Physics 344 Final Project

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1 Introduction

For the final project of Physics 344, I will be investigating the critical exponents of the same model as before (on a square lattice) in more depth. In Assignment 5 it seemed that the exponents associated with the correlation length of the bond percolation transition were different on the two sides of the transition line. Since correlation lengths are notoriously tricky, we will need to use some more sophisticated methods than before if we are to get any sort of clarity. We would also like to investigate the exponents associated with some of the different transitions that are present in this model. The most interesting would be 4-site percolation, since it doesn't reduce to a bond or site percolation model under small variations of μ, β as the other transitions. It is therefore not clear if this transition should be expected to belong to the same universality class as percolation (and by extension the other transitions in the model).

2 Context

In previous assignments we have investigated a model laid out in more detail below. The model defines a Hamiltonian on the edges of a graph, allowing us to consider the grand canonical ensemble of these graphs, and investigate ensemble averages parameterised by the 'inverse temperature' β and the 'chemical potential' associated with the number of edges μ. We have found 4 order parameters that are associated with what we have called the bond percolation, 0-site percolation, 4-site percolation and 8-site percolation transitions. These order parameters are also defined in detail below. This defines 5 distinct phases in our $\mu - \beta$ plane, which were previously investigated and found to agree well with some naive back-of-the-envelope calculations, as can be seen in Figure 1 below.

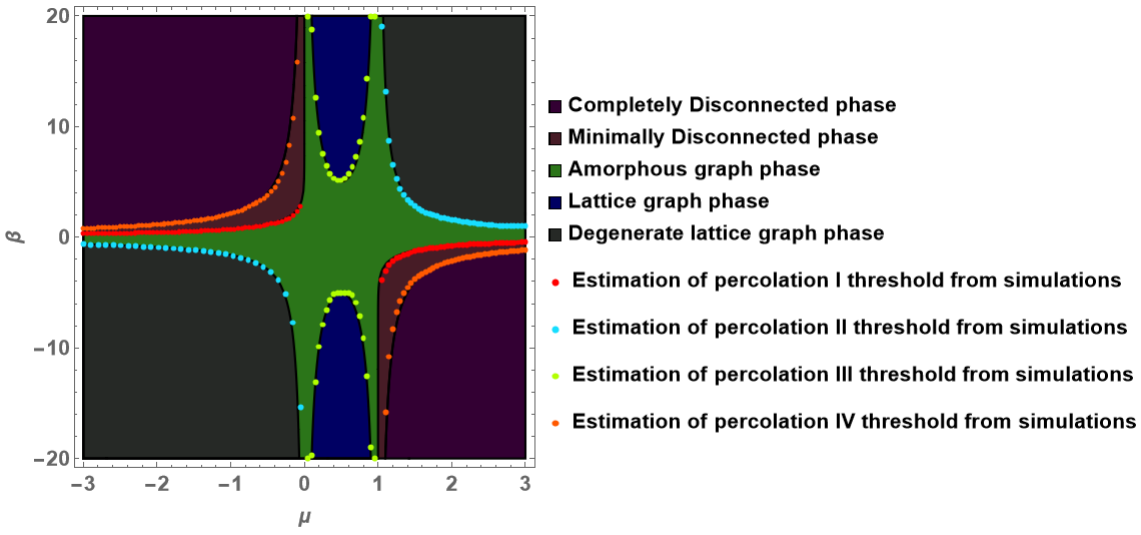

Figure 1: The phase diagram of the model. The different transitions are labelled where percolation I,II,III and IV are the bond, 8-site, 4-site and 0-site percolation transitions respectively.

To get a feel for the qualitative differences between these phases, let us look at some examples of typical graphs in each phase in Figure 2 below.

