Spectral Approach to Quantum Percolation on the Honeycomb Lattice

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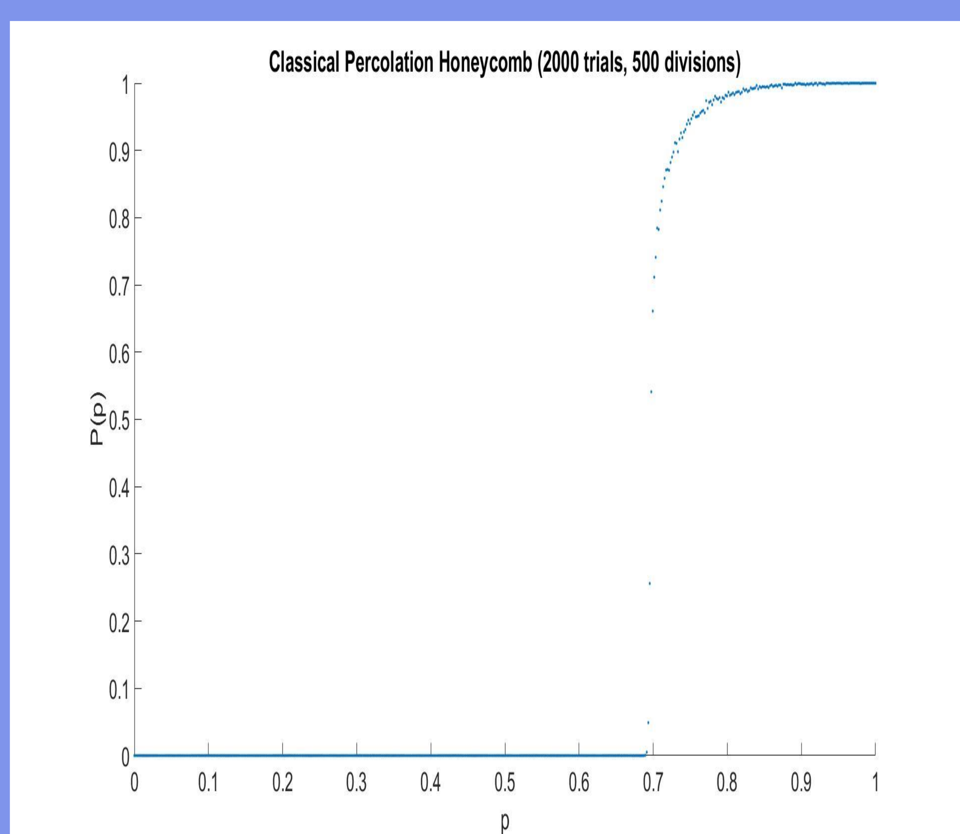
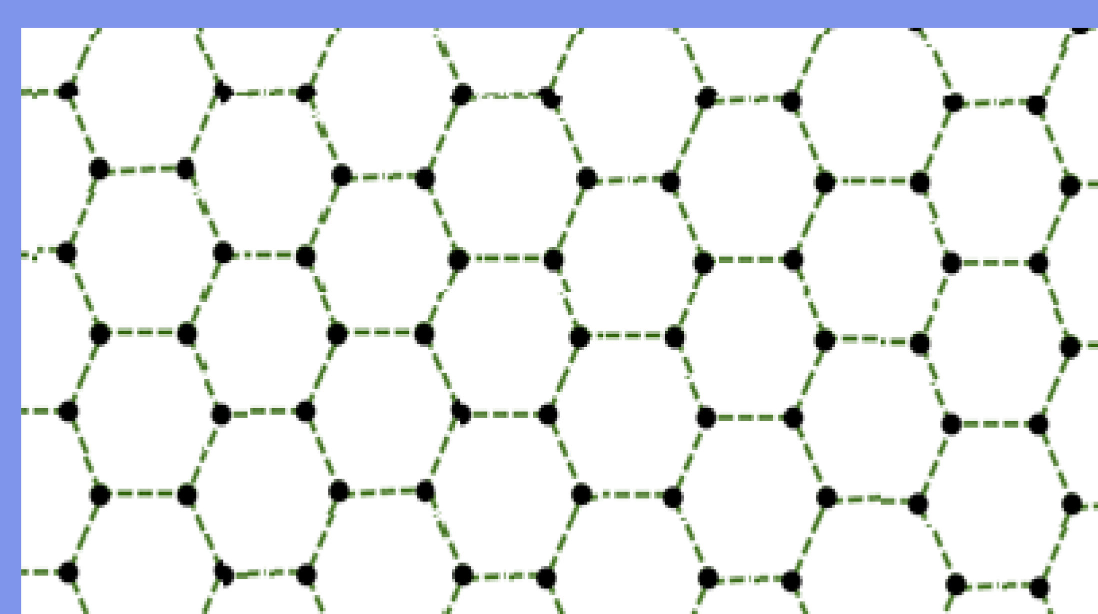
Classical Percolation



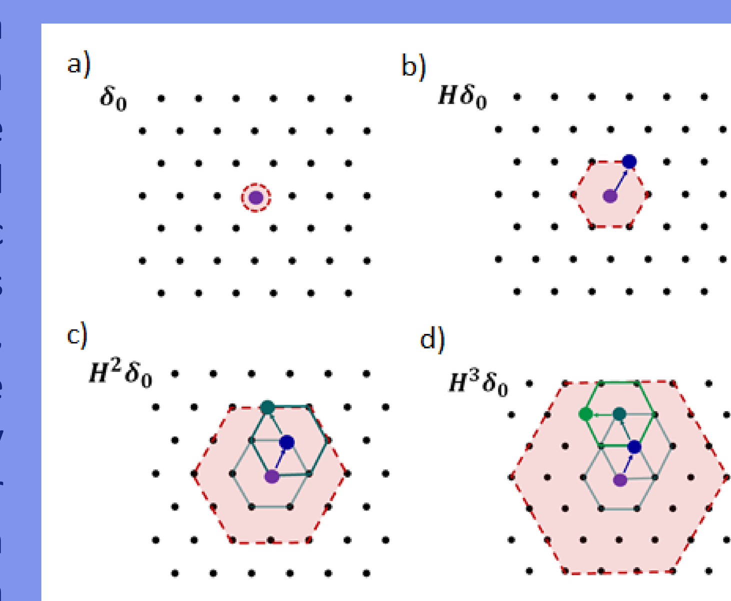
The graph above represents a simulation of classical percolation in a honeycomb shaped graph. p is the probability of any vertex being open and theta(p) is percolation probability. The critical point for this lattice structure is about 0.69, as can be seen. To the right is an example of the honeycomb structure.

