, percolation thresholds have also been computed in two of the most important quasilattices; the simple octagonal and dode-

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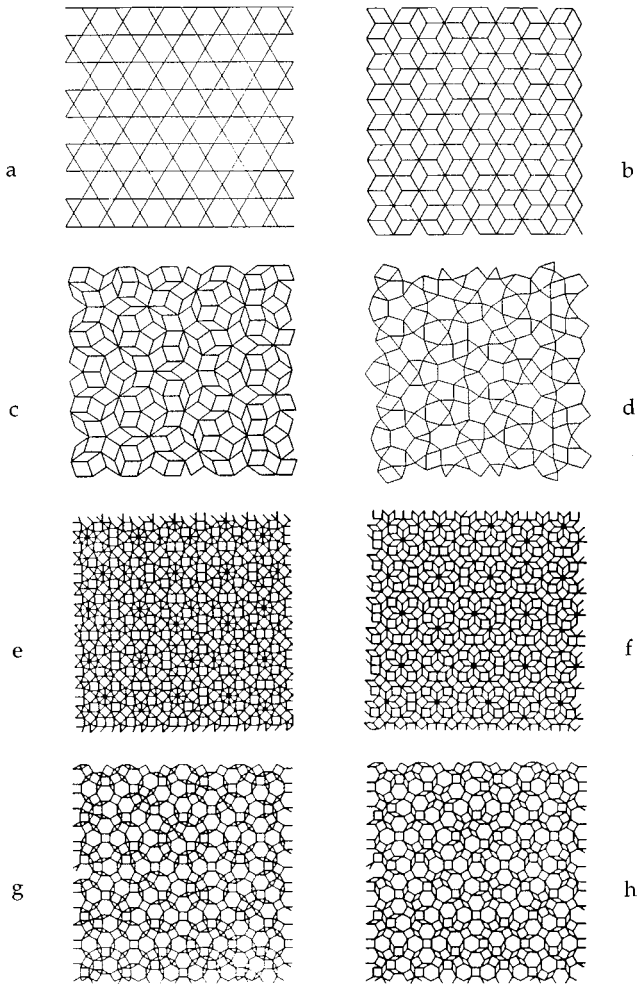

FIG. 1. Less-common lattices studied in this paper: Kagomé (a) and its dual, dice lattice (b); Penrose quasicrystalline lattice (c) and its dual (d); octagonal quasicrystalline lattice with ferromagnetic links (e) and chemical links (f); dodecagonal quasicrystalline lattice with ferromagnetic links (g) and chemical links (h).

cagonal tilings [7], which belong to the Penrose local isomorphism class.

In analogy to other lattices, one can require that lattice sites are connected only via the tile edges. The corresponding percolation problem is called chemical percolation. Adding the connection through the diagonals of tiles which are shorter than the tile edge leads to so-called ferromagnetic percolation [8]. Both these percolations will be considered here. These lattices are reproduced in Fig. 1.

Some lattices do not have a single-valued coordination number q. Lattices with mixed-valued coordination can be either periodic or nonperiodic. An example of a periodic lattice at $d=2$ is provided by the dice lattice, which mixes $q=3$ and 6. An example of a nonperiodic lattice is the Penrose tiling, which mixes $q=3$, 4, 5, 6, and 7. Note that the dual of the dice is the Kagomé lattice, and vice versa, while the dual of the Penrose tiling was called the Penrose dual lattice. Both the Kagomé and the Penrose dual are lattices with a single-valued coordination $q=4$. Octagonal and dodecagonal lattices have mixed-value coordinations. Numerical estimates of the percolation thresholds of dice can be found in Ref. [6].

III. EFFECTIVE NUMBER OF NEAREST NEIGHBORS

In the past, attempts have been made to generalize empirical relations such as the Scher and Zallen approximate [9], which depends on dimension. For instance at $d=2$, these are $qp_c(\text{bond})\simeq 2.0$ and $fp_c(\text{site})\simeq 0.45$, with f the lattice filling factor. Extension to quasilattices [6,7] consists of replacing q by the mean coordination number $\overline{z}$ in the invariant appropriate to bonds (the problem for sites is not solved, because there is no ambiguous definition of the filling factor in quasicrystals [7]).

In the same spirit, we propose to extend Eq. (1), replacing q by an effective value q_{eff}. The dependence of the percolation thresholds on site connectivity does not imply that the relevant variable should be the arithmetic average $\overline{z}$. Therefore, we regard q_{eff} as a parameter which has to be determined, rather than arbitrarily forced to be equal to $\overline{z}$.