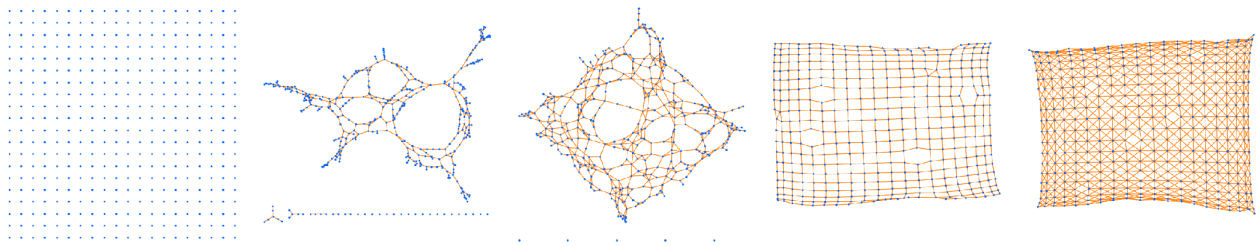

Figure 2: Examples of graphs in the different phases. The phases are in the same order as the labeling in Figure 1. They were generated with $(\mu, \beta) = (-2, 10), (-0.25, 1), (0.5, 0), (0.5, 10), (-1, -5)$ respectively.

3 Definitions

Given the context laid out above, we can now set out to more precisely define our model and some relevant concepts. A basic understanding of graph theory (in particular simple graphs) is assumed.

Definition 1. Our *underlying lattice* or *graph* is a square lattice graph of size $L \times L$ (without periodic boundary conditions, to ease detecting spanning clusters).

Definition 2. In a graph a *cycle* is a path that starts and ends at the same vertex. A *chord* of a cycle is an edge that connects two non-consecutive vertices in that cycle. A *chordless-cycle* is a cycle that contains no chords.

Definition 3. A *shortcut* on an underlying graph is an edge connecting two vertices that are part of a chordless-cycle of the underlying graph (which automatically makes all edges in the underlying graph shortcuts).

Definition 4. Our ensemble is the *grand canonical ensemble* of graphs on the underlying lattice, parameterized by the *inverse temperature* β and the *chemical potential* μ.

Definition 5. The *Hamiltonian* of the ensemble is defined as the sum of the weights of all edges in the graph, where the weight of an edge is given by $s - 1$, where s is the distance between the vertices of the edge in the underlying graph. For the square lattice this means the 'energy' of an edge is 0 if it is in the underlying graph and 1 if it is a shortcut that isn't in the underlying graph.

Remark. It can be straight-forwardly shown that we can generate a graph typical of a pair (μ, β) by generating a graph where each edge that is in the underlying graph is present with probability $\frac{1}{1+e^{\beta\mu}}$ and each shortcut not in the underlying graph is present with probability $\frac{1}{1+e^{\beta(\mu-1)}}$. This also makes clear the fermionic nature of edges in simple graphs.

Remark. It might seem like we can re-parametrize our ensemble in terms of the two probabilities $\frac{1}{1+e^{\beta\mu}}$ and $\frac{1}{1+e^{\beta(\mu-1)}}$ instead of μ and β. However, this is not the case in general, and we have previously shown that in more complicated lattices with weight 2 and more edges there is a lot of analogous behaviour, while obviously the three or more probabilities can no longer be made independent. In light of these interesting generalizations of the model and their corresponding behaviors, we will stick to the original parameters μ and β.

Having abstractly defined the instance of the model we will be using, we can now define the order parameters we will be using to investigate the model. We have found the following order parameters that correspond to phase transitions in the model:

- Percentage of vertices in largest cluster (order parameter for bond percolation transition)
- Percentage of vertices in the largest cluster in the sub-graph of the underlying graph induced by vertices which have no edges (order parameter for 0-site percolation transition)
- Percentage of vertices in the largest cluster in the sub-graph induced by vertices which have exactly 4 edges (order parameter for 4-site percolation transition)
- Percentage of vertices in the largest cluster in the sub-graph induced by vertices which have all 8 edges (order parameter for 8-site percolation transition)

Definition 6. The *correlation length* of a transition is defined in terms of the clusters associated with that parameter. Following [1] we define the correlation length

$$\xi^2 = \frac{\sum_n m_n I_n}{\sum_n m_n^2} \tag{1}$$

where $\sum_n$ is a sum over all non-spanning clusters, m_n is the number of vertices in cluster n and I_n is the moment of inertia of cluster n, defined as $I_n = \sum_i^{m_n} r_i^2$, where r_i is the distance (in the plane, not the graph) of vertex i from the center of mass of the cluster (defined in the usual way with all vertices with mass 1).

