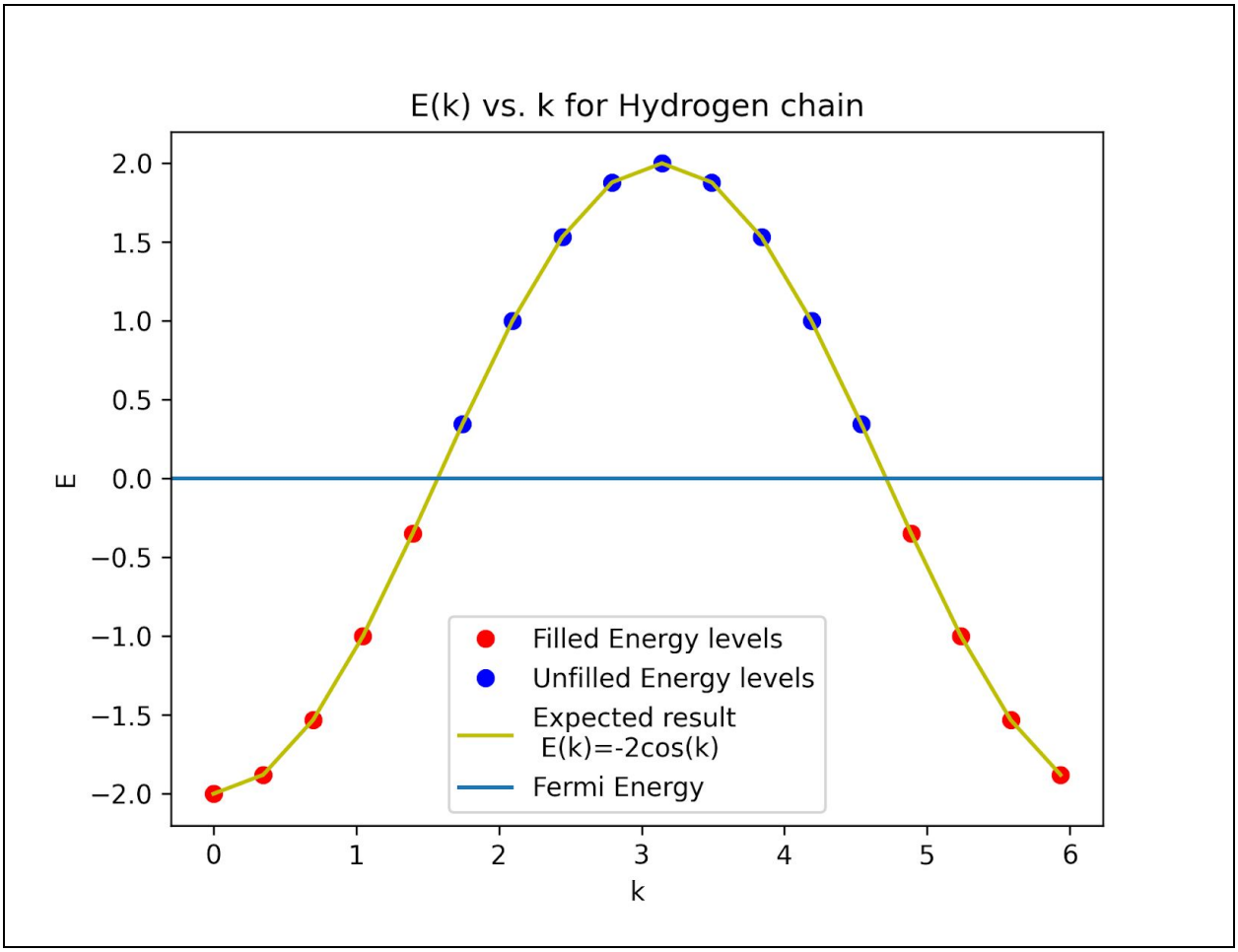
Tight-binding models

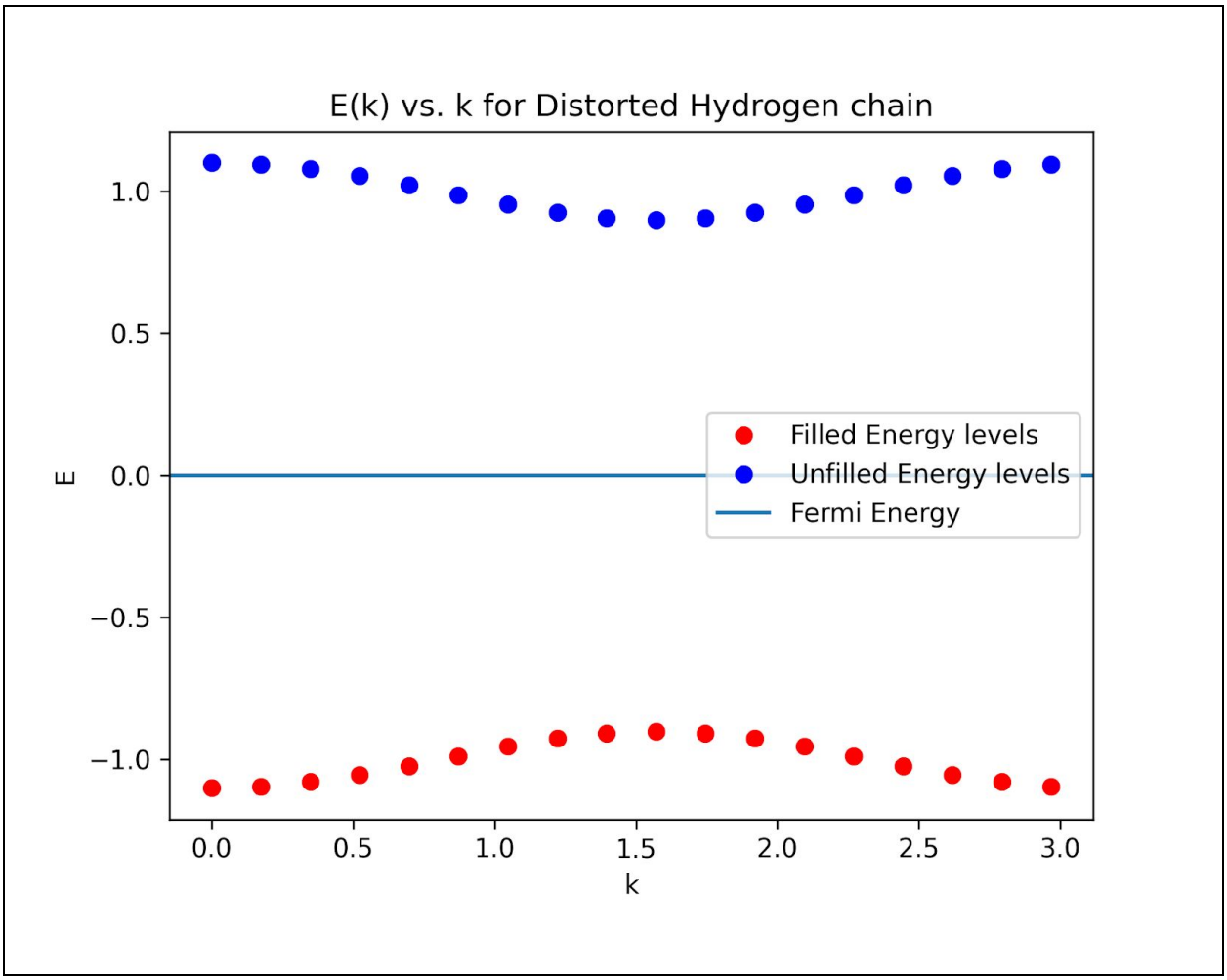
Hamiltonian I: Hydrogen chain

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.