Classical percolation is a problem in graph theory that seeks theta(p), the probability that the origin in an infinite graph will be part of an infinite open cluster. For site percolation all bonds are considered open, and the value p is the probability of any particular vertex being open. Study into this problem has revealed that there exists a critical point; any value of p below this point will result in theta(p) = 0. Any theta(p) greater than this point will result in theta(p) > 0.



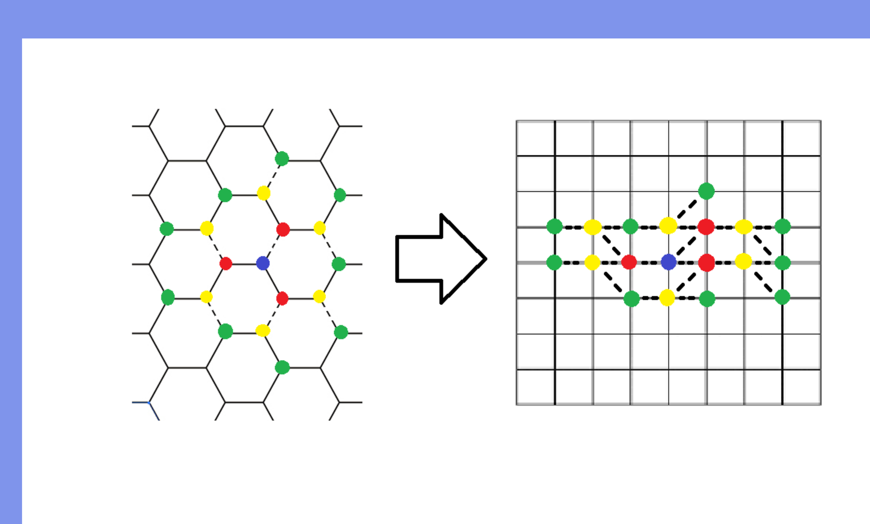
Quantum Percolation

Quantum percolation is a variation on regular percolation that attempts to take percolation and use it to model electron flow in atomic structures. Because electrons are subject to quantum effects, the more primitive classical site percolation which simply assigns vertices as open or closed is insufficient. Quantum percolation uses a Hamiltonian to represent the change in the wave over time. This method accounts for effects such as the electron being able to jump back and forth to previous sites.



Honey Comb Code

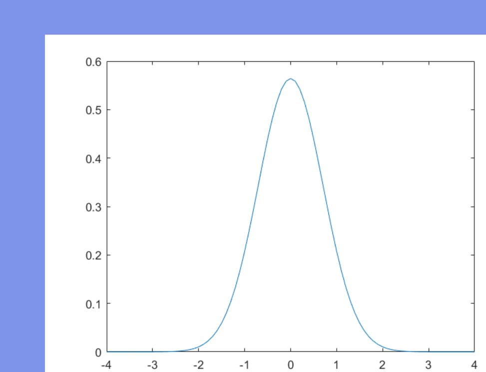
One of the challenges faced during this project was properly representing the graphene's 2D honeycomb structure within our program. This structure proved more difficult than the 2D square or triangular structures. To the right is a diagram that gives a rough idea of how it is done. The organic honeycomb structure is broken down into a more grid like structure that can be interpreted by the computer.

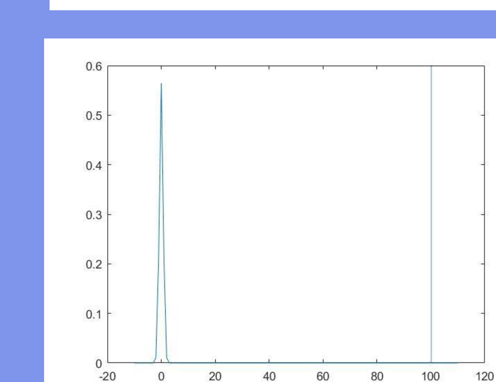


Distributions

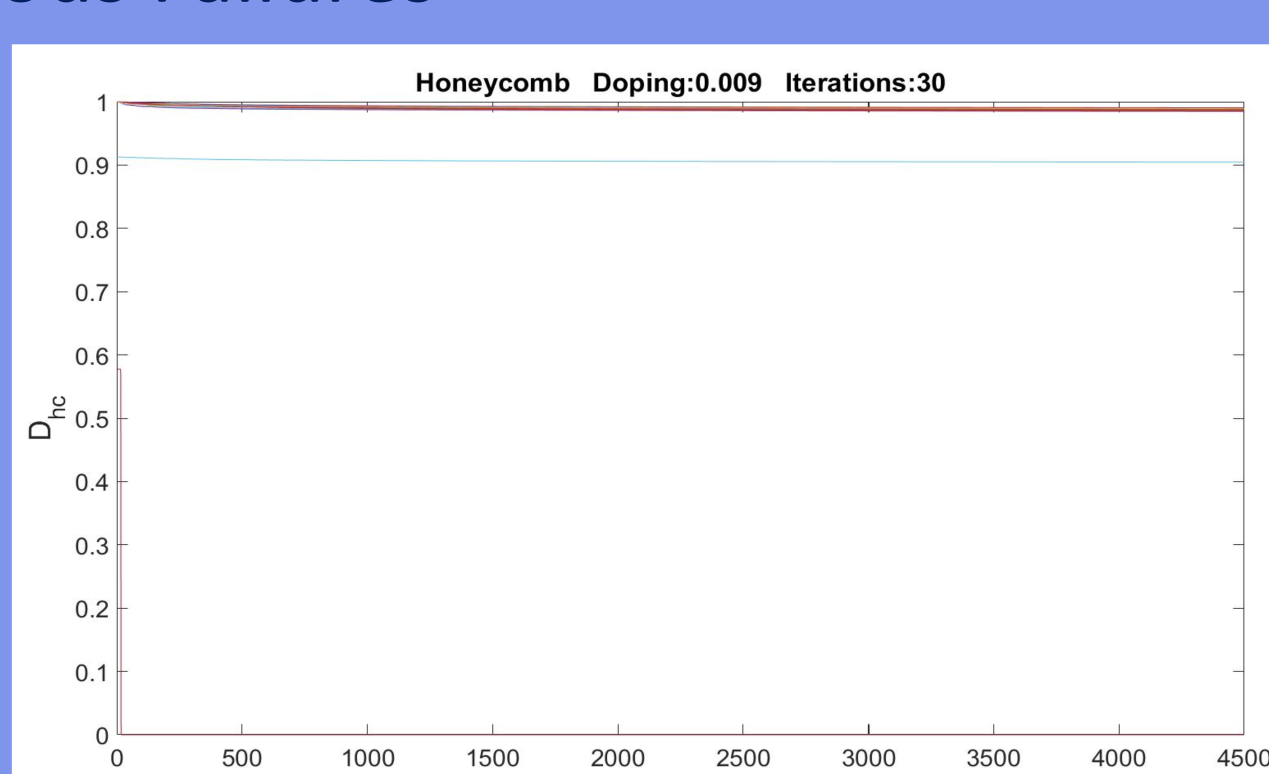
In our simulations, an energy must be assigned to each site. We decided to do this assignment according to a Gaussian distribution (left above).

