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LETTER TO THE EDITOR

Crossing probabilities in one, two or three directions for percolation on a cubic lattice

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Abstract. The probabilities of crossing in exactly one, two or three directions have been investigated using Monte Carlo simulations of percolation on cubic lattices with free boundary conditions. The crossing probability in exactly one given direction shows the least influence of finite-size effects and is best suited to obtain the percolation threshold (p_c). Finite-size effects are most important for simultaneous crossing in three directions. Crossing probabilities at p_c for large lattices are the same for site and bond percolation. The crossing probability in a given direction regardless of crossing in other directions, R_1, is 0.28. Exact results for small lattices agree with simulation results.

In Monte Carlo simulations of the percolation process a site or a bond of a lattice with size L is randomly occupied with probability p. Above a critical value (p_c) the bonds or sites percolate the lattice. The probability of percolation goes from zero for $p < p_c$ to one for $p > p_c$ with a transition that sharpens with increasing lattice size. Recently, Monte Carlo simulations have been done to obtain the probability of percolation at $p = p_c$ for $L \to \infty$. Before one can obtain the probability of percolation it is necessary to define precisely what counts as percolation of the lattice. The definition adopted in the past was introduced by Reynolds *et al* [1] and is the probability (R_1) that a cluster crosses the lattice in one fixed direction regardless of crossing in other directions.

Following this definition, Lin *et al* [2] calculated the so-called crossing probability for percolation in three dimensions at the percolation threshold. They considered both site and bond percolation on body-centred and simple cubic lattices using free boundary conditions. They found the same value $R_1 = 0.265$ for bond and site percolation and both types of lattices even though the value of p_c is different.

Acharyya and Stauffer [3] studied the effect of boundary conditions. They found different crossing probabilities if helical boundary conditions were applied in the directions not tested for crossing although the value of p_c is the same. In three dimensions they found $R_1 = 0.28, 0.41$ and 0.513 if helical boundary conditions were applied to zero, one and two other directions, respectively.

Lorenz and Ziff [4] studied the crossing probability on lattices which varied in size L' in the direction tested for crossing while keeping the length of the other two directions fixed at L. Using periodic boundary conditions in the directions not tested for crossing they found that R_1 decreased exponentially with the ratio L'/L. For $L = L'$, they found $R_1 = 0.573$ for $L \to \infty$.

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Table 1. Comparison between Monte Carlo and exact calculation of P_k at p_c for two small cubic lattices.

	$L = 3$, 27 sites, $p_c = 0.3116$ [4]		$L = 2$,12 bonds, $p_c = 0.2488$ [4]	
	Monte Carlo, 10^6 tests	Exact	Monte Carlo, 5×10^5 tests	Exact
P_1	$9.36 \times 10^{-2} \pm 0.06 \times 10^{-2}$	9.35×10^{-2}	$7.0 \times 10^{-2} \pm 0.5 \times 10^{-2}$	6.9×10^{-2}
P_2	$6.42 \times 10^{-2} \pm 0.05 \times 10^{-2}$	6.40×10^{-2}	$1.45 \times 10^{-1} \pm 0.07 \times 10^{-1}$	1.48×10^{-1}
P_3	$1.126 \times 10^{-1} \pm 0.006 \times 10^{-1}$	1.125×10^{-1}	$3.21 \times 10^{-1} \pm 0.09 \times 10^{-1}$	3.17×10^{-1}

The justification for using helical or periodic boundary conditions is that convergence to $L \to \infty$ is supposed to be faster. However, the limiting values of R_1 were all obtained for large values of L where the influence of finite-size effects is small for all boundary conditions. Thus, even for $L \to \infty$, the crossing probability in one direction is increased if periodic or helical boundary conditions are used in the other directions. This questions the validity of the use of periodic or helical boundary conditions to find the crossing probability. The dependence of R_1 on the boundary conditions was not anticipated and is probably the reason why Stauffer *et al* did not mention in [5] that they had used helical boundary conditions in one of the other directions. Lorenz and Ziff [4] mention that they believe that the helical and periodic boundary conditions should give the same result for R_1 if $L \to \infty$, but it is clear that boundary conditions influence the value of R_1 even for $L \to \infty$.