Definition 7. A *spanning cluster* is a cluster that contains at least one vertex from two opposing sides of the underlying graph, utilizing the lack of periodic boundary conditions to ease computation.

4 Methods

Following [1] we will use the so-called disjoint set data structure together with the parallel axis theorem to efficiently compute correlation lengths. The parallel axis theorem allows us to calculate the resulting moment of inertia of a cluster made up by merging two disjoint clusters. It gives us the following formula:

$$I_{\text{new}} = I_1 + I_2 + m_1(\overline{x}_{\text{new}} - \overline{x}_1)^2 + m_2(\overline{x}_{\text{new}} - \overline{x}_2)^2 \tag{2}$$

where $\overline{x}_1, \overline{x}_2$ are the centers of mass of the two clusters and $\overline{x}_{\text{new}}$ is the center of mass of the new cluster. This allows us to efficiently compute the correlation length of a transition by keeping track of the clusters in the graph and updating the moment of inertias of the clusters as well as updating the centers of mass of the clusters as we merge them. The new center of mass of the new cluster is given by

$$\overline{x}_{\text{new}} = \frac{m_1\overline{x}_1 + m_2\overline{x}_2}{m_1 + m_2} \tag{3}$$

as usual. We can track if a cluster is spanning by individually keeping track of which sides of the underlying graph the cluster is connected to (and when merging awith a cluster touching a given side, the resultant cluster will as well). We start with each vertex having $I_n = 0, m_n = 1$ and $\overline{x}_n$ is the coordinate of the vertex in the plane.

All that remains is to define how we will decide what and when to merge. This will depend on which transition we are considering. For bond percolation we will merge disjoint clusters when an edge is added that connects them. For 0-site percolation we will check which vertices have no edges and merge clusters that contain adjacent (in the underlying graph) such vertices. For 4-site percolation we will check which vertices have exactly 4 edges and merge clusters with edges between them that contain such vertices. Since 8-site percolation promised no interesting behavior not present in the other transitions, we will not consider it here.

5 Results

5.1 Bond percolation

We can start by investigating how the correlation length related to bond percolation ξ_b varies as a function of μ and β. We can

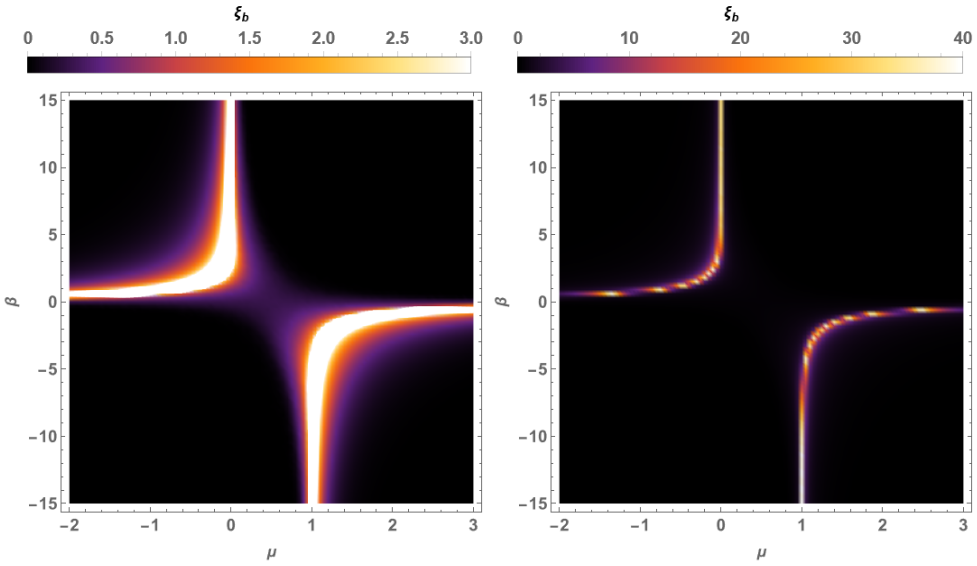

Figure 3: Correlation length of bond percolation as a function of μ and β, with a cutoff at 3 and without a cutoff respectively.