In order to account for the effect of doping in materials, we also used another distribution (right below). This distribution is a combination of a Gaussian curve centered at 0 and a delta function centered at 100. The delta portion represents the probability of a site being doped and therefore having a much higher energy and being far more difficult for an electron to jump to.





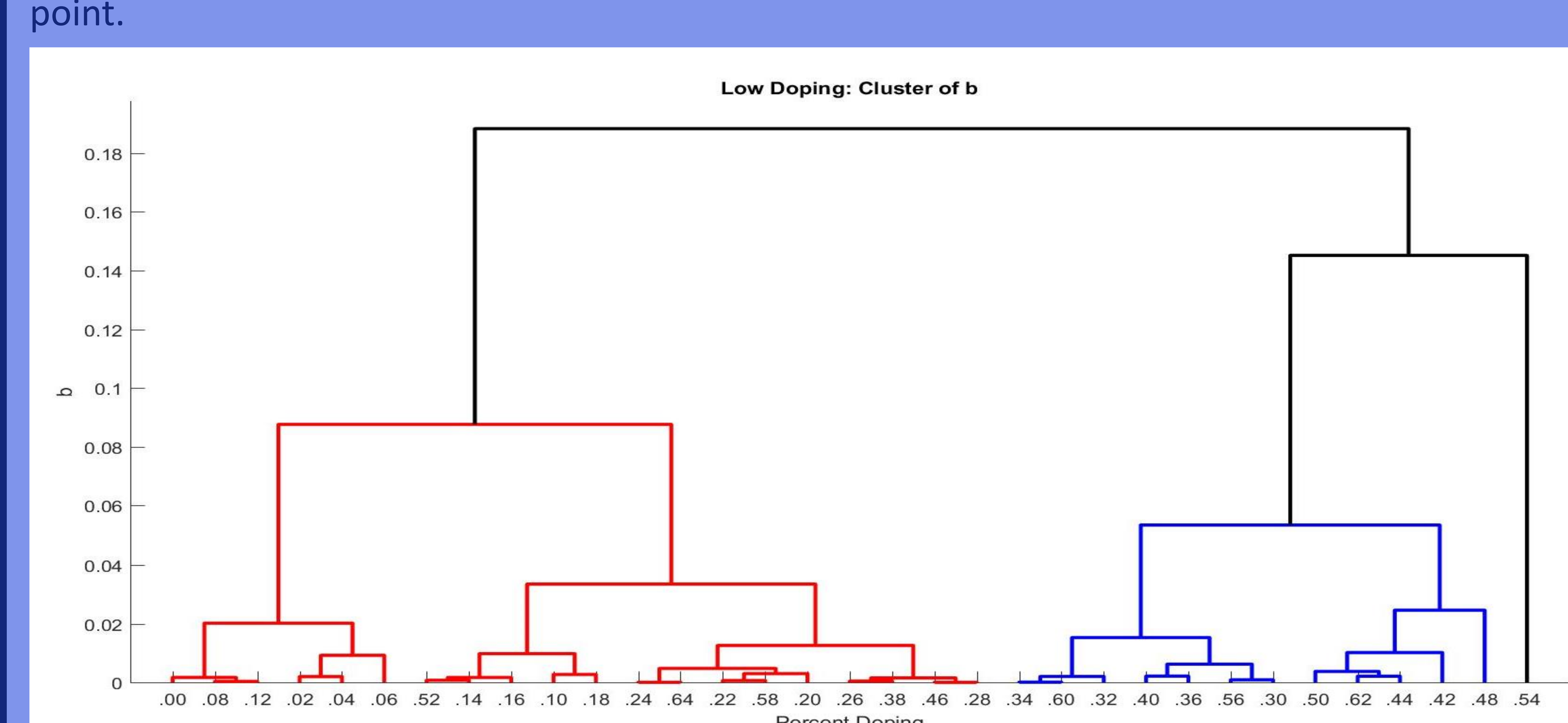
Ominous Failures



One effect noticed during analysis an was occasional sudden drop in the distance D. This frequently results in the function dropping almost immediately to zero. The above is the graph for 30 realizations of a the same doping (0.9%). Most of the realizations follow a similar course remaining very close to 1 during the whole run. One suddenly drops to about 0.9 and then remains steady. And, close inspection reveals that one drop to 0 almost immediately after the beginning of the simulation. The cause of these sudden drops is currently unknown. Is it a flaw in the simulation code or the mathematical method? Or, does it represent some unusual yet legitimate phenomena? In any case, finding the reason for this behavior will be key to getting good results and properly interpreting them. Since it does seem to occur less often for lower doping, the remainder of our results come from very small doping simulations and avoid this behavior.

0.30% Region

For sufficient doping, electron transport will not be possible, but it is hoped that the critical point in percolation can be connected to an amount of doping that serves as a transition point between conductivity and insulation in actual materials. It has been speculated that this point might be around .3%. In the below graph, the end values of different simulations are clustered together, with two main clusters emerging. It does seems that the blue cluster consists entirely of doping values above 0.30%. The correlation is not perfect though as there are some values above 0.30% in the red cluster. Further study will be required to see if this is the desired critical point.



Conclusions

- Unexplained failures exist for doping above 0.08%. These will require further study.
- 0.30% doping may be a transition point in the quantum percolation problem corresponding to a change in the electron transport properties of 2D materials

Application to Material Science

The main application of these studies into percolation is finding a way of modeling the electron transport properties of 2D materials, such as graphene. Graphene is a recently discovered allotrope of carbon that is truly 2-dimensional. It has a honeycomb structure the same as that used in our simulations. It is hoped that graphene will demonstrate useful electronic properties, such as semi conductivity. However graphene defies the current model for electron transfer, which is based on Anderson localization. In order to take advantage of the exciting properties of graphene, a new electron transfer model will be needed. It is hoped that this work with quantum percolation and the spectral method will lead to such a model.

