Percolation - A Numerical Approach

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ABSTRACT

Percolation theory is an important method in many different areas of science. In this paper I have simulated clusters by connecting lattice sites through bonds for studying bond percolation. I found that the number of nearest neighbors in a lattice affects the critical probabilities, although the critical behavior itself is similar for two-dimensional lattices. The results indicates also that the triangular lattice is the dual lattice of the honeycomb lattice.

Keywords: Percolation, FSS, Critical exponents.

I. INTRODUCTION

A. Percolation theory

Percolation theory describes the formation and behavior of clusters. Its range of application is wide, as it is being used in conductor-physics[3], growth modeling[6] and epidemiology[1]. Percolation is a random process, tightly connected to critical phenomena and renormalization theory[5]. This paper treats bond percolation, meaning that bonds can be opened or closed and that a cluster is defined as a group of sites connected by open bonds[7]. The goal of this paper is to calculate the critical behavior for two dimensional square, triangular and honeycomb lattices. What differs between the structure of these lattices is number of bonds per site, which are correspondingly two, three and three halves. Each type of lattice had the same number of sites, namely L^2 for $L = 100, 200, 300, ..., 1000$.

B. Finite-Size Scaling

The critical behavior investigated is described through the physics of finite-size scaling. The quantities taken into account were the giant component, P_∞, describing the size of the largest cluster, the average cluster size $\langle s \rangle$, and the correlation length, ξ. The percolation transition takes place when the system goes from a state of small clusters to a state where a cluster connects the boundaries. P_∞, $\langle s \rangle$, and ξ can be describes by the power laws defined in Equation 1 near the critical probability p_c:

$$P_\infty \propto (q - p_c)^\beta, \tag{1a}$$

$$\langle s \rangle \propto |q - p_c|^{-\gamma}, \tag{1b}$$

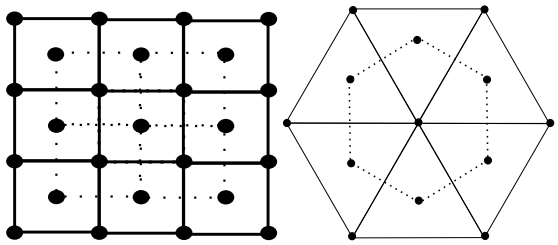
$$\xi \propto |q - p_c|^{-\nu}, \tag{1c}$$

where q is the probability to activate bond and β, γ and ν are the critical exponents[7]. There are more quantities which can be described by similar power-laws, such as the total number of clusters, with critical exponent $2 - \alpha$, characteristic cluster size, described by the exponent $-\frac{1}{\sigma}$[4]. The reason for not calculating these other quantities is that the critical exponents are coupled through relations such as the hyperscaling relation $2\beta + \gamma = d\nu = 2 - \alpha$, where d is the number of dimensions[4]. Therefore knowing the three exponents calculated in this paper, one can calculate the critical behavior of other cluster quantities.

1. *Dual lattices*

Lattices can be dual, meaning that two different lattices are coupled in a way such that one can know the critical behavior of one by knowing the behavior of the other. In Figure 1a and Figure 1b a lattice and its dual lattice are drawn. The dual lattice of a square lattice is also a square, meaning it is self-dual, while the triangular lattice and the honeycomb lattice are dual lattices. Two active bonds cannot cross, so if the bond of the original lattice is active, then the perpendicular bond, belonging to the dual lattice must be non-active. Since activating bonds are done randomly, the probability of activating a bond in the dual lattice must be:

$$p_c^{dual} = 1 - p_c^{original}. \tag{2}$$



(a) (b)

FIG. 1: Dual lattices. The dotted lines are drawn between the midpoints between lattice sites. These dotted shapes are the dual lattice of the the solid shapes. In figure a) the square and its dual lattice is drawn, while in b) a triangular lattice is shown with its dual lattice.

II. MODEL AND METHODS

A. Activating bonds

To generate a list of bonds between lattice sites without over-counting, only a portion of the neighboring sites were added through bonds. For the square lattice, only the sites to the right and below were added as bonds, while for the triangular one the right, the down left and the down right sites were added as bonds. Lastly, for the hexagonal lattice, the bonds

added alternated between solely the right one and the upright-down-right ones, depending on if the coordinates were odd or even. This method produced $2N$, $3N$ and $\frac{3}{2}N$ bonds for correspondingly square, triangular and honeycomb lattices, where N is the number of sites.

