Square-lattice site percolation at increasing ranges of neighbor bonds

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We report site percolation thresholds for square lattice with neighbor bonds at various increasing ranges. Using Monte Carlo techniques we found that nearest neighbors (NN), next-nearest neighbors (NNN), next-next-nearest neighbors (4N), and fifth-nearest neighbors (6N) yield the same $p_c=0.592\ldots$. The fourth-nearest neighbors (5N) give $p_c=0.298\ldots$. This equality is proved to be mathematically exact using symmetry argument. We then consider combinations of various kinds of neighborhoods with (NN+NNN), (NN+4N), (NN+NNN+4N), and (NN+5N). The calculated associated thresholds are respectively $p_c=0.407\ldots$, $0.337\ldots$, $0.288\ldots$, and $0.234\ldots$. The existing Galam-Mauger universal formula for percolation thresholds does not reproduce the data showing dimension and coordination number are not sufficient to build a universal law which extends to complex lattices.

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I. INTRODUCTION

Calculating percolation thresholds has been an ongoing challenge for decades [1–6]. While very few lattices allow an exact analytical calculation, large scale simulations have been very valuable to determine a large spectrum of them for both Bravais' [4,7,8] and disordered [9] lattices. The drastic increase in computer capacities has recently permitted the calculation of thresholds at rather high dimensions up to $d=13$ for the hypercube [4,10]. In parallel, not much work has been devoted to regular lattices with neighbor links which are not nearest neighbors (NN, von Neumann's neighborhood). Some scarce results are available for simultaneous nearest and next-nearest neighbors (NN+NNN, Moore's neighborhood) [4,11].

In this paper we report a systematic calculation of site percolation thresholds for the square lattice with neighbor bonds at successive increasing range. We consider the series of nearest neighbors (NN), next-nearest neighbors (NNN), next-next-nearest neighbors (4N), fourth-nearest neighbors (5N), and fifth-nearest neighbors (6N). It should be stressed that for each one of the considered distance of bonds, all others are not active. For instance, in the case of next-nearest neighbors (NNN), the nearest-neighbors (NN) sites are not connected, only the NNN are. This principle applies to all our calculations. We found that the threshold is the same for all of them with $p_c=p_c(\mathrm{NN})$ except at 5N. An explanation in terms of symmetry is provided.

We then consider combinations of various ranges of neighborhoods with (NN+NNN), (NN+4N), (NN+5N), and (NN+NNN+4N). In these cases we have simultaneous range of bonds but they are necessarily compact. For instance, for (NN+4N) all nearest-neighbors sites are connected as well as all next-next-nearest-neighbor ones but next-nearest neighbors are not active.

Comparing our numerical estimates with the predictions from the Galam-Mauger (GM) universal formula for percolation thresholds [12], we found significant discrepancies. It strengthens the earlier claim that only dimension and coordination number could not be sufficient to build a universal law which extends to complex lattices [7,13].

II. CALCULATIONS

There exist several computational techniques which allow us to perform calculations of percolation thresholds [14–17]. Here we are using the Hoshen-Kopelman algorithm (HKA) [17]. Once the lattice is given with the occupied sites, it allows us to recognize which sites belong to which clusters. With HKA one can assign to each occupied site a label and sites in the same cluster have the same labels. Different labels are assigned to different clusters. The HKA is particularly efficient when we check if the site at distance ℓ from the first line—often fully occupied—is still connected to that line through the sites at the distances smaller than ℓ. The algorithm requires storing only a single line of sites and goes through the lattice only once. In such a case HKA becomes extremely efficient as it saves memory and time [4]. However, when links between sites at distances larger than ℓ from a top border are desired, the whole lattice must be stored [4,18–20]. With the HKA on a square lattice when we assign the labels for the investigated site (black sites in Fig. 1), we need to check already labeled and occupied sites in its neighborhood (slashed sites in Fig. 1). The possible links to remaining sites in the neighborhood (backslashed sites in Fig. 1) may be checked later, basing on the neighborhood's point symmetry.

The percolation threshold values p_c are evaluated from the crossing point of three curves showing dependences of the percolation probability P on the site occupation probabil-