The need to substitute q with q_{eff} in the equations is easily understood in both the case of quasilattices and the case of lattices which mix different values of q. It is also needed in anisotropic lattices. Let us again consider the hexagonal lattice with spacings a, b, and c in the three lattice directions. In the limit $c\rightarrow+\infty$, one is left with decoupled ab planes for physical systems having a finite range of interaction. Therefore, the percolation threshold of the hexagonal lattice must depend somehow on the ratio c/a. It is expected to range between that of an isotropic bcc lattice with $d=3$ and $q=8$, and that of the $d=2$ triangular lattice, associated with the limit $c/a\rightarrow+\infty$. Note that in this limit one recovers an isotropic lattice with $q=6$ instead of $q=8$, which suggests an effective coordinance $6\leqslant q_{\text{eff}}\leqslant 8$. In view of such considerations, we propose to extend Eq. (1) substituting q by some q_{eff} for any lattice.

Note that within the two classes defined by the set (a,p_0), q_{eff} is the unique unknown parameter. For each lattice, we find a value of this fitting parameter which, when inserted into Eq. (1), reproduces both the site and the bond percolation threshold within ∓ 0.01. Values of q_{eff} are reported for different lattices in Table I, together with site and bond percolation thresholds p_c^s, p_c^b obtained when q is replaced by q_{eff} in Eq. (1). The mean coordination $\overline{z}$ and p_c^e for site and bond percolation are also reported for comparison. Exact or numerical estimates p_c^e are obtained from Refs. [6,7,10].

IV. RESULTS

For lattices at $d=2$, q_{eff} differs from $\overline{z}$ by 1% in the case of the dual Penrose lattice, and is smaller than 0.5% for all the other lattices. These data corroborate that two-dimensional lattices are divided into the two distinct classes defined in Ref. [1]. This is illustrated in Figs. 2 and 3, where p_c^e's are reported in a log-log plot such that the experimental points for lattices in the same class align on a straight line according to Eq. (1).

The pertinent variable after Eq. (1) is $(d-1)(q_{\text{eff}}-1)$ for sites and $(d-1)(q_{\text{eff}}-1)/d$ for bonds. Those are the variables in abscissa in Fig. 3, which reports data for lattices in dimensions $d=2$ and 3 (data in higher dimensions have been already displayed in a similar plot in Ref. [1], with

TABLE I. Percolation thresholds from this work p_c compared to ''exact estimates'' p_c^e taken from Refs. [6,7,10]. $\Delta \equiv p_c - p_c^e$. $*$ refers to a multivalued coordination number (mean coordination $\overline{z}$). All the lattices are in dimension $d=2$, except for the last six ones in the second class which have $d=3$. We completed the table caption as follows: q_{eff} has been chosen as the arithmetic average of the parameters q which reproduces p_c^e for the site and bond, respectively, when inserted into Eq. (1).

			First class					
			Site			Bond		
Lattice	$\overline{z}$	q_{eff}	p_c^e	p_c	Δ	p_c^e	p_c	Δ
Square	4	4.02	0.5928	0.5970	+0.0042	0.5	0.4935	−0.0064
Honeycomb	3	2.99	0.6962	0.6938	−0.0024	0.6527	0.6581	+0.0054
Triangular	6	5.98	0.5	0.4986	−0.0014	0.34729	0.34955	+0.0023
Dice*	4	4.189	0.5851	0.5854	+0.0003	0.476	0.4754	−0.0006
Penrose*	4	4.194	0.5837	0.5851	+0.0014	0.477	0.4748	−0.0022
Octa. chem. links*	4	4.170	0.585	0.5867	+0.0017	0.48	0.4773	−0.0027
Octa. ferro. links*	5.17	5.013	0.543	0.5389	−0.0041	0.40	0.406	+0.0057
Dode. chem. links*	3.63	3.638	0.628	0.6269	−0.0011	0.54	0.5419	+0.0019
			Second class					
			Site			Bond		
Lattice	$\overline{z}$	q_{eff}	p_c^e	p_c	Δ	p_c^e	p_c	Δ
Kagomé	4	3.980	0.6527	0.6567	+0.0040	0.5244	0.5195	−0.0049
Dual Penrose	4	4.04	0.6381	0.6487	+0.0106	0.5233	0.5099	−0.01341
Dode. ferro. links*	4.27	4.218	0.617	0.6264	+0.0094	0.495	0.4835	−0.0115
Hex. compact	12	11.146	0.204	0.2015	−0.0025	0.124	0.1263	+0.0023
Stac. triangle	8	7.661	0.2623	0.2611	−0.0012	0.1859	0.1872	0.0013
Diamond	4	4.0087	0.43	0.4260	−0.0040	0.1859	0.3935	+0.0055
sc	6	5.9558	0.3116	0.3132	+0.0016	0.2488	0.2468	−0.0020
bcc	8	8.1355	0.246	0.2502	+0.0042	0.1803	0.1755	−0.0047
fcc	12	11.626	0.198	0.1958	−0.0022	0.119	0.1210	0.0020