see there is quite a sharp divergence of the correlation length on the transition line as one would expect. It is also interesting

to note the 'residual' correlation length around the origin. We can now choose some lines along which to cross the transition line, in order to investigate how the critical exponents related to ξ_b depend on the side of the transition line, the location of the transition, and the angle at which we cross the transition line. We can define the critical exponents $\nu_{b1}(\theta), \nu_{b2}(\theta)$ by

$$\xi_b(\mu, \beta = -\mu \tan\theta) \sim |\mu - \mu_c(\theta)|^{\nu_{b\text{-}}(\theta)} \tag{4}$$

where $\mu_c(\theta)$ is the location of the transition line at angle θ, and $\nu_{b1}(\theta)$ is the exponent above the transition (in this case for $\mu > \mu_c(\theta)$) and $\nu_{b2}(\theta)$ is the exponent below the transition (in this case for $\mu < \mu_c(\theta)$). We can calculate the correlation

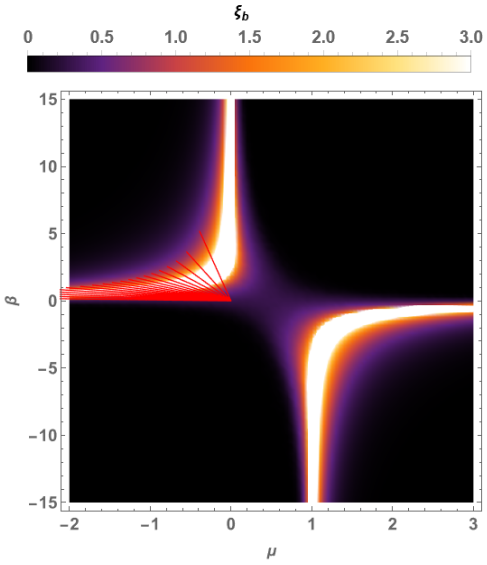

Figure 4: Lines along which we will gather larger amounts of data, in order to investigate the critical exponents $\nu_{b1}(\theta), \nu_{b2}(\theta)$

length along these lines parametrized by $\beta = -\mu \tan\theta$ and plot the results in the following figure. For each line we can fit the

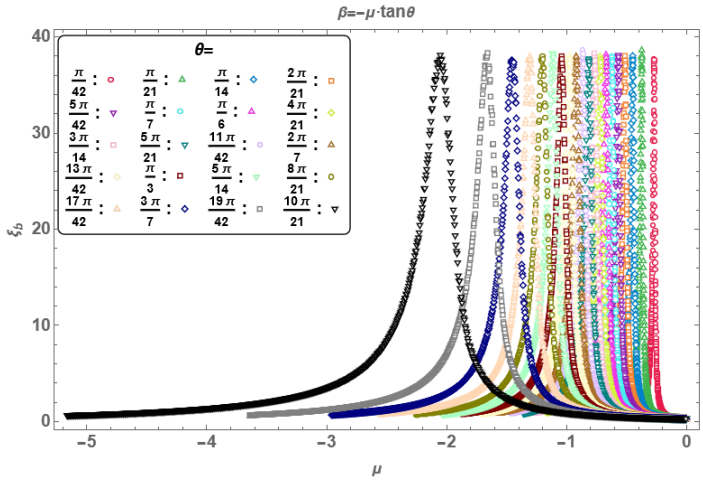

Figure 5: The correlation length ξ_b as a function of μ for different values of θ along the lines in figure 4, each data point is the average of 1024 graphs.

data to a power law and extract the critical exponents $\nu_{b1}(\theta), \nu_{b2}(\theta)$, by splitting the data onto two parts, above and below the μ where it attains its maximum value. This allows us to take the $\log - \log$ data, and use the second numerical derivative to isolate the linear part of the $\log - \log$ data, whose slope gives us the relevant critical exponent.

If we calculate these critical exponents by smoothing out the logged data by using a moving average over 50 data points at a time, and choose data points that yield a second numerical derivative of less than 0.5 we get the very reasonable results seen in Figure 6. We can see that the exponents are seemingly independent of θ, and very similar on the two sides of the transition line (taking into account that the error bars only quantify the uncertainty of the final fit, not systematic and statistical uncertainties before that).