To effectively activate random bonds, the list of bonds was shuffled randomly, by swapping the order of bonds. Then bonds were activated by iterating through the shuffled list. This procedure saved time, as random numbers do not have to be picked multiple times.

To save information on connections in a cluster, a network of pointers was generated. If the pointer was negative, then the corresponding site was a root node. Else, a pointer to the root node of the relevant cluster was used. To effectively merge clusters a dictionary was used, where keys consisted of the root nodes, while the values were the sites connected to this root node.

Bonds were activated one by one. If one of the sites in the activated bond belonged to a cluster, the other part of the bond was added to the dictionary of the cluster, while a pointer to the root node was added. If both sites were connected to their own cluster, these were merged such that the root of the larger cluster became the root of the combined cluster. The values of the larger cluster root node key were updated with the new sites, while the key belonging to the root node of the smaller cluster was deleted. The network was also updated such that the root nodes of the larger cluster became more negative, corresponding to the number of sites in the cluster, while the sites of the smaller cluster were updated to point to the root node of the larger cluster. The procedure of activating bonds was done for each bond in the shuffled bond list, or until all of the nodes belonged to one cluster. Stopping as this point instead iterating through the whole list of bonds was done to reduce the computational time. For each bond activated, the giant cluster P_∞ and the variable s_{avg}, later used to calculate the average cluster size $\langle s \rangle$, were calculated using Equation 3 and Equation 4:

$$P_\infty(n) = \frac{M_\infty(n)}{n}, \tag{3}$$

where n is the number of activated bonds and $M_\infty(n)$ is number of bonds in largest cluster,

$$s_{avg} = s_{avg} - network[r_i]^2 - network[r_j]^2 + (network[r_i] + network[r_j])^2, \tag{4}$$

where r_i and r_j is the root node of the two clusters being merged. After activating bonds the average cluster size for all probabilities was calculated as Equation 5:

$$\langle s \rangle = \frac{s_{avg} - (NP_\infty)^2}{N(1 - P_\infty)}. \tag{5}$$

As $P_\infty \to 1$, when the system merges to just one cluster, $\langle s \rangle \to \infty$ due to the denominator in the Equation 5. To avoid NaN-values all indices $P_\infty > 0.999$ were found and the corresponding values of $\langle s \rangle$ were set to zero. To avoid sampling statistical outliers the procedure of activating bonds was done 100 before the mean of P_∞ and $\langle s \rangle$ was calculated.

Equation 6

$$\chi = N\sqrt{\langle P_\infty^2 \rangle - \langle P_\infty \rangle^2}, \tag{6}$$

which may be seen as the autocorrelation of the variable P_∞.

B. Convolution

To further validate the values of P_∞ and $\langle s \rangle$ statistically, the result was embedded into the right statistical ensemble, through convolution using Equation 7:

$$Q(q) = \sum_{n=0}^{M} \binom{M}{n} q^n (1-q)^{M-n} Q_n, \tag{7}$$

where $\{Q_n\}$ is the set of quantities previously calculated, P_∞ and $\langle s \rangle$, M the number of bonds and q is the probability of activating a bond. The resolution of q used was 10000 values. Equation 7 was used in a logarithmic form as M is a large number, up to a million, and q small, down to a ten-thousandth. Thus precision error was reduced.

1. *Finite-size scaling*

To calculate the critical probability p_c, the Equation 1a was used in logarithmic form. A line was fitted through the data points $(\log \xi, \log P_\infty)$, one for each value of q. The probability q with the highest R^2-coefficient was chosen as p_c, since that would be the best fit for $\log P_\infty$ as a power-law function of $\log \xi$. The slope of the corresponding fitted line was set to be the fraction $-\frac{\beta}{\nu}$, which can be derived if using Equation 1c in Equation 1a. Using the same p_c, a line was fitted through the data points $(\log \xi, \log(\max \langle s \rangle))$ for each q. The slope of the line gave the exponent $\frac{\gamma}{\nu}$. Lastly a line was fitted to the data $(\log \xi, \log q_{max})$, where q_{max} is the probabilities that give maximal value to $\langle s \rangle$. The slope of this line gave the exponent $-\frac{1}{\nu}$. Combining the three mentioned exponents, the critical exponents β, γ and ν could be calculated, resulting in Table I.

