Solid State Physics
Electron Localization

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Non-interacting electrons in periodic potentials form eigenstates in bands, because of the conservation of crystal momentum k. In disordered materials (e.g., silicon doped with phosphorous) the random potential energy makes crystal momentum no longer a good quantum number. What happens to the extended plane–wave eigenstates as the disorder is turned on?

Conversely, suppose we start from the other limit: independent atomic orbitals, each with their own energy E_i. The eigenstates in this limit are localized on individual atoms. As we turn on a hopping t between atoms (as in a tight–binding model), how do the localized states mix and spread out?

We can answer both of these questions in the context of a one–dimensional model. Let the eigenstate localized on site n be denoted $|n\rangle$. The Hamiltonian for a one–dimensional chain of atoms is

$$H = \sum_{n=1}^{N} E_n |n\rangle\langle n| - t|n\rangle\langle n-1| - t|n\rangle\langle n+1|.$$

In matrix form,

$$H = \begin{pmatrix} E_1 & -t & 0 & \dots & 0 \\ -t & E_2 & -t & \dots & 0 \\ 0 & -t & E_3 & \dots & 0 \\ 0 & 0 & -t & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & E_N \end{pmatrix}.$$

(a) Write a routine which generates this matrix and solves for the eigenvalues and eigenvectors. Pick the eigenvalues E_n with a uniform distribution between $-W$ and W, using the Numerical Recipes routines ran2 and scaling the result, or using Random[ ] in Mathematica. The Hamiltonian is tridiagonal; use the routine tqli to find the eigenvalues and eigenvectors, or use Eigensystem. Since only the ratio W/t matters, let $t = 1$. Starting with $N = 50$ and $W = 0$, plot a few eigenstates and show that they are plane waves. With $W = 10$, show by plotting that the eigenstates are nearly localized on individual sites. Plot a few eigenstates for $W = 2$. They should fall off exponentially from their peak value at n_0: $\psi(n) \sim e^{-\lambda|n-n_0|}$. Estimate λ for a few energies by plotting with semi-logarithmic axes.

(b) Using a histogram, plot the density of states for $W = 0, 2$, and 10. (PLOT has a histogram option; using Mathematica, we will provide one.) Briefly discuss the form for small and large W. Can you see why the spectrum extends from $-W - 2t$ to $W + 2t$?

(c) We can estimate the spreading of the eigenstate ψ by using the participation ratio:

$$P(\psi) = \frac{(\sum_n |\psi(n)|^2)^2}{\sum_n |\psi(n)|^4}.$$

Show that a state extended uniformly over M sites has $P = M$. If all of our eigenstates have $P << N$, we can reasonably expect that they are all localized. For $W = 2$, calculate the participation ratio for the eigenstates, and plot it as a function of their energy. You may want to reduce the scatter in the plot by averaging over small ranges in energy (as in the histogram). Is there a systematic dependence of the localization length on energy? Are any of the eigenstates extended?

It has been proven for this model that all states are localized for any non-zero disorder W. In two dimensions, all states are also disordered (but just barely); in three dimensions, the states in the center of the band (near $E = 0$) can be extended. The study of the *mobility edge* separating the localized and extended states in three dimensions has been one of the exciting research topics of the last decade.