PHZ 5156 Final project

Random resistor network

We saw in class that hopping in a disordered semiconductor has a rate given by,

\[ \Gamma_{i,j} = \gamma_{i,j} \exp\left(-\frac{2r_{ij}}{a}\right) \exp\left(-\frac{\epsilon_{ij}}{k_B T}\right) \]

This accounts for the overlap of local wave functions of size \( a \), and also the activated hopping (through phonon emission/adsorption) of carriers between sites with energy difference \( \epsilon_{ij} \). This leads to a resistance between sites \( i \) and \( j \),

\[ R_{ij} = R_{ij}^0 \exp(\xi_{ij}) \]

where \( \xi_{ij} = \frac{2r_{ij}}{a} + \frac{\epsilon_{ij}}{k_B T} \) and \( R_{ij}^0 = \frac{k_B T}{\gamma_{i,j}} \). In the random resistor model, we assume that we can treat the problem as a regular network (e.g., a square array) connected by random resistances. Take the distribution \( F(\xi') \) of the values \( \xi \) to given by \( F(\xi') = \frac{1}{2\xi_0} \) for \( |\xi'| < \xi_0 \), and \( F(\xi') = 0 \) for \( |\xi'| > \xi_0 \). Each resistance then is assigned based on the random numbers \( \xi' \) drawn from the range \( -\xi_0 \) to \( \xi_0 \), with \( R = R_0 e^{\xi'} \).

Begin with an \( N \times N \) square lattice of nodes with random resistors connecting each node. You can represent in your code the voltage at each node by an array \( \text{volt}(n) \) which will have dimension \( N^2 - 2N \). We want to determine what happens when we connect opposing ends of the system to a source with potential difference \( V \). To do this, take the top row of nodes to each have potential \( V \), and the bottom row to be at ground (i.e., zero potential). To determine the current, and hence the resistance of the network, we will solve Kirchoff’s current law for each node. In particular, if we consider a node at potential \( V_0 \), with the surrounding four nodes at potentials \( V_1, V_2, V_3, \) and \( V_4 \), with the resistors connecting the nodes \( R_1, R_2, R_3, \) and \( R_4 \), Kirchoff’s current law yields,

\[ \frac{V_1 - V_0}{R_1} + \frac{V_2 - V_0}{R_2} + \frac{V_3 - V_0}{R_3} + \frac{V_4 - V_0}{R_4} = 0 \]

You may use periodic boundary conditions for the direction perpendicular to the applied potential difference.

Because the potential of the top and bottom row of nodes is fixed by the external source, there are \( N^2 - 2N \) unknown potentials to determine for the \( N \times N \) square lattice. Therefore, the problem becomes one of solving \( N^2 - 2N \) coupled linear equation to determine the unknown potentials.
You can index the nodes by row \( i \) and column \( j \). Then, node \( i, j \) is connected to nodes \( i \pm 1, j \) and \( i, j \pm 1 \). You may use periodic boundary conditions for the direction perpendicular to the applied potential difference. To get the number of the resistor, you can use \( k = (i - 1)N + j \). Then the unknown potentials are \( \text{volt}(k) \) with \( k = 1, 2, \ldots, N^2 - 2N \). To solve the system of linear equations, use the \text{ludcmp} and \text{lubksb} subroutines from Numerical Recipes for LU decomposition and forward/backward substitution, as we discussed in class.

We showed in class that we can start by cutting all the connections between the nodes, and then turn on the lowest resistances one at a time. When we have turned on all resistances with \( \xi' < \xi \), then the fraction \( x \) of unbroken connections is given by,

\[
x(\xi) = \int_{-\xi_0}^{\xi} F(\xi')d\xi'
\]

which just gives \( x(\xi) = \frac{\xi_0 + \xi}{2\xi_0} \). Once \( x(\xi) \) becomes large enough to form an infinite percolating cluster, current will be able to flow across the system. For a square lattice in two dimensions, the critical threshold value for percolation is \( x_c = 0.5 \). This corresponds to a critical value \( \xi_c = 0 \). Once we have turned on about 1/2 of the connections in this way, turning on more does little to increase the conductivity. We assume that the resistance of the network is determined by the biggest resistances, so that the conductivity should be

\[
\sigma(\xi_0) = \sigma_0 e^{-\xi_c}
\]

For a two-dimensional square lattice, since \( \xi_c = 0 \), this suggests that the conductivity is independent of the \( \xi_0 \), and hence the range of the resistances. Test this surprising result by computing the conductivity as a function of \( \xi_0 \) from \( \xi_0 = 1 \) to \( \xi_0 = 15 \) for a \( 50 \times 50 \) square lattice of nodes. For each value of \( \xi_0 \), you should determine an average \( \sigma(\xi_0) \) over many (\( \sim 10^4 - 10^6 \)) realizations of the random network. You should find that \( \sigma(\xi_0) \) is independent of \( \xi_0 \). Plot \( \ln(\frac{\sigma(\xi_0)}{\sigma(0)}) \) vs. \( \xi_0 \) and determined the slope. You should find approximately that the slope is zero.