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Overview

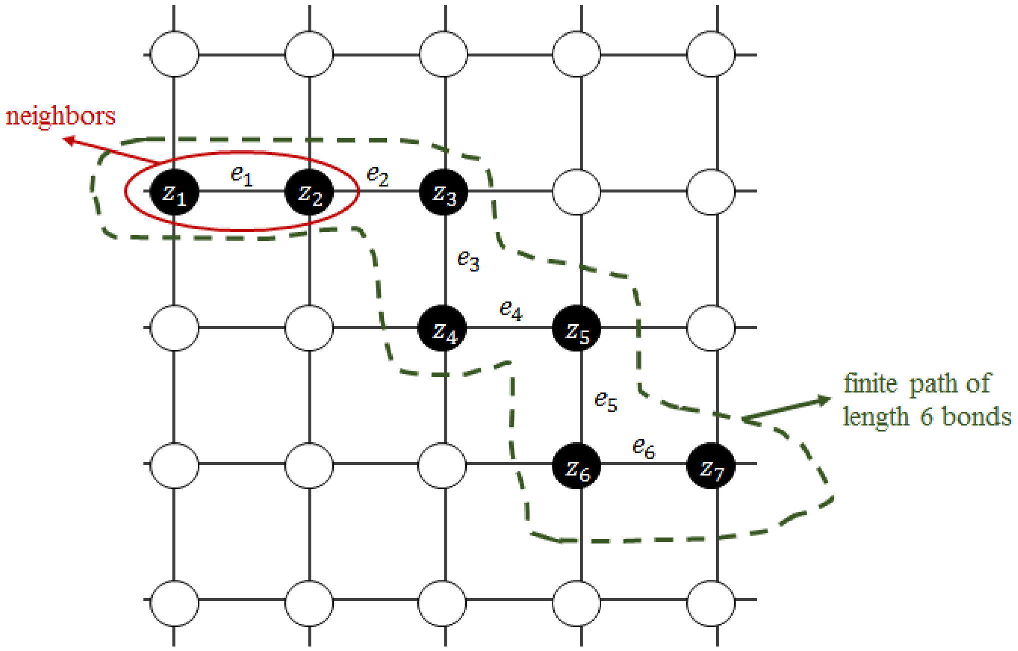
- Background – Graphene, Classical Percolation, Quantum Percolation
- Method – New Honey Comb Code, Distributions, Spectral Analysis
- Results – .3% Region, Failures
- Conclusions

Background – Graphene

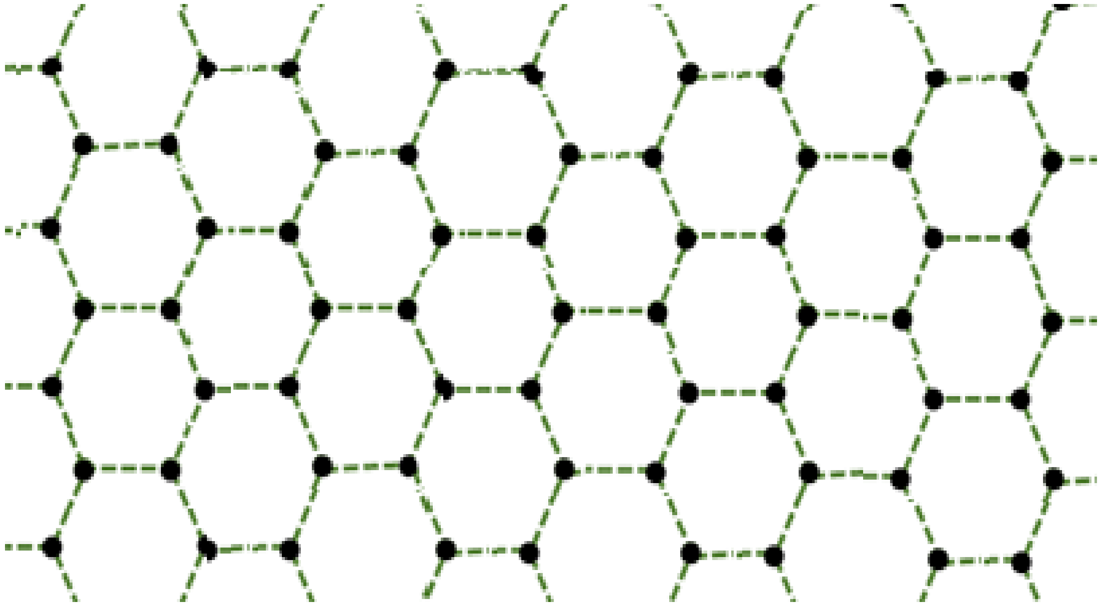
- Graphene is an exciting, newly discovered 2D material.
- Electrical properties defy expectations from the current model.
- Anderson localization
- New model will be required.