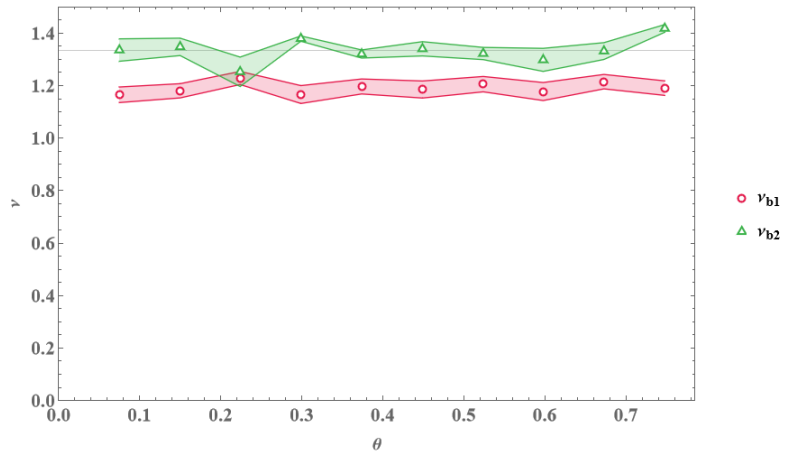

Figure 6: The critical exponents $\nu_{b1}(\theta), \nu_{b2}(\theta)$ as a function of θ.

5.2 0-site percolation

We can start by investigating how the correlation length related to 0-site percolation ξ_0 varies as a function of μ and β. We can

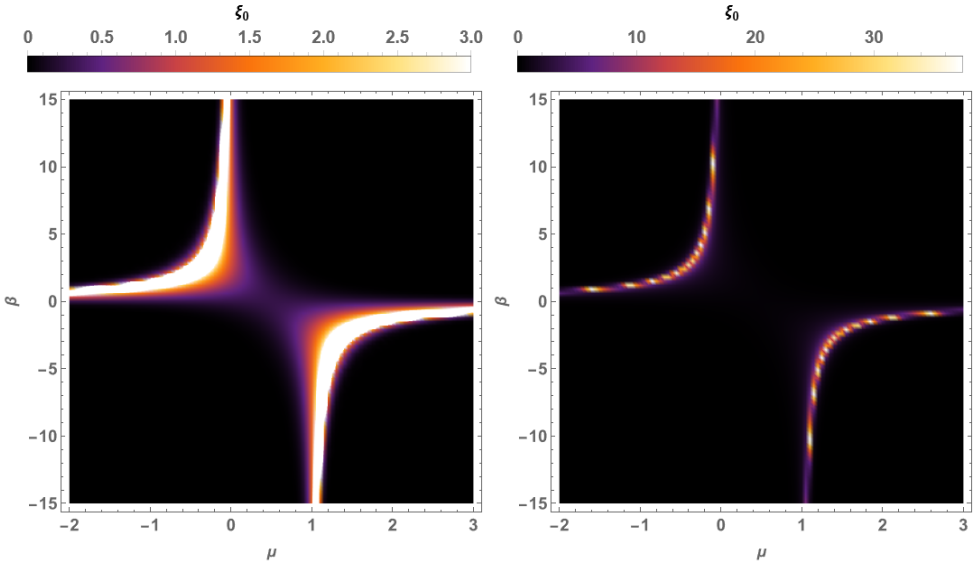

Figure 7: Correlation length of 0-site percolation as a function of μ and β, with a cutoff at 3 and without a cutoff respectively.

see there is quite a sharp divergence of the correlation length on the transition line as one would expect. It is also interesting to note the 'residual' correlation length around the origin. We can now choose some lines along which to cross the transition line, in order to investigate how the critical exponents related to ξ_0 depend on the side of the transition line, the location of the transition, and the angle at which we cross the transition line. We can define the critical exponents $\nu_{01}(\theta), \nu_{02}(\theta)$ by

$$\xi_0(\mu, \beta = -\mu \tan\theta) \sim |\mu - \mu_c(\theta)|^{\nu_{0\_}(\theta)} \tag{5}$$

where $\mu_c(\theta)$ is the location of the transition line at angle θ, and $\nu_{01}(\theta)$ is the exponent above the transition (in this case for $\mu > \mu_c(\theta)$) and $\nu_{02}(\theta)$ is the exponent below the transition (in this case for $\mu < \mu_c(\theta)$). We can calculate the correlation length along these lines parametrized by $\beta = -\mu \tan\theta$ and plot the results in the following figure. For each line we can fit the data to a power law and extract the critical exponents $\nu_{01}(\theta), \nu_{02}(\theta)$, by splitting the data onto two parts, above and below the μ where it attains its maximum value. This allows us to take the $\log - \log$ data, and use the second numerical derivative to isolate the linear part of the $\log - \log$ data, whose slope gives us the relevant critical exponent.