In the work mentioned above [1–5], other definitions of percolation were not considered. For percolation in three dimensions we can consider crossing probabilities in just one fixed direction (P_1), in just two fixed directions (P_2) or in all three directions (P_3). The probability of other crossing events follows from combinations of these elementary probabilities. For example, $R_1 = P_1 + 2P_2 + P_3$ and the probability of crossing in any direction is $R_0 = 3P_1 + 3P_2 + P_3 = 1 - P_0$, with P_0 the probability of no crossing. We note that simultaneous crossing in two or three directions does not necessarily mean that one cluster spans the cubic lattice in two or three directions. It is possible that two or three clusters span in only one direction. We restrict ourselves to the case of free boundary conditions in all directions as we do not know how to unambiguously define crossing in the case of periodic or helical boundary conditions.

For a given lattice with N sites or bonds the total number of configurations is 2^N and the elementary probabilities are given by: $P_k = \sum_{i=0}^{N} A_{k,i} \cdot p^i \cdot (1-p)^{N-i}$. $A_{k,i}$ is the number of configurations corresponding to the events indexed by k using i bonds or sites. $A_{k,i}$ can, in principle, be calculated exactly, but for the current generation of PCs it is impossible to enumerate in a reasonable time all the configurations for $L > 3$ for site percolation and $L > 2$ for bond percolation. For $L = 4$ there are $2^{64} \approx 1.8 \times 10^{19}$ configurations of sites and for $L = 3$ there are $2^{54} \approx 1.8 \times 10^{16}$ configurations for bonds. For larger lattice size Monte Carlo simulations are unavoidable. Nevertheless, the exact calculation on small lattices is useful as a check of the Monte Carlo simulation. Values of P_k at p_c obtained from Monte Carlo simulations are equal to the exact values within the experimental error, see table 1.

We conducted Monte Carlo simulations of both bond and site percolation on simple cubic lattices using free boundary conditions and the Hoshen and Kopelman labelling technique [6]. For L up to 342 we used a PC with 512 Mb of memory. For the calculation of R_0 for $L = 511$ and $L = 1023$, we used the T3E from IDRIS (Orsay, France). The number of trials depends on L and varies between 10^4 and 10^6.

Figure 1 shows the dependence of P_1, P_2 and P_3 on p for site percolation on cubic lattices with L between 10 and 80. P_1 and P_2 go through a maximum at $p_{\max}$ while P_3 increases to

