This problem is a simple but very powerful model for impurity states in a semiconductor. As impurities (i.e. dopants) increase in concentration, the can form an impurity band. In principle the impurity band might be metallic, but disorder can result in localized states at the Fermi level and the system is semiconducting. In other words, disorder can result in trapped electrons that only conduct due to thermally-activated hopping processes.

The simplest model is due to Anderson. The Hamiltonian can be represented by a matrix with diagonal elements

\[ \hat{H}_{j,j} = \epsilon_j \]

and off-diagonal elements for neighboring sites

\[ \hat{H}_{j,j+m} = I \]

The sites themselves represent impurity ions. The diagonal elements of \( \hat{H} \) represent the energy of placing an electron on an impurity. The off-diagonal elements that connect neighboring sites represent the overlap between neighboring states and permit electrons to hop from site to site.

The key element of this simple model is that the diagonal site energies \( \epsilon_j \) are chosen randomly with a uniform distribution

\[
P(\epsilon) = \begin{cases} 
\frac{1}{W}, & |\epsilon| \leq W/2 \\
0, & |\epsilon| > W/2 
\end{cases}
\]

This random disorder will tend to localize the electrons. Electrons want to sit in low-energy sites, but they spread out somewhat because they can lower their energy by spending some time at neighboring sites due to the hopping energy \( I \).

The critical parameter in the Anderson model is the dimensionless ratio \( \frac{W}{I} \). For large \( \frac{W}{I} \), all states become localized. At some critical value \( \frac{W}{I} \) states are believed to become delocalized. Because everything is controlled by \( \frac{W}{I} \), we will take \( I = 1 \) and just vary \( W \) in our simulation.

The localization can be studied using the participation \( p_\lambda \) ratio defined as

\[
p_\lambda^{-1} = \sum_{i=1,N} (c_{i,\lambda}^* c_{i,\lambda})^2
\]
where $\lambda$ labels the eigenstates, $c_{i,\lambda}$ are the expansion coefficients of the wave-function in the tight-binding basis states $\phi_i(\vec{r})$, and $N$ is the total number of impurity sites. Each wave function then takes the form

$$\phi(\vec{r}) = \sum_{i=1,N} c_{i,\lambda} \phi_i(\vec{r})$$

Notice that we never explicitly define the basis states $\phi_i(\vec{r})$, but we can assume they are just localized orbitals centered on site $i$.

1. Code in the Anderson model calculation. Use standard library routines for matrix diagonalization to obtain the eigenvalues and eigenvectors for a system with $N$ sites

$$\sum_{j=1}^{N} H_{ij} c_{j,\lambda} = E_{\lambda} c_{i,\lambda}$$

The system will be finite size, but you can apply periodic boundary conditions to approximate an infinite system (i.e. one without surfaces or edges). Use the standard random number generator to generate a random distribution of site energies $\epsilon_j$.

2. For a three-dimensional system, the critical localization threshold has been computed to be about $W_c = 15$. Study the system on either side of this localization threshold. Again consider an ensemble of systems by performing the diagonalization for different realizations of the disorder. Compute the participation ratios to try and identify the edges between the localized and delocalized states (this might be rather hard but we should get some idea). Since the threshold is only clearly defined in an infinite system, we will look at how the participation ratio depends on system size by analyzing lattices with dimensions $8 \times 8 \times 8$, $9 \times 9 \times 9$, and $10 \times 10 \times 10$. In general, if the participation ratio is decreasing as system size increases, the states are localized. Plot out the participation ratio vs. energy and also the density of states, each averaged over a large ensemble of systems.