III. RESULTS AND DISCUSSION

In Table I one can see that all analytical expressions are included in the 95%-confidence interval, except β for the square lattice. The confidence intervals are large, and most of the numerical results do differ much from the analytical expression, meaning that more precision is welcomed. When picking the critical probability, p_c the value of the R^2-coefficient differed slightly, meaning that many values of q gave almost the same R^2-coefficient, but could have lead to a different slope for the variables of interest. This could have been avoided by running the convolution with an increased number of steps, beyond the

TABLE I: Critical exponents for finite-size scaling. The analytical exponents are from table 2 of[7], while the critical probabilities p_c is calculated in[2].

	Type of lattice	Analytical	Numerical	95%-Confidence interval
p_c	square	$1/2$	0.501	
	triangular	$2\sin(\pi/18)$	0.346	
	honeycomb	$1-2\sin(\pi/18)$	0.652	
γ	square	$43/18$	2.639	$[2.216, 3.220]$
	triangular	$43/18$	1.572	$[1.123, 2.509]$
	honeycomb	$43/18$	2.305	$[1.859, 2.977]$
β	square	$5/36$	0.099	$[0.074, 0.133]$
	triangular	$5/36$	0.175	$[0.108, 0.315]$
	honeycomb	$5/36$	0.172	$[0.118, 0.254]$
ν	square	$4/3$	1.490	$[1.287, 1.769]$
	triangular	$4/3$	0.899	$[0.665, 1.386]$
	honeycomb	$4/3$	1.331	$[1.107, 1.670]$

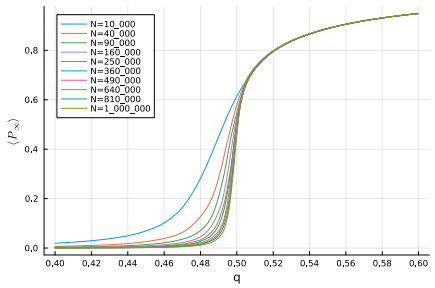
10000 used in this paper, though it be computational demanding. Calculating the difference between adding the critical probability of the triangular and the honeycomb lattice, the result is almost one, meaning that Equation 2 is fulfilled, confirming the duality between these two lattices.

When comparing the value of p_c for each of the lattices, it can be observed that the higher the number of neighbors, the lower the critical probability. The number of neighbors in the honeycomb lattice is $\frac{3}{2}N$, $2N$ for the square lattice and $3N$ for the triangular lattice. Even though the critical probabilities are different, the critical behavior themselves are rather similar, as can be observed by the similarities between the values for the critical exponents in Table I. The similarities of the critical behavior are also visible in the shape of the three curves in Figure 2 and Figure 3, as they are similar.

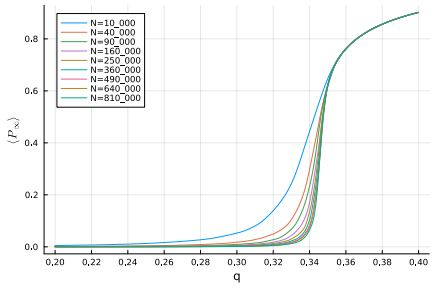
IV. CONCLUSION

In two dimensions, the number of neighbors in a lattice influences the critical probabilities p_c. The critical behavior is though similar for square, triangular and honeycomb lattices, as they share the same critical exponents and curve shape. The algorithms described in this paper produced critical exponents in which the analytical results are included in the 95%-confidence interval, for all lattices and exponents, excluding β for square lattice.

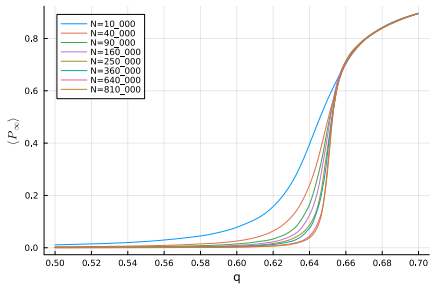
Further investigations of increased resolution of the probability q could be of interest, as this could have given more accurate results, although it is computationally demanding. Calculating more exponents like α from the total number of clusters and σ for the characteristic cluster size and comparing them with analytical expressions would also be interesting. The same could be said about increasing the number of dimensions and also tracking the second largest cluster and its behavior.



(a) Square lattice



(b) Triangular lattice



(c) Honeycomb lattice

FIG. 2: Giant component, P_∞ for three types of lattices. The first axis, the probability q is plotted, while the giant component is shown on the secondary axis. The legend describes the number of sites in the lattice.