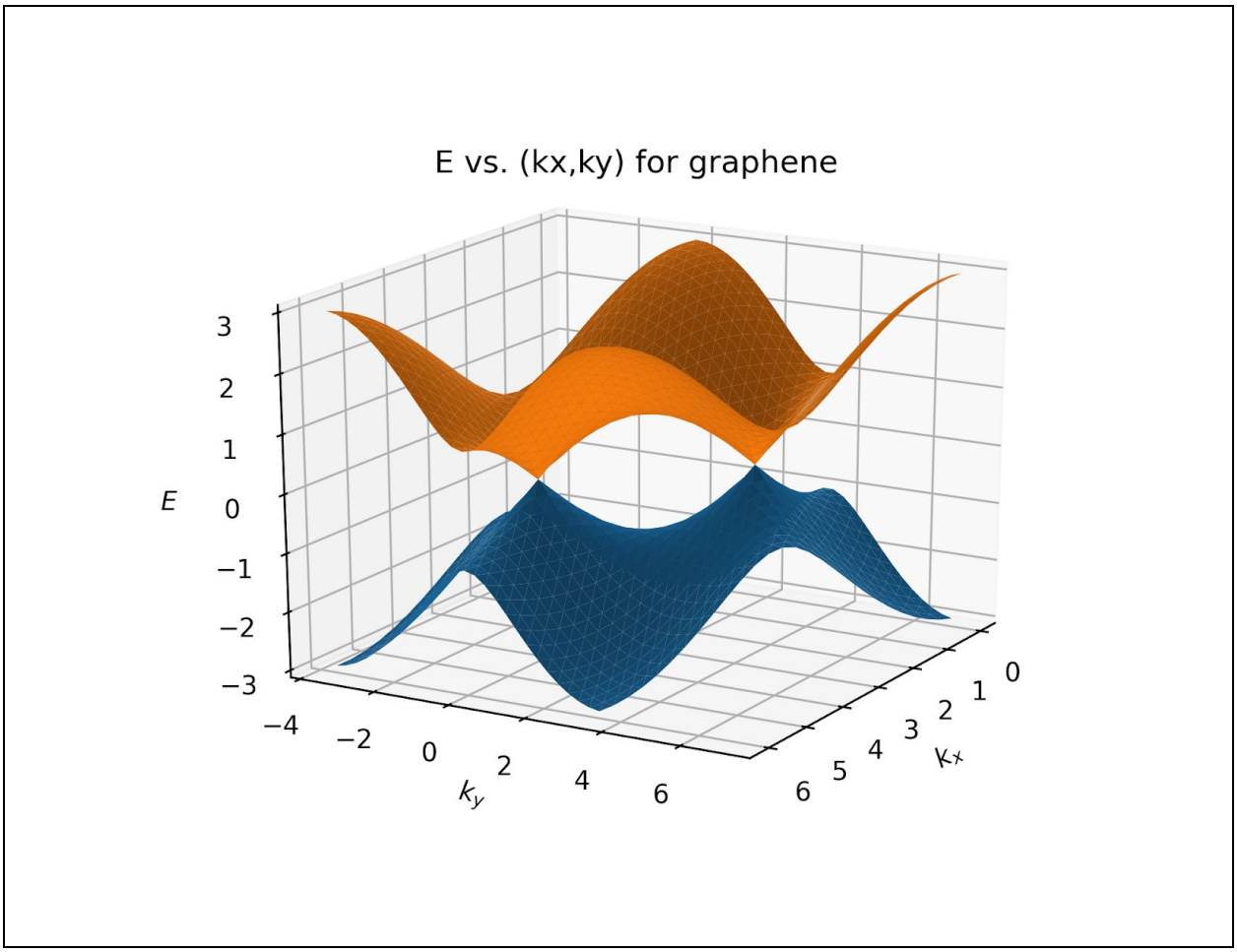
Hamiltonian II: Distorted hydrogen chain

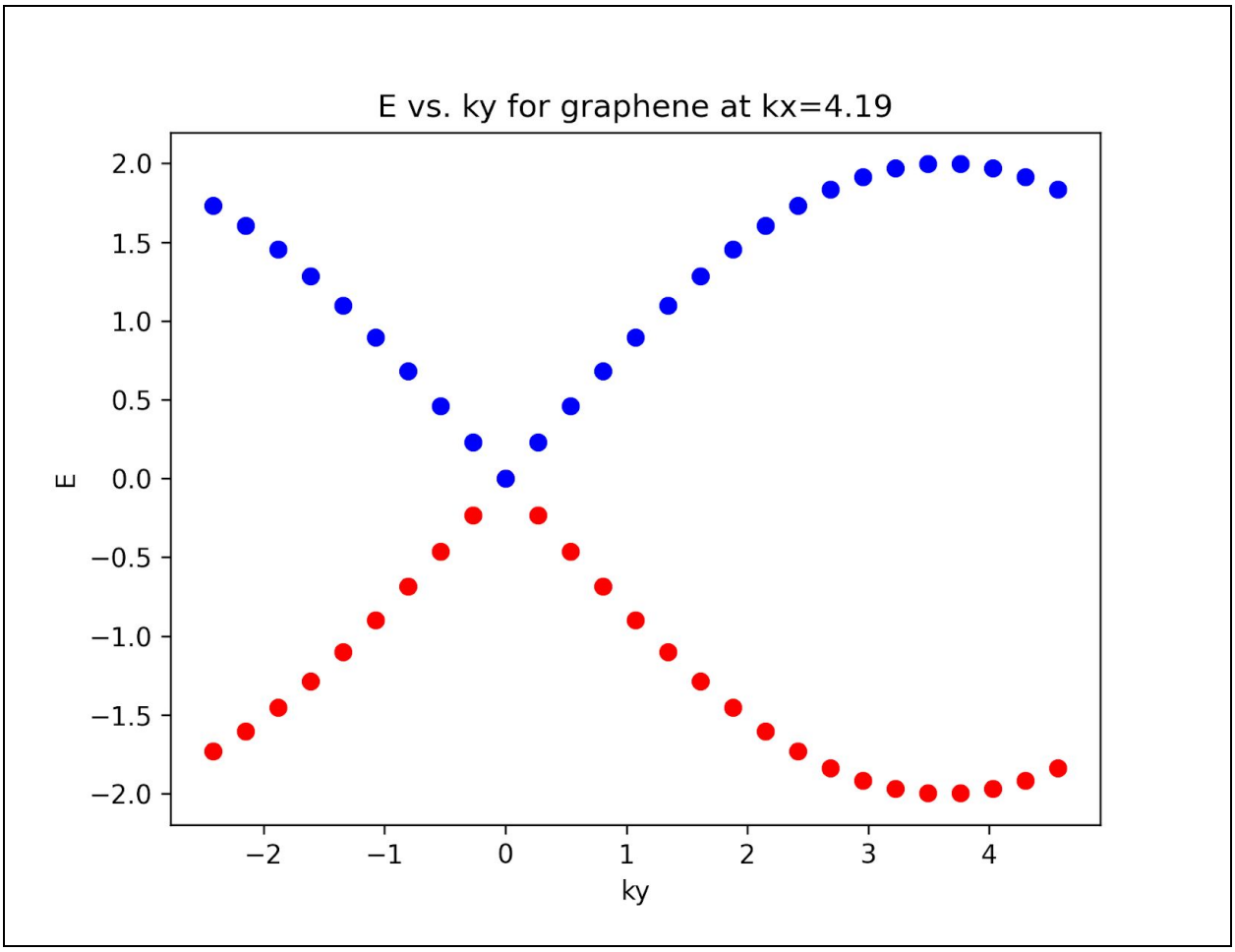
Plot the band structure (E(k) vs. k) for the two bands. Indicate the Fermi energy with a horizontal line.