Background – Classical Percolation

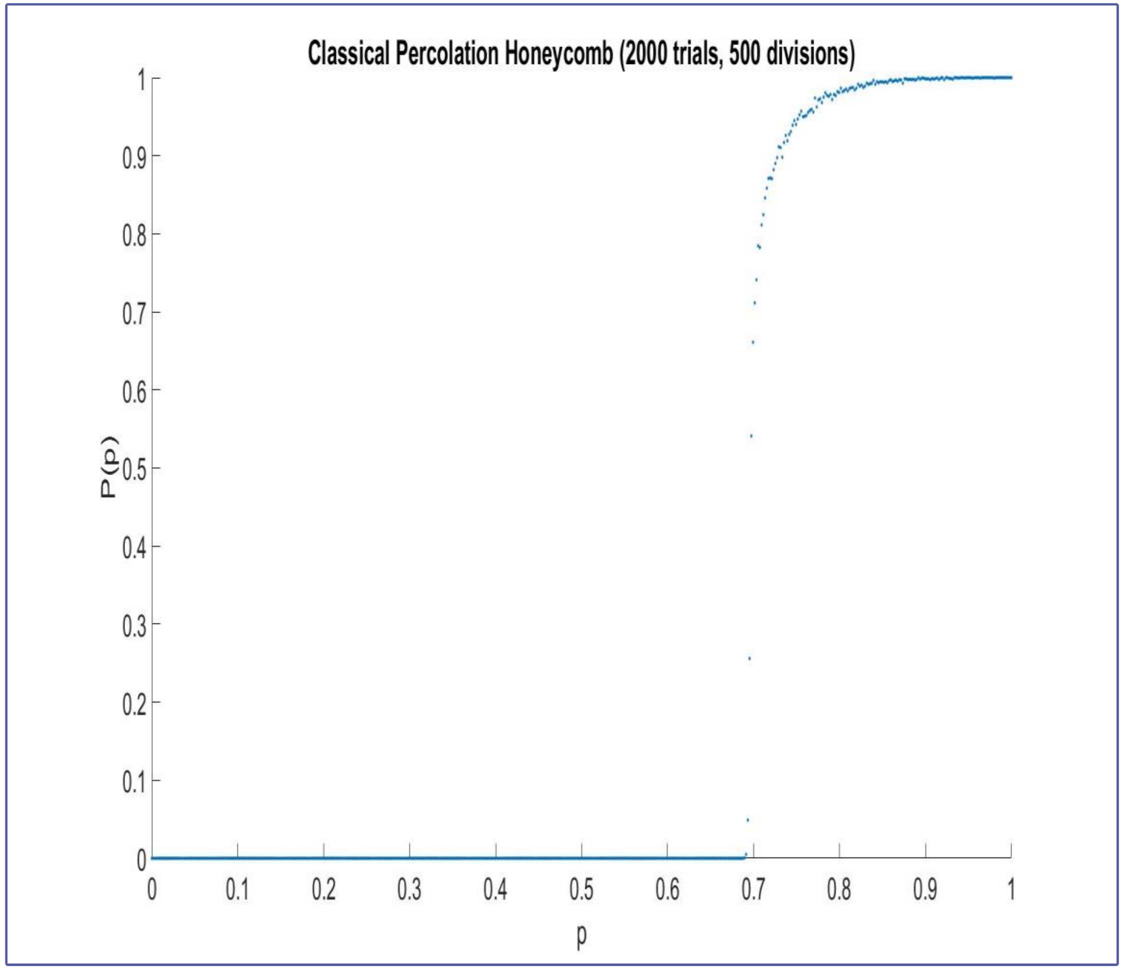
Connected Open Path



Honeycomb Structure



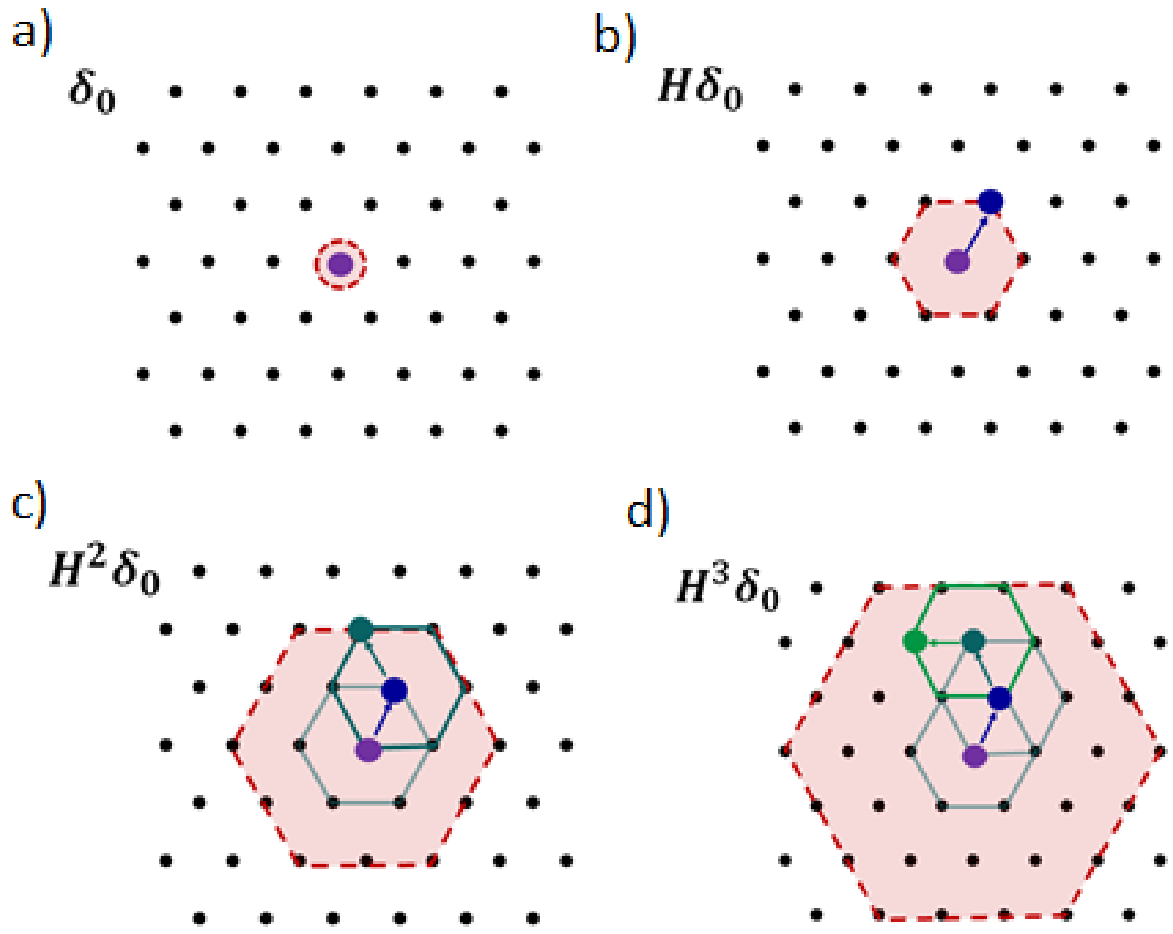
Background – Classical Percolation



- Behavior of Percolation
  - theta(0) = 0
  - theta(1) = 1
- Interest in critical point
  - Below theta(p) = 0
  - Above theta(p) > 0

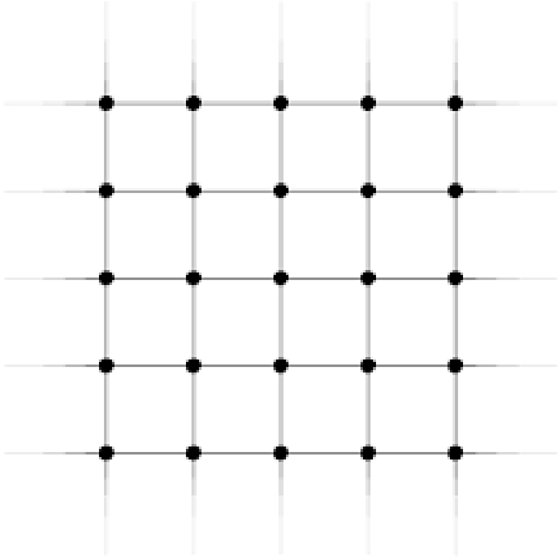
Background – Quantum Percolation

- Similar to classical percolation but accounts for quantum effects.
- Uses Hamiltonian to preform jumps.
- Can jump to previous locations.