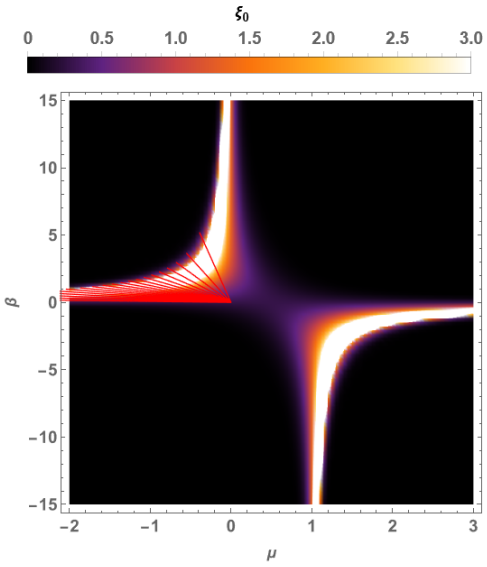

Figure 8: Lines along which we will gather larger amounts of data, in order to investigate the critical exponents $\nu_{01}(\theta), \nu_{02}(\theta)$

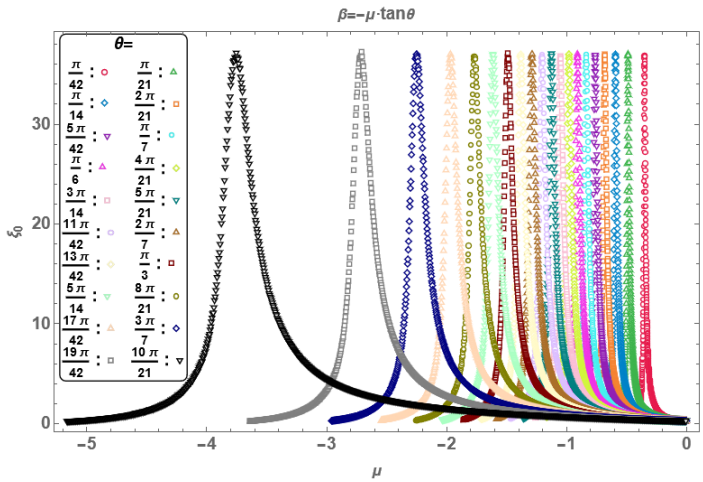

Figure 9: The correlation length ξ_0 as a function of μ for different values of θ along the lines in figure 8, each data point is the average of 4096 graphs.

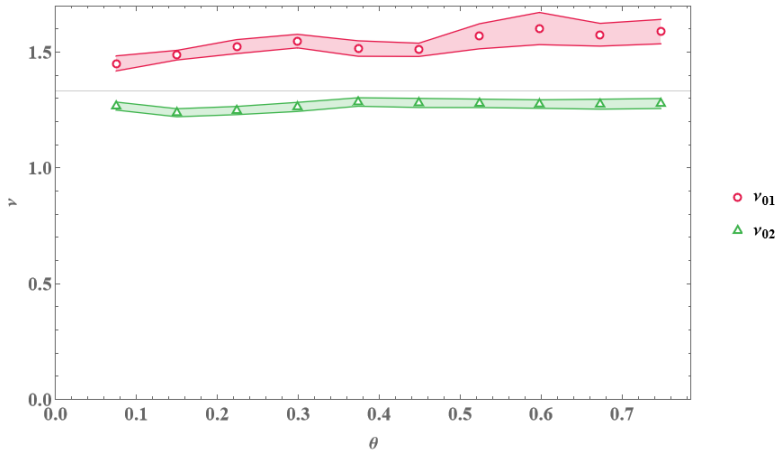

Figure 10: The critical exponents $\nu_{01}(\theta), \nu_{02}(\theta)$ as a function of θ.