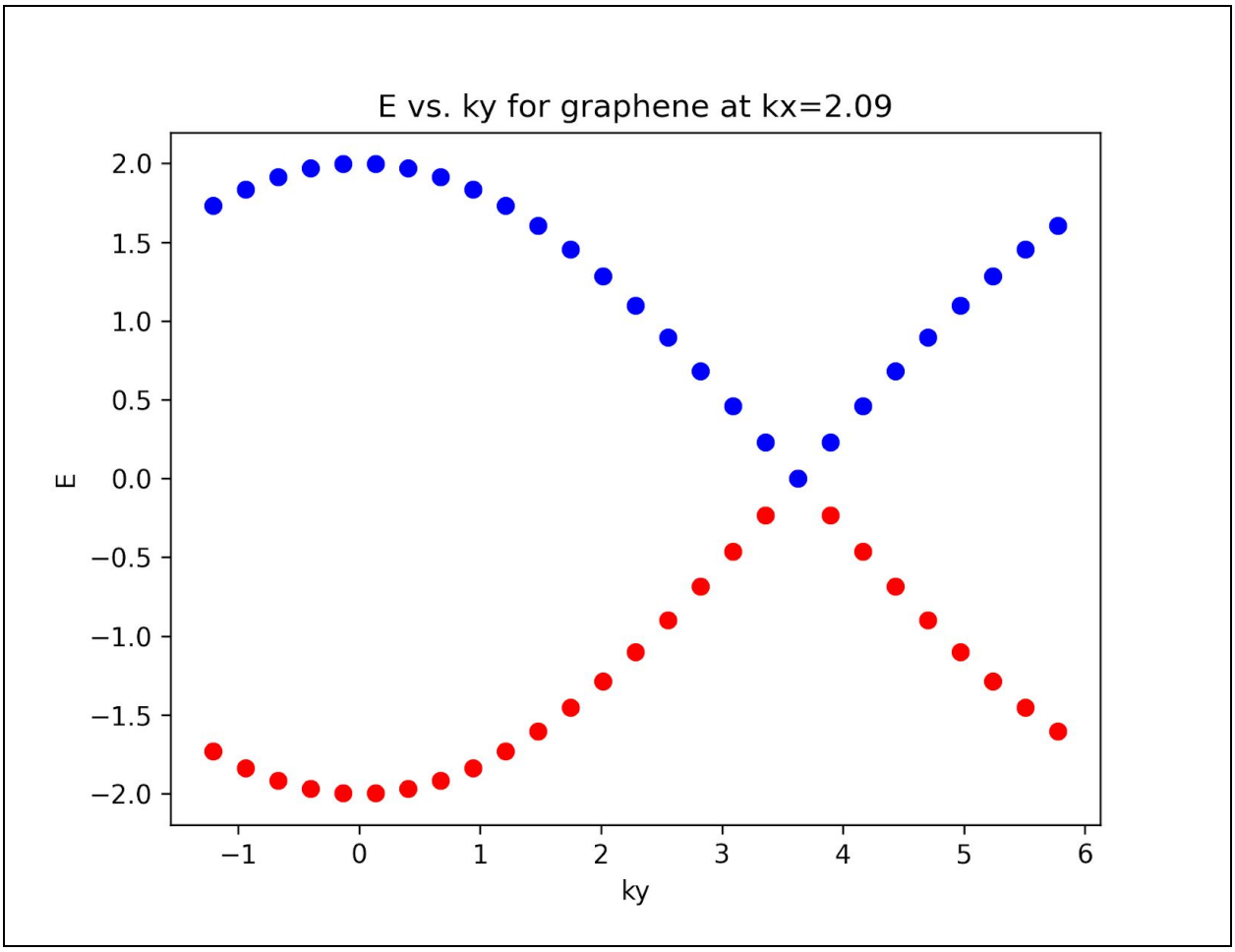


Hamiltonian III: graphene

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.

