Tight-binding models

Hamiltonian I: Hydrogen chain

Plot the band structure E(k) vs. k sites with the expected theoretical result E(k)=-2 cos(k) plotted on top of it for comparison and the Fermi energy indicated with a horizontal line.

Hamiltonian II: Distorted hydrogen chain

Plot the band structure (E(k) vs. k) for the two bands. Indicate the Fermi energy with a horizontal line.

Hamiltonian III: graphene

Plot E(k_x, k_y) vs. k_x, k_y on a 27 x 27 lattice for the E>0 and E<0 bands. Make a 3d plot or and a 2d plot that includes a point where the two bands touch at E=0.

Hamiltonian IV: Boron nitride

Plot E(k_x, k_y) vs. k_x, k_y on a 27 x 27 lattice for the E>0 and E<0 bands. Make a 3d plot or many 2d plots (or both).

Hamiltonian V: Haldane honeycomb model

For t'=0.3, theta=0.7, M=0.1, plot E(k_x, k_y) vs. k_x, k_y on a 27 x 27 lattice for the E>0 and E<0 bands. Make a 3d plot or many 2d plots (or both).

Two forms of insulators

For Hamiltonian V, plot the minimum gap between the two bands as you tune M from M=0 to M=2. Do M=0, 0.8, 1.0, 1.2, 2.0. There is a transition when the gap becomes zero. At what M does this happen?

Make contour plots of the berry curvature vs. (k_x,k_y) for M=0.8 and M=1.2.

M=0.8	M=1.2

Plot the Chern number vs. M. You should see it transition between 0 and 2 at the same M that the gap became zero.

Make Hamiltonian V be periodic in the x-direction, but open in the y-direction. Plot E(k_x, y) versus k_x for each y on the same diagram. Make this plot with M=0.2 **(left)** and M=2.0 **(right)**. You should see zero-energy edges modes at M=0.2 and not at M=2.0

M=0.2	M=2.0