$q_{\text{eff}}=q$). Since the first class concerns only lattices which are all at $d=2$, the above variables for sites and bonds, respectively, may reduce to one single common variable q_{eff}, as shown in Fig. 2. $|\Delta|$ reaches 0.01 only in the dodecagonal lattice with ferromagnetic links, and in the dual Penrose lattice. In all the other cases, the error in the percolation threshold estimates is only on the third decimal.

Note the larger error in the dodecagonal lattice. We attribute it to an actual bond percolation threshold $p_c^e(\text{bond})=0.495$ [6] larger than *a priori* expected. One would indeed have expected $p_c(\text{bond})=0.475$ from the

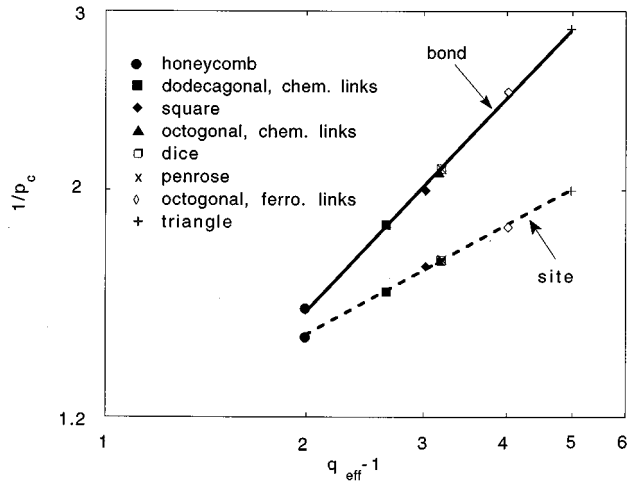

FIG. 2. Inverse of percolation thresholds as a function of the variables $(d-1)(q_{\text{eff}}-1)$ and $(d-1)(q_{\text{eff}}-1)/d$ which reduce here $(d=2)$ to the single variable q_{eff} in logarithmic scales for lattices belonging to the first class.

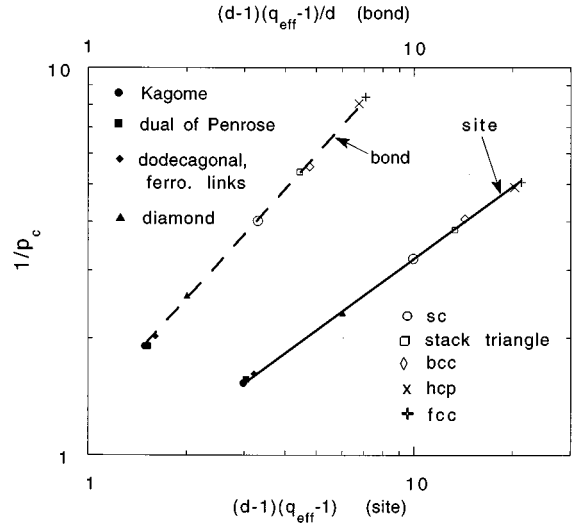

FIG. 3. Inverse of percolation thresholds as a function of the variables $(d-1)(q_{\text{eff}}-1)$ and $(d-1)(q_{\text{eff}}-1)/d$ appropriate to site and bonds, respectively, in logarthmic scales for lattices belonging to the second class.

straight line in Fig. 3, in which case a value $q_{\rm eff}=4.289$, close to $\overline{z}=4.27$, would have reproduced both site and bond percolation thresholds within $|\Delta|=0.001$. The problem with the estimate $p_c^e(\text{bond})=0.495$ is also evident from the Scher and Zallen invariant. It yields $\overline{z}\,p_c^e(\text{bond})=2.11$, the largest value of this parameter among all the lattices investigated [6]. Conversely $p_c(\text{bond})=0.475$ would yield $\overline{z}\,p_c(\text{bond})=2.028$, close to the invariant value 2.0 at $d=2$.