If we calculate these critical exponents by smoothing out the logged data by using a moving average over 50 data points

at a time, and choose data points that yield a second numerical derivative of less than 0.5 we get the very reasonable results seen in Figure 10. We can see that the exponents are seemingly independent of θ, and very similar on the two sides of the transition line (taking into account that the error bars only quantify the uncertainty of the final fit, not systematic and statistical uncertainties before that).

5.3 4-site percolation

We can start by investigating how the correlation length related to 4-site percolation ξ_4 varies as a function of μ and β. We

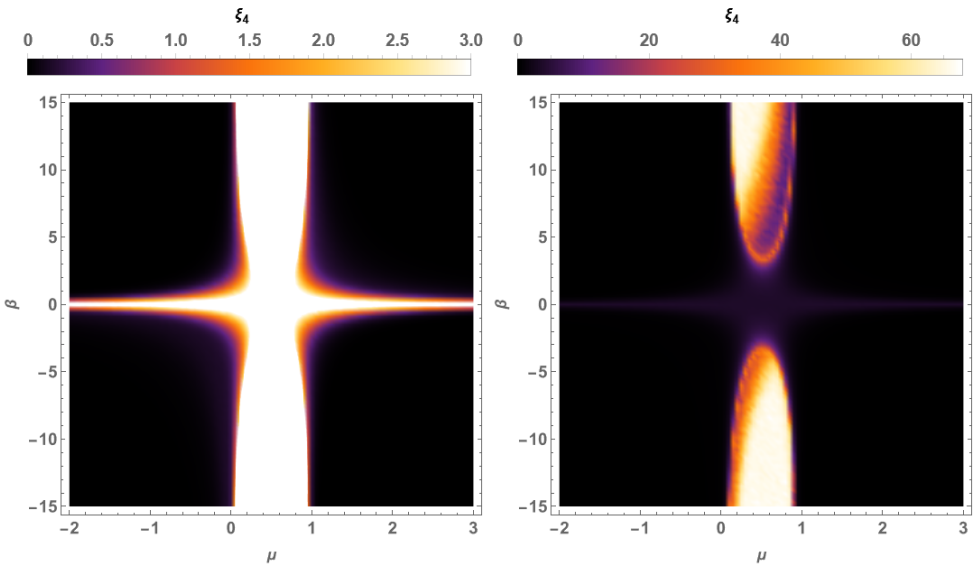

Figure 11: Correlation length of 4-site percolation as a function of μ and β, with a cutoff at 3 and without a cutoff respectively.

can see in Figure 11 that the calculated correlation length diverges in the ordered phase, when one would expect it to go down again. This is presumably due to difficulties in identifying spanning clusters, seeing as vertices on the edges of the underlying graph only has 5 possible edges, so it is significantly less likely to have exactly 4 edges, making spanning clusters less likely than they should be. This messes with the data gathered to such an extent that no useful exponents can be extracted from it. We again note the 'residual' correlation length around the origin.

6 Conclusion

We have found a great improvement to previous results on the universality of the investigated model, which strongly suggested different exponents on the two sides of the bond percolation transition line. Furthermore, we have found that the critical exponents related to the bond percolation transition are independent of the angle at which we cross the transition line, and that they are very similar on the two sides of the transition line. We have also found that the critical exponents related to the 0-site percolation transition are independent of the angle at which we cross the transition line, and that they are very similar on the two sides of the transition line, as well as the exponents found for bond percolation. We finally also note how close the found critical exponents are to the universal exponent $\hat{=}\frac{4}{3}$ for percolation in general. The method of disjoint sets is a great speed up that enabled the accuracy of the data that was necessary to get sensible results. The code developed can also be quite easily adapted to investigate several other critical exponents (which can then be used to investigate the hypersaline relations) as well as other underlying graphs, such as hexagonal and cubical lattices. By improving the detection of spanning clusters, all transitions can also be investigated further (and ideally periodic boundary conditions can also be implemented).

7 Acknowledgements

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References

[1] Michael M. Danziger, Bnaya Gross, and Sergey V. Buldyrev. Faster calculation of the percolation correlation length on spatial networks. *Phys. Rev. E*, 101:013306, Jan 2020.