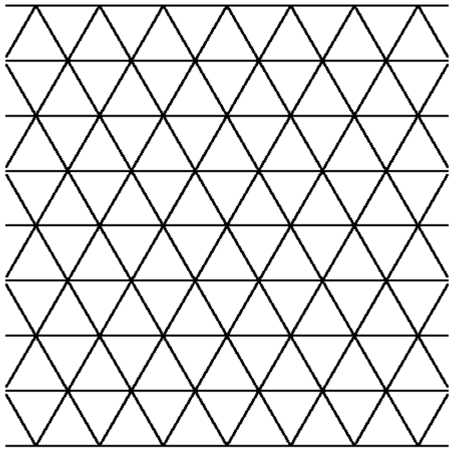


Method – Honeycomb Code

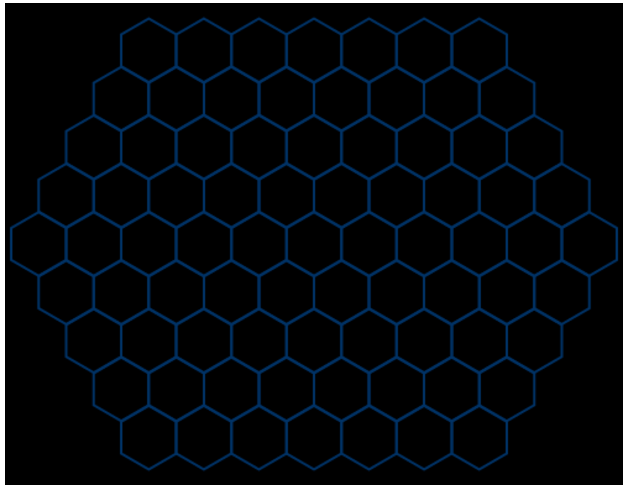
- Hoped to improve honeycomb lattice code to run at same speed as square and triangle lattice code
- Replaced conditionals with carefully aligned vector arithmetic. (Using Matlab's double colon notation)