At $d=3$, percolation values are reproduced with a very good accuracy, since $|\Delta|\leqslant 0.004$ for all the lattices. The difference between $q_{\rm eff}$ and $\overline{z}$ is not negligible, as it reaches a few percent in some cases. This is easily understood in the case of the hexagonal (stack triangle) case, where we argued earlier that a value $q_{\rm eff}$ smaller than 8 is expected. Actually, we find $q_{\rm eff}=7.66$, as a consequence of the anisotropy. The hexagonal-close-packed (hcp) lattice has percolation thresholds which are different from those of the fcc lattice, as expected since the hcp lattice is not a Bravais lattice.

However, differences are small, which may be attributed to the fact that both lattices are indeed isotropic, each site being surrounded by 12 equivalent neighbors. In this context, the small value of $q_{\rm eff}$ close to 11 in the hcp lattice is not only due to the non-Bravais nature of the lattice. It is also related to the fact that in the fcc lattice, $q_{\rm eff}$ is only 11.6, significantly smaller than $q=12$, although the coordination number is single valued.

On the other hand, $q_{\rm eff}$ differs from q by only 1% in the other lattices (sc, diamond, bcc). Still one would expect $q_{\rm eff}=q$ in such isotropic lattices with a single-valued coordination number. The difference between $q_{\rm eff}$ and q in this case illustrates that our formula for the percolation thresholds is not exact, as we already stated in Ref. [1], and as was shown convicingly in Ref. [2]. Nevertheless, both site and bond percolation thresholds for all the lattices in any dimension are provided within 1% by our universal law involving only two parameters: the dimension d and a parameter $q_{\rm eff}$ which contains more information on the geometry than the mean coordination.

V. CONCLUSION

We have shown that the universal formula for percolation threholds we reported earlier [1] for periodic Bravais lattices with equivalent nearest neighbors does extend to any kind of lattice, provided the coordination number is replaced by an effective value $q_{\rm eff}$. We then conclude that a good estimate of both site and bond percolation thresholds can be obtained from the formula in Eq. (1) involving only the dimension d of the lattice, and one parameter $q_{\rm eff}$ which contains geometric information about the lattice. This parameter however, does not reduce to the mean coordination number $\overline{z}$, although $\overline{z}$ and $q_{\rm eff}$ differ by a few percent only. Indeed, we find that the universality does include different numerical values for $q_{\rm eff}$, and thus different percolation thresholds for lattices which have the same set $(d,\overline{z})$. This is evident from Table I, which reports results for as many as six lattices with $(d=2,\overline{z}=4)$, two lattices with $(d=3,\ \overline{z}=8)$, and two other ones with $(d=3,\overline{z}=12)$.

In our previous work, we had only three lattices belonging to the first class. The present work extends this class from three to eight lattices. We might have invoked chance for three points aligned on a same line, but not for eight points as in Fig. 1. Therefore, we confirm the existence of two different classes: one for some of the two-dimensional lattices, the second for all the other two-dimensional lattices and all the lattices up to $d=7$.

We do not have a scheme to derive the relevant variable $q_{\rm eff}$ from the geometry of the lattice. However, an important result of this work is that this variable does exist. It means that there exists a single value for $q_{\rm eff}$ which accounts for both the site and bond percolation thresholds for any given lattice within ∓ 0.01. This result is sufficient to give our formula a predicting ability for percolation thresholds of other lattices which have not yet been computed. For example, the knowledge of one site (bond) percolation threshold for a given lattice is sufficient to determine a point on the relevant straight line in Figs. 2 or 3. Then $q_{\rm eff}$ can be found from the abscissa of this point, which in turn allows for a determination of the bond (site) percolation threshold from our universal formula, within ∓ 0.01. Depending on whether p_c^s or p_c^b is known, the value of $q_{\rm eff}$ deduced from Figs. 2 or 3 will be different. However, this difference corresponds only to the deviation of the p_c^e's with respect to the universal law, i.e., to less than 1% with the exception of only a few outlying values.

The robustness of our formula suggests an extension to more complex problems such as directed percolation. Also, anisotropic percolations with different bond probabilities in different directions may be addressed in the near future.

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