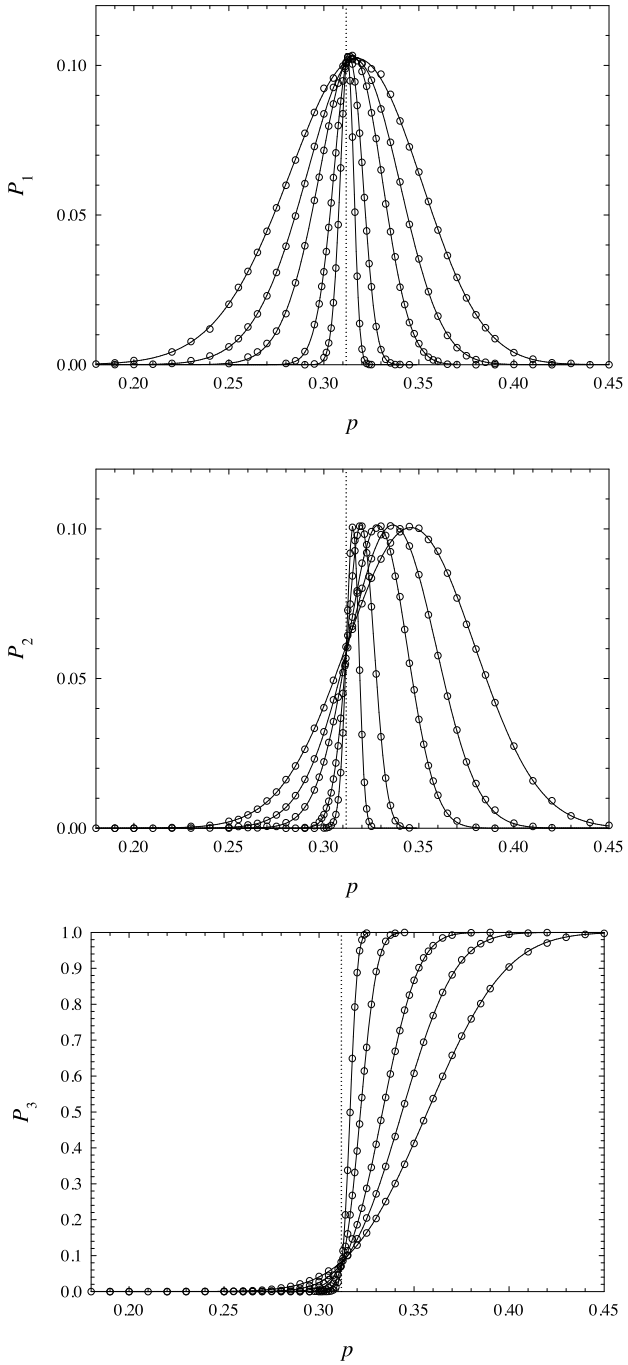

Figure 1. Crossing probabilities for site percolation for $L = 10$, 14, 20, 40 and 80 in exactly one (P_1), two (P_2) or three (P_3) directions. The dotted line indicates the position of p_c. The solid curves are fits to a GMG (P_1 and P_2) or a cumulative Gaussian (P_3).

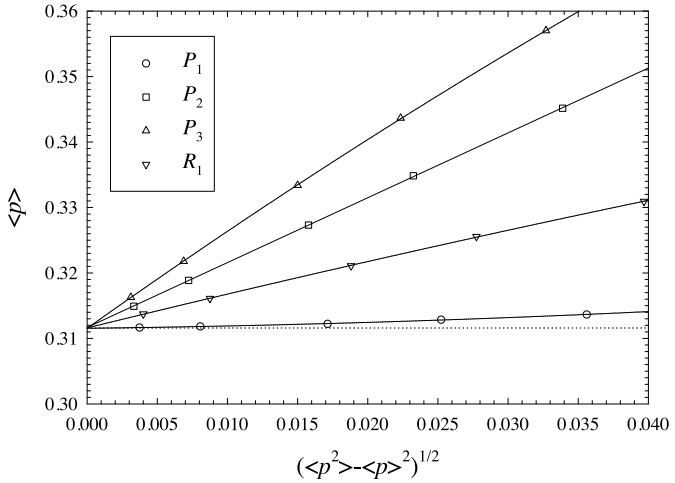

Figure 2. Comparison of $\langle p \rangle$ as a function of the standard deviation for different crossing probabilities as indicated in the figure. The dotted line indicates the position of p_c, while the solid curves are fits to a second-degree polynomial.