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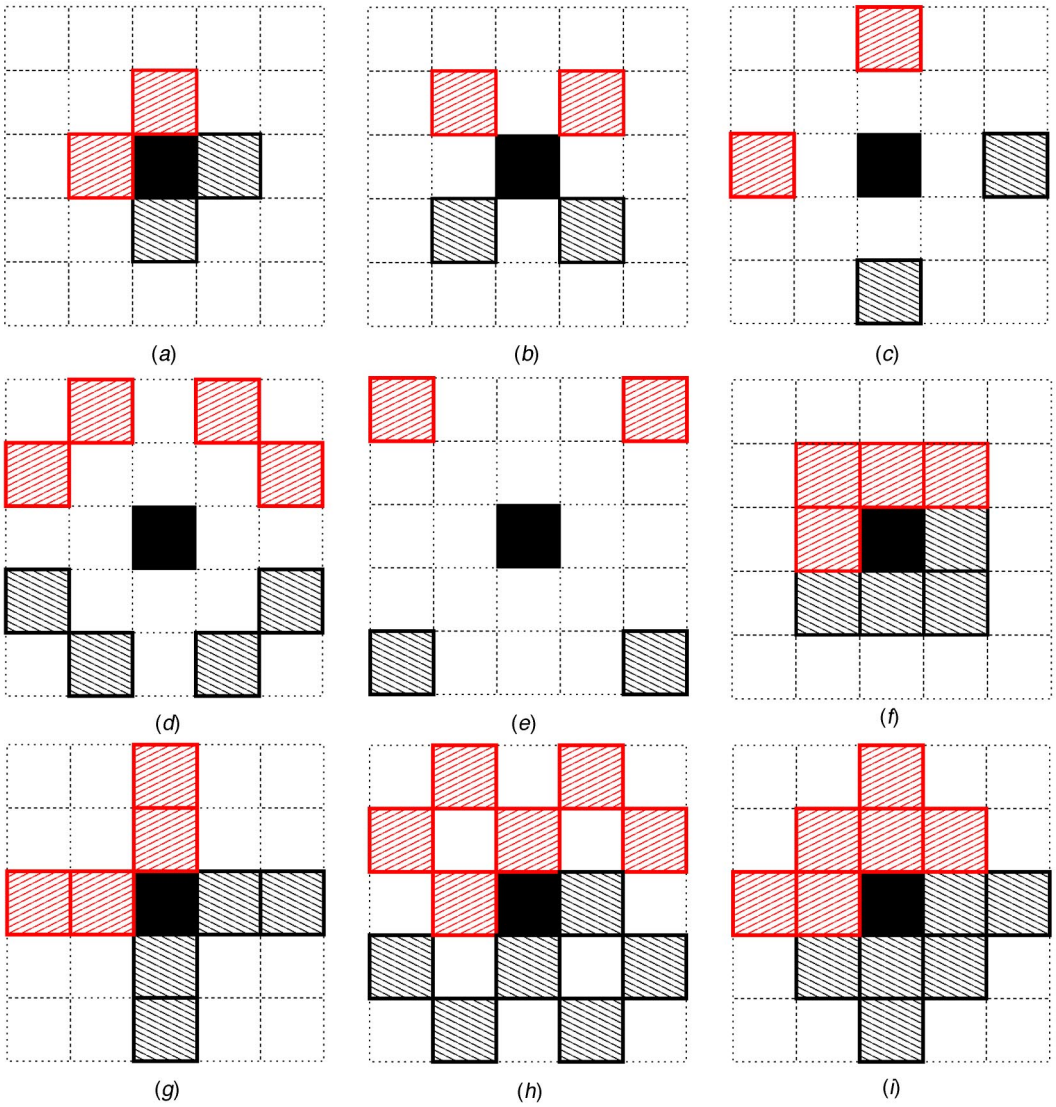

FIG. 1. Various site neighborhoods on the square lattice: (a) NN—von Neumann's neighborhood, (b) NNN, (c) 4N, (d) 5N, (e) 6N; and the examples of their combinations: (f) NN+NNN—Moore's neighborhood; (g) NN+4N, (h) NN+5N, and (i) NN+NNN+4N.

ity p for lattices of linear sizes $L=100$, 500, and 1000. The results are averaged over $N_{\mathrm{run}}=10^3$ and 10^4 for $L=1000$ and 100, respectively. With enlarging the lattice size L the curve $P(p)$ becomes steeper and steeper and tends to Heaviside's function $\Theta(-p_c)$ when $L\to\infty$, as expected.

III. RESULTS

We present our results in Table I. The percolation thresholds p_c for the square lattice are computed with HKA for a series of neighborhoods. First only one type of neighbor is considered at a time, increasing repeatedly the range with NN, NNN, 4N, 5N, and 6N. It turns out that the threshold $p_c=0.592\ldots$ is the same for all of them except at 5N where $p_c=0.298\ldots$.

We now demonstrate mathematically that the above equality of the percolation thresholds for NN, NNN, 4N, and 6N neighborhoods is indeed exact. Using symmetry argu-

TABLE I. The percolation threshold p_c for various neighborhoods on square lattice and sites coordination number z and the theoretical values p_c^{GM}.