Square



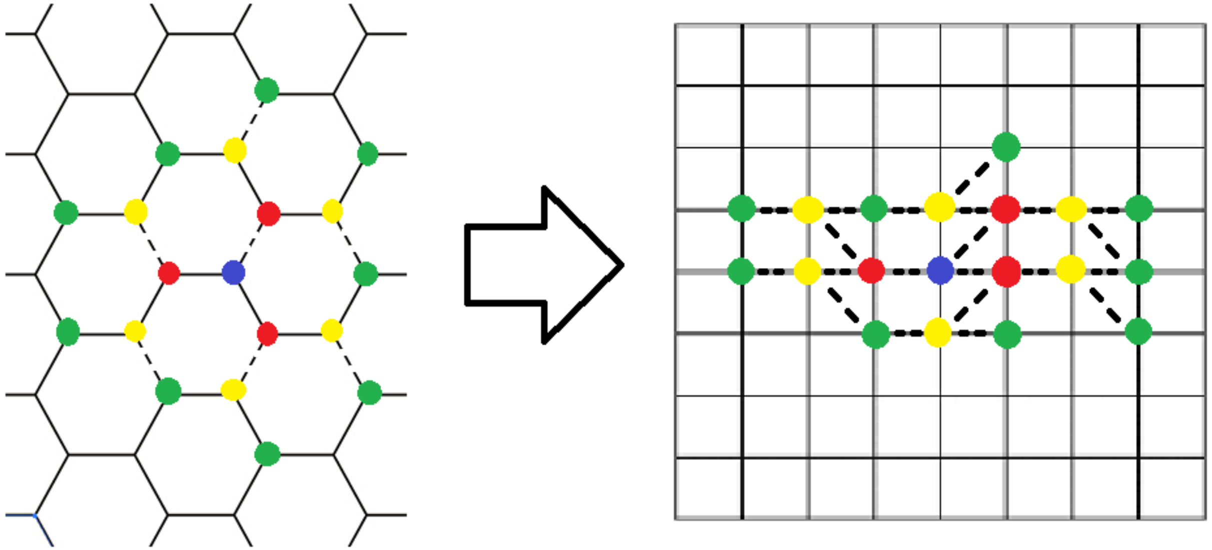
Triangular



Honeycomb

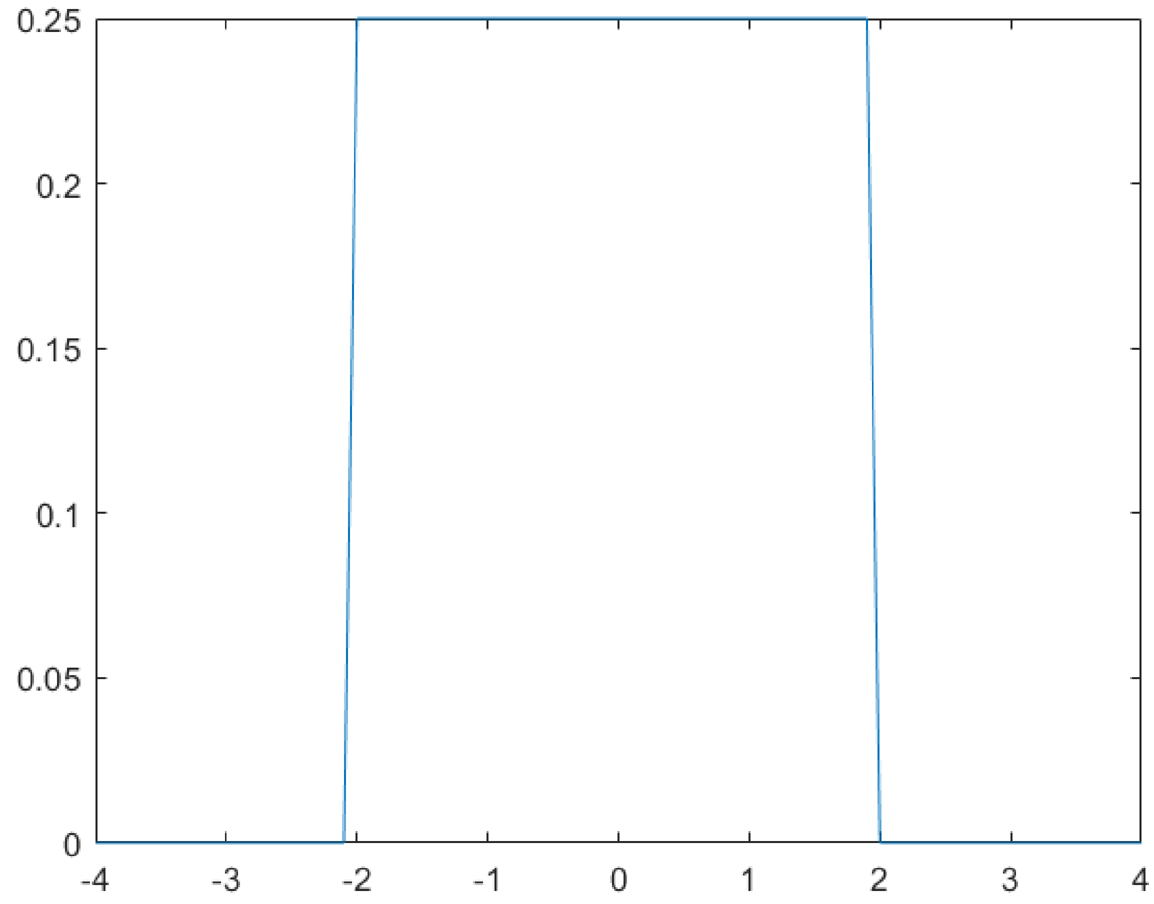
Method – Honeycomb Code

- Honeycomb represented in grid form.
- Dashed lines in grid represent connections
- Grid then transferred to 1D array



