

# Physics 5403: Computational Physics – Project 4a

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due date: Oct 4, 2022

## Anderson model of localization

The electronic states in a periodic crystal are extended in space because of Bloch's theorem. In the presence of randomness, the theorem does not hold anymore, and the wavefunctions can localize, a phenomenon called Anderson localization. A prototypical model to study localization is the Anderson model, defined by the Hamiltonian

$$H = \sum_{i=1}^N \epsilon_i |i\rangle\langle i| - t \sum_{i=1}^N (|i\rangle\langle i+1| + |i+1\rangle\langle i|) .$$

Here  $|i\rangle$  represents an orbital on lattice site  $i$ . The first term in  $H$  is a random potential with  $\epsilon_i$  being a random number drawn from a probability distribution

$$P(\epsilon) = \begin{cases} 1/(2W) & \text{for } -W < \epsilon < W \\ 0 & \text{otherwise} \end{cases} .$$

The second term describes the particle hopping from one site to its neighbor.

In this project, you will explore the quantum eigenstates of the Anderson model of localization by turning it into a matrix eigenvalue problem and solving it using an eigenproblem solver.

- Write a program which does the following: Set up the Hamiltonian matrix for the above problem (treating the number  $N$  of sites as a parameter). Think about the boundary conditions. How do you want to treat the first and last sites? Solve the resulting matrix eigenvalue problem. Output all eigenvalues and selected eigenvectors (in the band tails and in the band center).
- Perform the simulation for  $t = 1$ , and  $W = 0$ . What would be a good value for the number of site,  $N$ ? For  $W = 0$ , the Hamiltonian is solvable analytically. Compare your numerical eigenvalues and eigenstates to the exact solution. Plot a few eigenstates.
- Repeat the simulation for different disorder strengths,  $W = 0.25, 0.5, 1, 2, 4$ . Describe the eigenstates both in the band tail and in the band center. Does their character change; if so, how? Plot a few characteristic states.
- The degree of localization of a normalized eigenstate  $|\psi\rangle = \sum_{i=1}^N a_i |i\rangle$  can be characterized by the so-called inverse participation number

$$R^{-1} = \sum_{i=1}^N |a_i|^4 .$$

Why is this a good measure of localization? Think about the extreme cases of a state being complete localized on a single site, or a state equally distributed on  $N$  sites. What does  $R$  measure?

Calculate  $R$  for states exactly in the band center for the different disorder strengths suggested above. Also calculate  $R$  for one disorder strength (e.g.,  $W = 1$ ) as function of the eigenenergy.