Neighborhood	z	p_c	p_c^{GM}
NN	4	0.592…	0.5984…
NNN	4	0.592…	0.5984…
4N	4	0.592…	0.5984…
5N	8	0.298…	0.4411…
6N	4	0.592…	0.5984…
NN+NNN	8	0.407…	0.4411…
NN+4N	8	0.337…	0.4411…
NN+5N	12	0.234…	0.3748…
NN+NNN+4N	12	0.288…	0.3748…

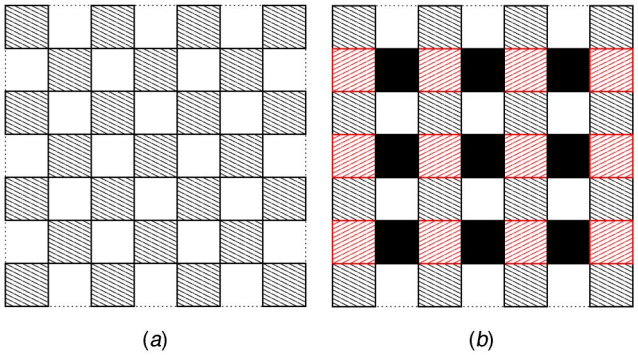

FIG. 2. The lattices with (a) NNN and (b) 4N neighborhoods may be mapped to (a) two or (b) four parallel NN situations but with (a) $\sqrt{2}$ and (b) two times larger lattice constants.

ments all lattices with neighborhoods shown in Figs. 1(b), 1(c), and 1(e), can be mapped into a NN situation as in Fig. 1(a). The only difference is a larger and larger lattice constant. To implement the mapping, we take a square lattice and build on it the lattice from only NNN bonds. Two independent interpenetrated squares sublattices appear. Therefore the percolation of NNN is split onto two parallel NN problems on each one of these two square sublattices. Accordingly the p_c on each one is the p_c of NN. Moreover, as the site must be distributed homogeneously on the initial lattice, we will have the same density of occupied sites on each one of the sublattices making both percolations occur simultaneously at the same p_c [see Fig. 2(a)]. Such a scheme can be repeated with 4N [Fig. 2(b)] and 6N but not with 5N. As shown in Fig. 1(d) the 5N lattice has eight neighbors while NN, NNN, 4N, and 6N have four. It is worth stressing that our demonstration applies to the exact equality of the percolation thresholds but does not hint to an exact calculation to the common percolation value since it uses only symmetry arguments. However, these symmetry properties may become instrumental in underlining interesting physical properties associated to some exotic materials. In particular, if one is able to discriminate between the two interpenetrated lattices, it may open a way to reach percolation at a much lower critical density, down to half the value of p_c. But such a search is outside the scope of the present work.

We also consider several combinations of various ranges of neighborhoods. First, an increasing compact neighborhood with (NN+NNN) and (NN+NNN+4N). The calculated threshold numerical estimates are respectively $p_c=0.407\ldots$ and $0.288\ldots$ (Table I). Then more complex ones with (NN+4N) and (NN+5N) for which we obtained $p_c=0.337\ldots$ and $0.234\ldots$ (Table I). The fact that p_c of (NN+5N) is smaller than p_c of (NN+NNN+4N) is consistent with 5N $z=8$ instead of $z=4$ for all the others.

The obtained percolation threshold values $p_c(\mathrm{NN})=0.592\ldots$ and $p_c(\mathrm{NN+NNN})=1-p_c(\mathrm{NN})=0.407\ldots$ are consistent with the values reported in Refs. [4,11,21] We have also revised the value of p_c(NN+NNN+4N) which has been studied in an earlier paper [22] and it was set at 0.292 to compare to our value of 0.288….

IV. DISCUSSION

At this stage it is interesting to check the validity of the GM universal formula for percolation thresholds [12,23] in the case of these complex neighborhoods. Comparing our numerical estimates with its predictions as shown in Table I we found a good agreement for NN, NNN, 4N, and 6N ($\Delta=0.006$) but not for 5N ($\Delta=0.123$). It is also fair for (NN+NNN) with $\Delta=0.034$ but not for all other combinations. The significant discrepancies occur for complex and noncompact neighborhoods. It strengthens the earlier claim that only dimension and coordination number could not be sufficient to build a universal law which extends to complex lattices [13].

Indeed above failures could be anticipated due to the fact that several lattices have both identical z and d though they exhibit different thresholds as seen from Table I. In particular 5N, (NN+NNN), (NN+4N) have $z=8$ and $d=2$ while all p_c are different. The same occurs for (NN+5N) and (NN+NNN+4N) with $z=12$ and $d=2$.

A similar situation occurs for T_C in the Ising model where even with the same number of interacting spins in the neighborhood and the same dimensionality we have different T_C [24]. On the other hand, the Bragg-Williams approximation [25] predicts T_C to be a unique function of coordination number z, i.e., $k_BT_C=zJ$ [26]. The GM universal formula which also extends to T_C includes a dependence on both d and z [27].

To conclude, we have reported numerical estimates for site percolation thresholds for the square lattice with NNN, 4N, 5N, 6N, (NN+4N), (NN+5N), and (NN+NNN+4N) neighborhoods. Our estimates may prove useful in the search for a robust universal formula for percolation thresholds which would apply to complex lattices. In particular on how to extend the GM law by including some additional topological ingredient besides coordination z and dimension d.

These results may prove useful to some of the large spectrum of physical and interdisciplinary topics where the percolation theory may be applied such as forest fires spreading [20,28], immunology [29], liquid migration in porous media [30], econophysics [31], and sociophysics [32].

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