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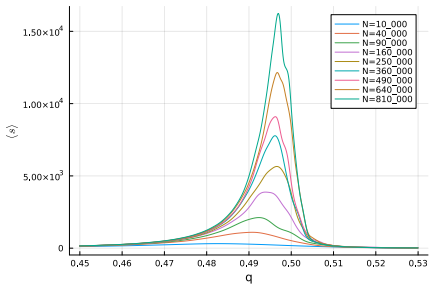
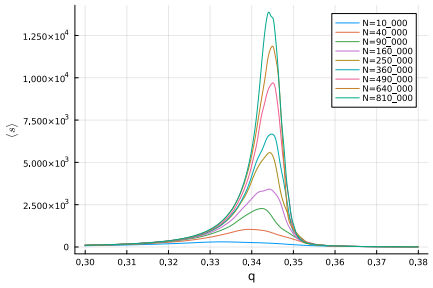
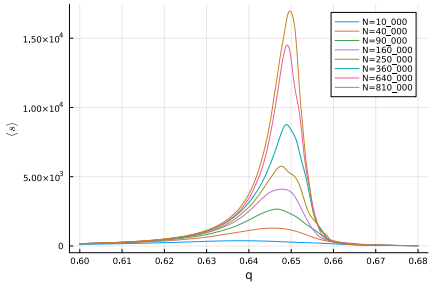


(a) Square lattice

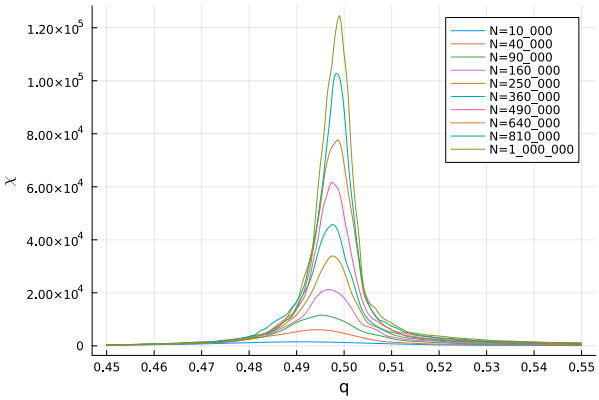


(b) Triangular lattice

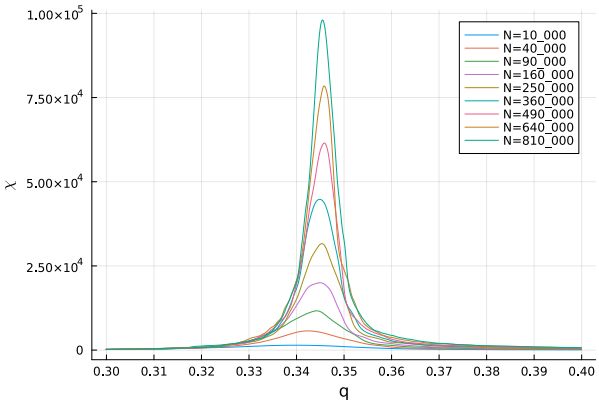


(c) Honeycomb lattice

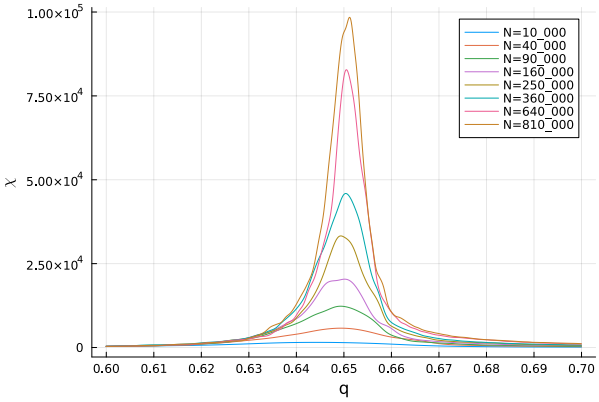
FIG. 3: Average cluster size, $\langle s \rangle$ for three types of lattices. The first axis, the probability q is plotted, while the average cluster size is shown on the secondary axis. The legend describes the number of sites in the lattice.



(a) Square lattice



(b) Triangular lattice



(c) Honeycomb lattice

FIG. 4: Susceptibility, χ for three types of lattices. The first axis, the probability q is plotted, while the susceptibility is shown on the secondary axis. The legend describes the number of sites in the lattice.