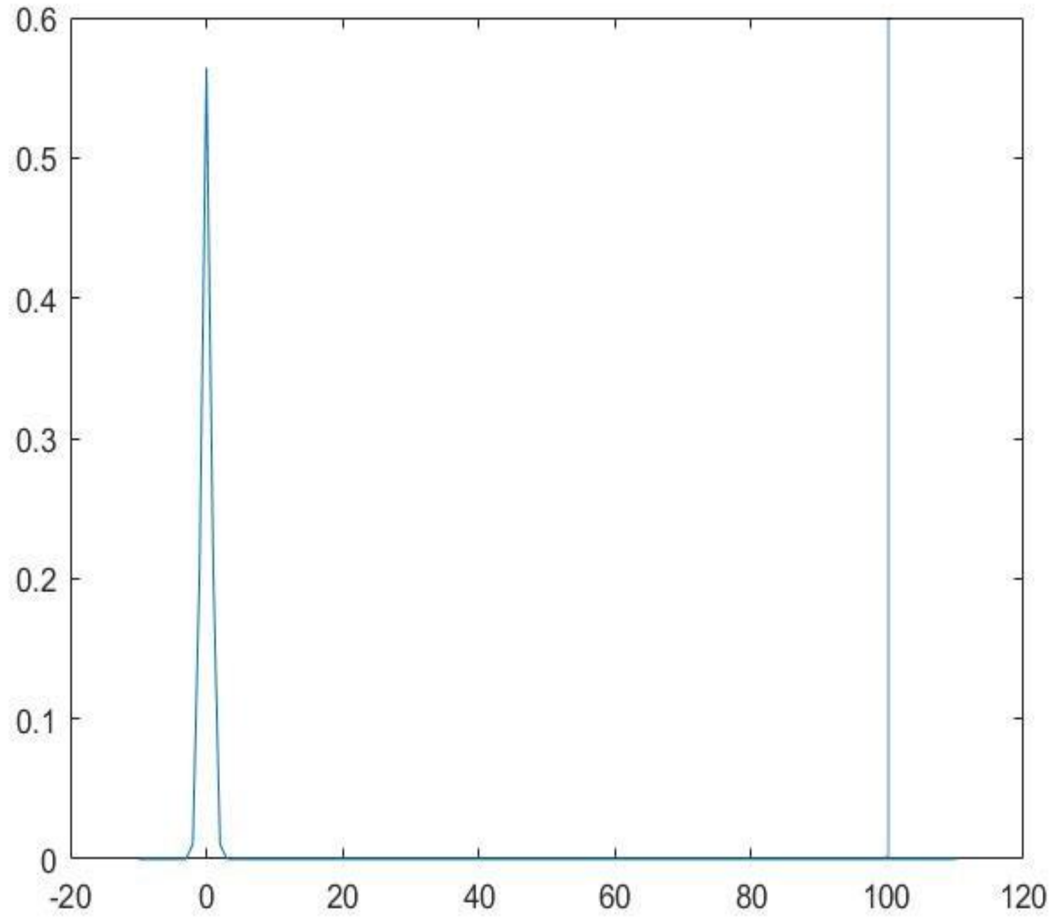
Method – Old Distributions

- The old distribution used was uniform
- Gaussian would be much more realistic



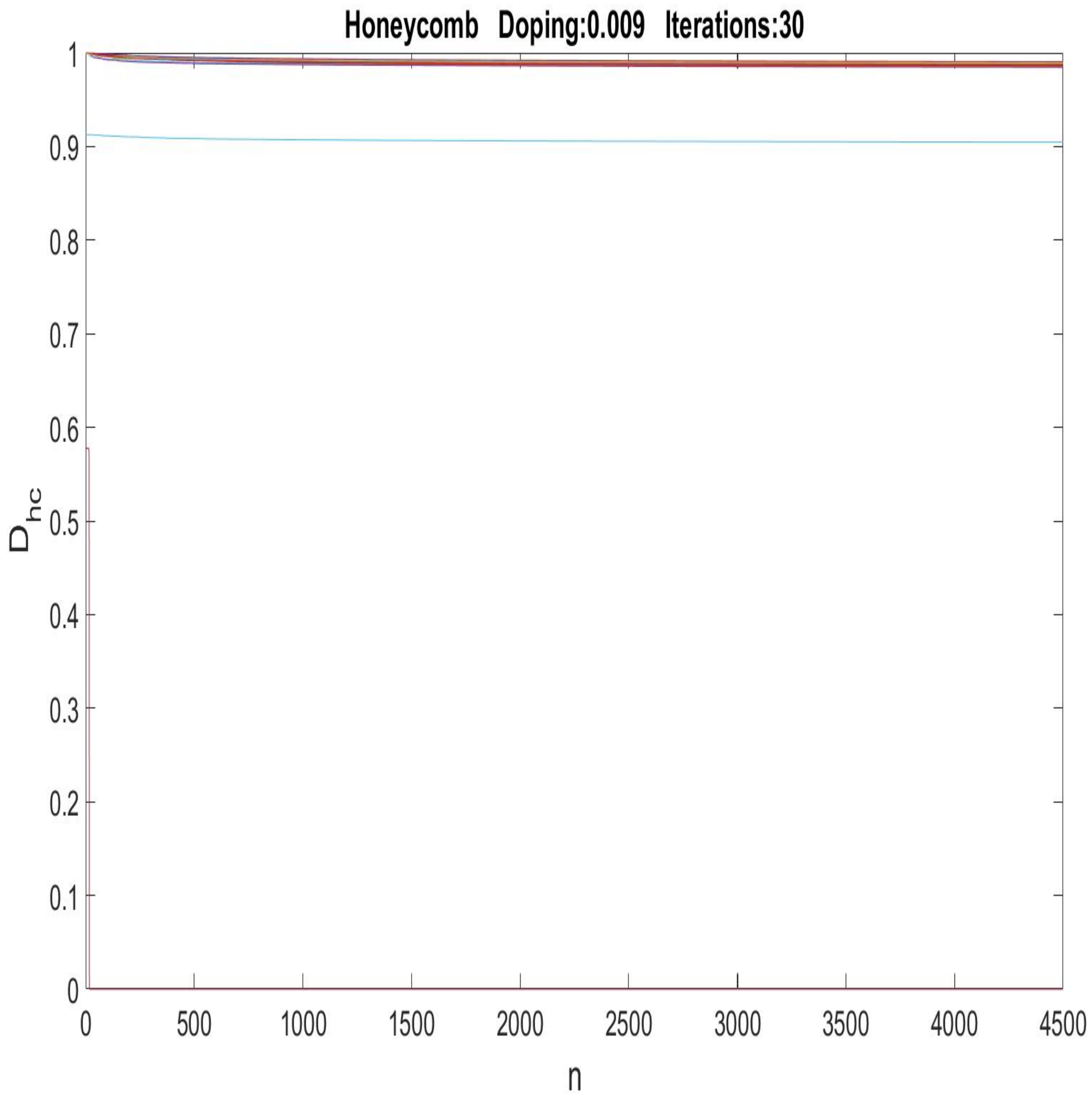
Method – New Distribution

- Gaussian curve representing energy variation
- Delta function representing doped particles
- Doped particles are difficult to jump to



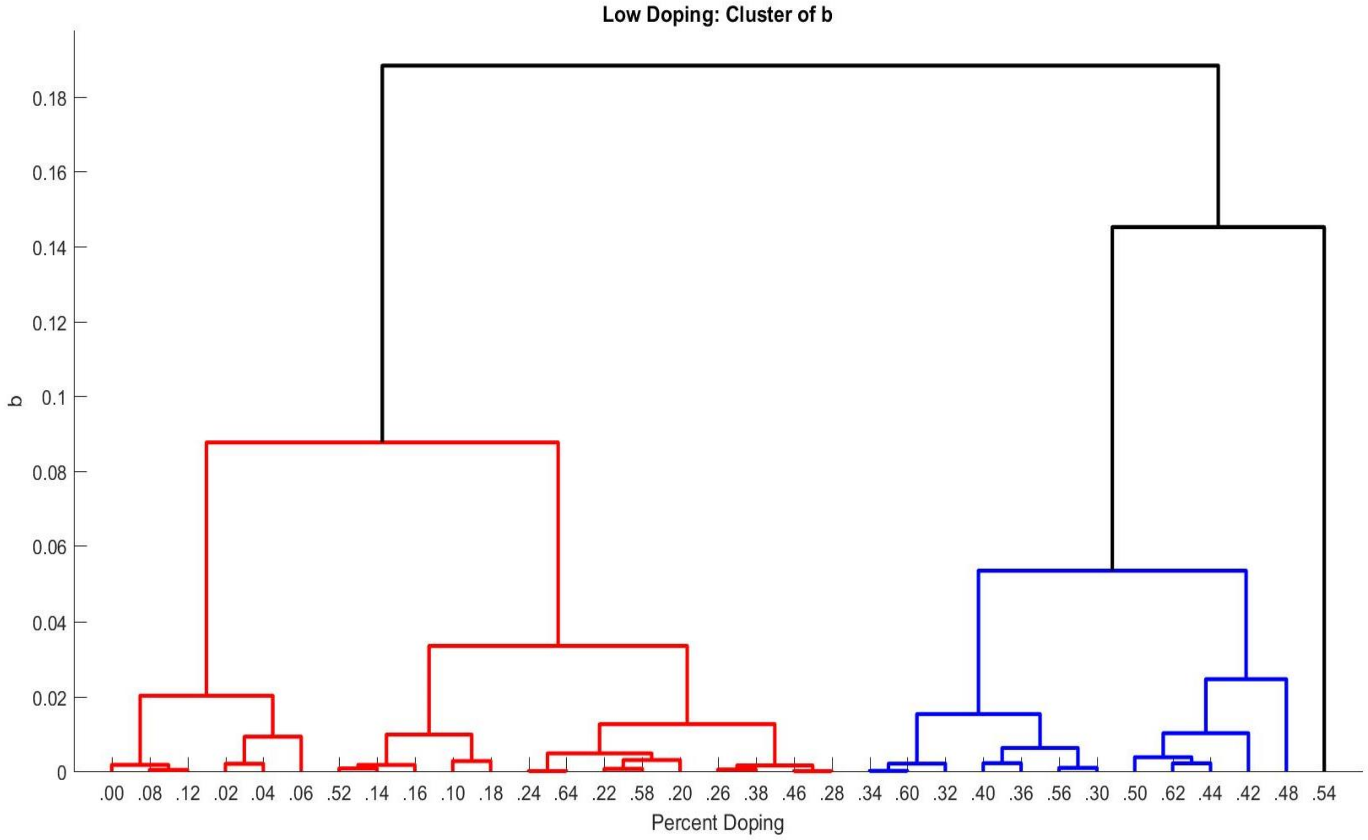
Results – Failures

- Occasional sudden drops
- Some go straight to 0
- Make analysis difficult
- May be caused by classical blocks
- Will require further study



Results – 0.3% Region

- Blue cluster consists only of doping 0.3%+
- Red cluster also contains some
- May be affected by partial failures
- Possibly exciting, but requires another look



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