unity. We have used half-Gaussian modified Gaussian (GMG) functions to describe P_1 and P_2 and a cumulative Gaussian function to describe P_3, see the solid curves in figure 1. GMG is the convolution of a Gaussian with a half-Gaussian response function. Values of the average probability ($\langle p \rangle$) and the standard deviation ($\Delta = (\langle p^2 \rangle - \langle p \rangle^2)^{1/2}$) can be calculated either by directly integrating over P_1 and P_2: $\langle p^n \rangle = \int_0^1 p^n P_k(p)\,\mathrm{d}p (\int_0^1 P_k(p)\,\mathrm{d}p)^{-1}$ with $k = 1, 2$ or by integrating over the derivative of P_3: $\langle p^n \rangle = \int_0^1 p^n \frac{\mathrm{d}}{\mathrm{d}p} P_3(p)\,\mathrm{d}p$. In figure 2 we show $\langle p \rangle$ as a function of Δ. In the past, only R_1 has been used as a criterion for percolation. For comparison we have included in figure 2 values based on integration over the derivative of R_1. Figure 2 shows that finite-size effects are not the same for the different definitions of the percolation event. Clearly, the most accurate value of p_c is obtained using P_1 and not R_1. In addition, using P_1 there is no need to take the derivative which increases the noise. Of course, extrapolation to $\Delta \to 0$ and thus $L \to \infty$ gives p_c whatever the definition. We find $p_c = 0.3116 \pm 0.000\,05$ in agreement with literature results [4], using lattice sizes up to only $L = 80$. In figure 3 P_k, R_0 and R_1 at p_c are plotted as a function of L for site percolation. The values become independent of the lattice size for $L > 100$ within the statistical error. We note that the most important finite-size effects occur for P_3, i.e. the probability of simultaneous crossing in three directions. Mean values of P_k, R_0 and R_1 for both site and bond percolation at large L are summarized in table 2. We confirm earlier observations that the limiting values are the same for site and bond percolation. A comparison of P_k at large L shows that while the crossing in just one fixed direction is always more likely, simultaneous crossing in just two fixed directions is less likely than simultaneous crossing in all three directions.

The value of R_1 is in agreement with that reported by Acharyya and Stauffer [3] and slightly larger than the results reported by Lin *et al* [2]. We checked that the difference is not due to the use of the so-called histogram method used by Lin *et al* .

It is interesting to note that the maximum values of P_1 and P_2 at $p = p_{\max}$ are the same and almost independent of L for $L > 10$. However, even if in both cases $p_{\max} \to p_c$ for $L \to \infty$, the values at $p_{\max}$ are not the same as the values at p_c even for $L \to \infty$. This is obvious for P_2 (see figure 1) but it is also true for P_1.

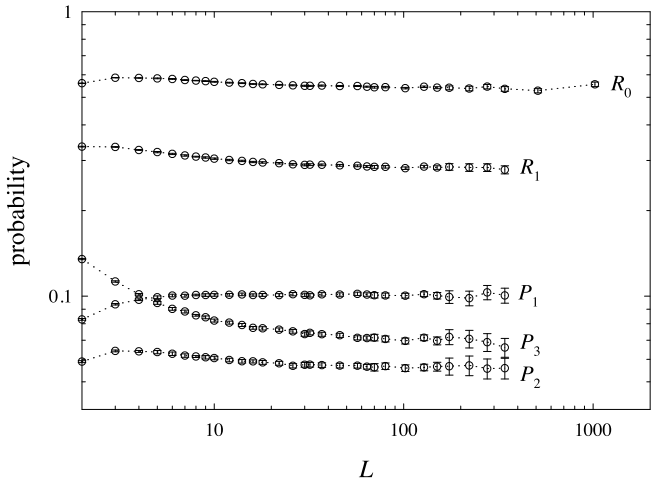

Figure 3. Lattice-size dependence of different crossing probabilities as indicated in the figure for cubic site percolation at the percolation threshold $p_c = 0.3116$.

Table 2. Comparison of the different probabilities at large L for site and bond percolation on a cubic lattice.

	Site, $p_c = 0.3116$	Bond, $p_c = 0.2488$
P_1	$0.101 \pm 1 \times 10^{-3}$	$0.102 \pm 2 \times 10^{-3}$
P_2	$0.057 \pm 1 \times 10^{-3}$	$0.056 \pm 1 \times 10^{-3}$
P_3	$0.070 \pm 2 \times 10^{-3}$	$0.071 \pm 2 \times 10^{-3}$
R_1	$0.283 \pm 2 \times 10^{-3}$	$0.285 \pm 4 \times 10^{-3}$
R_0	$0.541 \pm 6 \times 10^{-3}$	$0.543 \pm 8 \times 10^{-3}$

In summary, we have confirmed that the crossing probabilities at the percolation threshold are the same for bond and site percolation. The crossing probabilities obtained from our Monte Carlo simulations on small lattices are the same as the exact values within the experimental error. Finite-size effects depend on the definition of the percolation event. Smallest finite-size effects are found for crossing in exactly one given direction.

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