Reply to ''Comment on 'Universal formulas for percolation thresholds' ''

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In a recent paper, we reported a universal power law for both site and bond percolation thresholds for any lattice of cubic symmetry. Extension to anisotropic lattices is discussed. [S1063-651X(97)06101-1]

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In Ref. [1], we have found a power law for both site and bond percolation thresholds, which writes

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

with d the space dimension and q the coordination number. For site dilution $b=0$ while $b=a$ for bond dilution. Then a class of lattices is defined by the set of parameters $\{p_0;a\}$. One class includes two-dimensional triangle, square, and honeycomb lattices, 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 symetry (for $d\geqslant 3$) constitute the second class, characterized by $\{p_0=1.2868;\ a=0.6160\}$ and $\{p_0=0.7541;\ a=0.9346\}$ for sites and bonds, respectively. At high dimensions a third class for hypercubes (sc and fcc) is found, which recovers the infinite Cayley tree limit.

In the above Comment van der Marck reports the interesting observation that the stacked triangular lattice (also called hexagonal lattice) with the lattice parameters $a=b=c$ ($d=3$, $q=8$) does not fit into the second class. In particular, the percolation thresholds reported are different from those associated to the $d=3$, $q=8$ bcc lattice.

This is indeed an interesting observation which, however, does not contradict our previous work for the following reason. Within a given class, the percolation threshold according to Eq. (1) depends only on d and q, which implicitly requires that the q nearest neighbors of any site are equivalent. This is indeed the case in all lattices we have mentioned in the definition of the classes, but that is not the case of the stacked triangular lattice, which is anisotropic. There, a lattice site has six equivalent nearest neighbors in the a,b plane (bonding angle is 60°) and two nonequivalent sites along the c axis (bonding angle is 90°).

Actually, the percolation threshold of an anisotropic lattice must depend on the degree of anisotropy. This can be viewed on the stacked triangular lattice, if we note that this lattice is defined by lattice parameters $a=b\neq c$ (the case $a=c$ considered in the Comment is only a very particular case). Then in the limit where the c parameter goes to infinity, one is left with ab planes which will become decoupled for physical systems with finite ranges of interaction. Therefore, the percolation threshold of the stacked triangular lattice must depend on the ratio c/a and the percolation threshold will shift continuously from the numerical values given by van der Mark in the particular case ($c/a=1$, $q=8$), to those of the triangular lattice in $d=2$, in the limit $c/a\rightarrow\infty$. Note in this limit one recovers an isotropic lattice with $q=6$ instead of $q=8$.

However, it should be stressed that the above interpolation should not be taken literally. Percolation thresholds do depend on site connectivity and not on length between them. Then, if one wishes to generalize the Galam-Mauger formula, anisotropy should be taken into account by replacing the q parameter by some effective value between $q=8$ and $q=6$. Indeed, we found that a unique value of $q=6.65$ reproduces within the second universality class at $d=3$ both percolation thresholds 0.2614 (site) and 0.1875 (bond) in agreement with the result of Van der Marck for the stacked triangular lattice with $c=a$, which are 0.2623 and 0.1859, respectively.

According to these consideration, we can now discuss the limits of validity for the Galam-Mauger formula, which was lacking in Ref. [1]. Along the stacked triangular lattice case, one may also construct anisotropic percolation problems by having, for instance, two different bond probabilities in the two different lattice directions of the square lattice. Directed percolation would be another example. All these problems are more complicated that the isotropic percolation problem considered in Ref. [1], and were not considered in this prior work.

Extension of the formula, in view of above discussion, seems, however, possible, if one replaces q by an effective value. However, this value has to be determined for each case, depending on the nature and strength of the anisotropy. Nevertheless, the Galam-Mauger formula preserves a capacity of prediction. Knowledge of one (either site or bond) percolation threshold allows the determination of the effective value of q for each anisotropic percolation problem investigated. Then this value can be used to estimate the other percolation threshold. Otherwise the direct estimate of the effective q is required to yield both percolation thresholds.

Note that the Galam-Mauger formula actually applies not only to lattices with cubic symetry investigated in Ref. [1], but also to all isotropic lattices in general. This can be illustrated with the hexagonal compact (hcp) lattice. This is actually not a Bravais lattice, because, on a topologic viewpoint, it is a simple hexagonal lattice with two atoms per unit cell. However, each atom in this structure has $q=12$ nearest neighbors with the same bonding angle for each of them. We are then in the isotropic case with $d=3$, $q=12$ so that we predict the same percolation thresholds as in the case of the fcc lattice at $d=3$, namely, 0.192 and 0.117 for site and bond percolation thresholds, respectively according to the Galam-Mauger formula.

Percolation thresholds for the hcp were given by Shante and Kirpatrick [2] two decades ago, giving 0.204 (site) and 0.124 (bond). These authors report for the fcc site and bond percolation thresholds 0.199 and 0.125, respectively. Comparison with modern values available for the fcc shows that their last digit is not accurate. We can then conclude that the agreement between fcc and hcp percolation thresholds is good and actually much better than hexagonal and bcc ones, as expected.

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[1] S. Galam and A. Mauger, Phys. Rev. E **53**, 2177 (1996).

[2] V. K. S. Shante and S. Kirpatrick, Adv. Phys. **20**, 326 (1971).