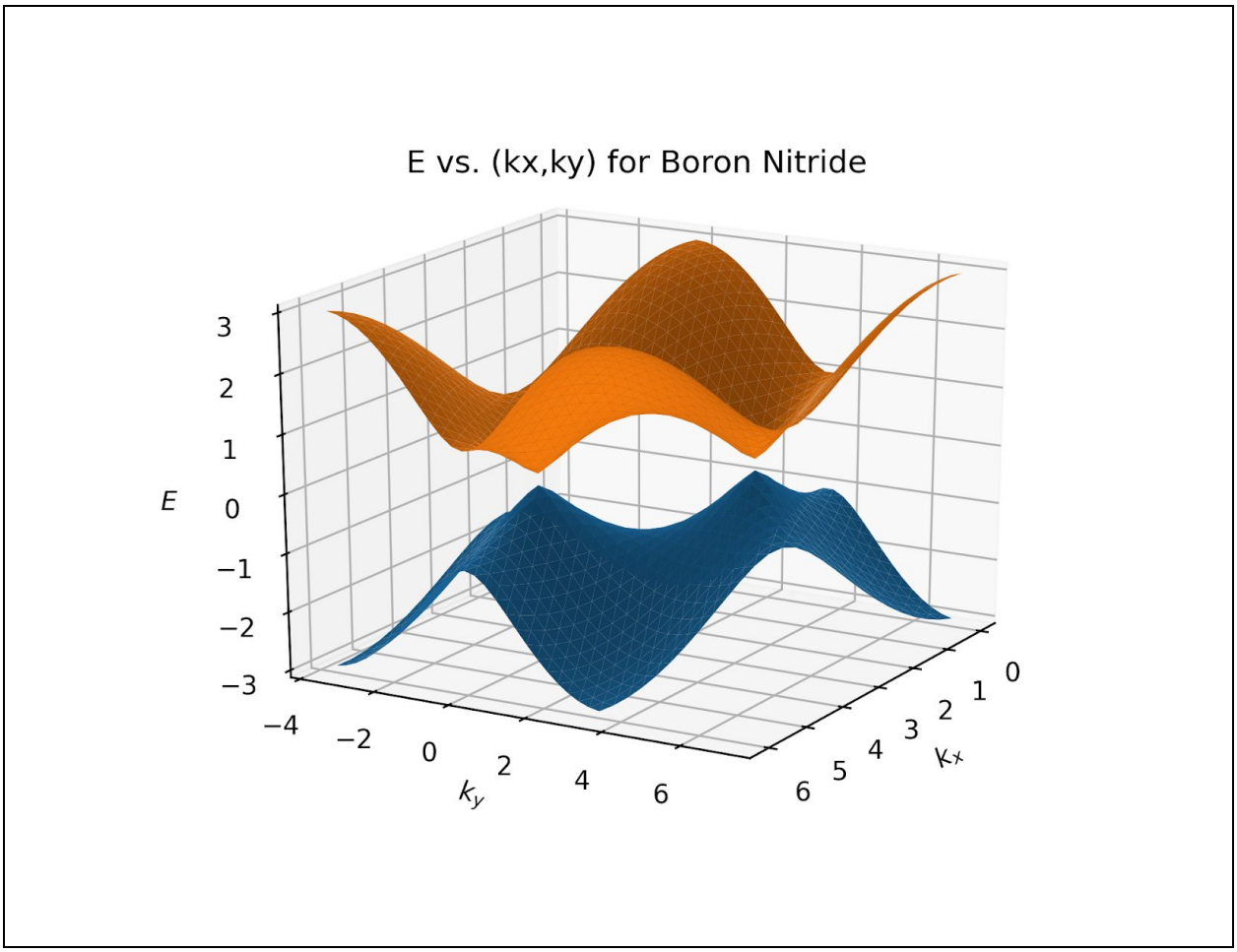

E vs. (kx,ky) for graphene
E
3
2
1
0
−1
−2
−3
−4
−2
0
2
4
6
k_y
0
1
2
3
4
5
6
kx

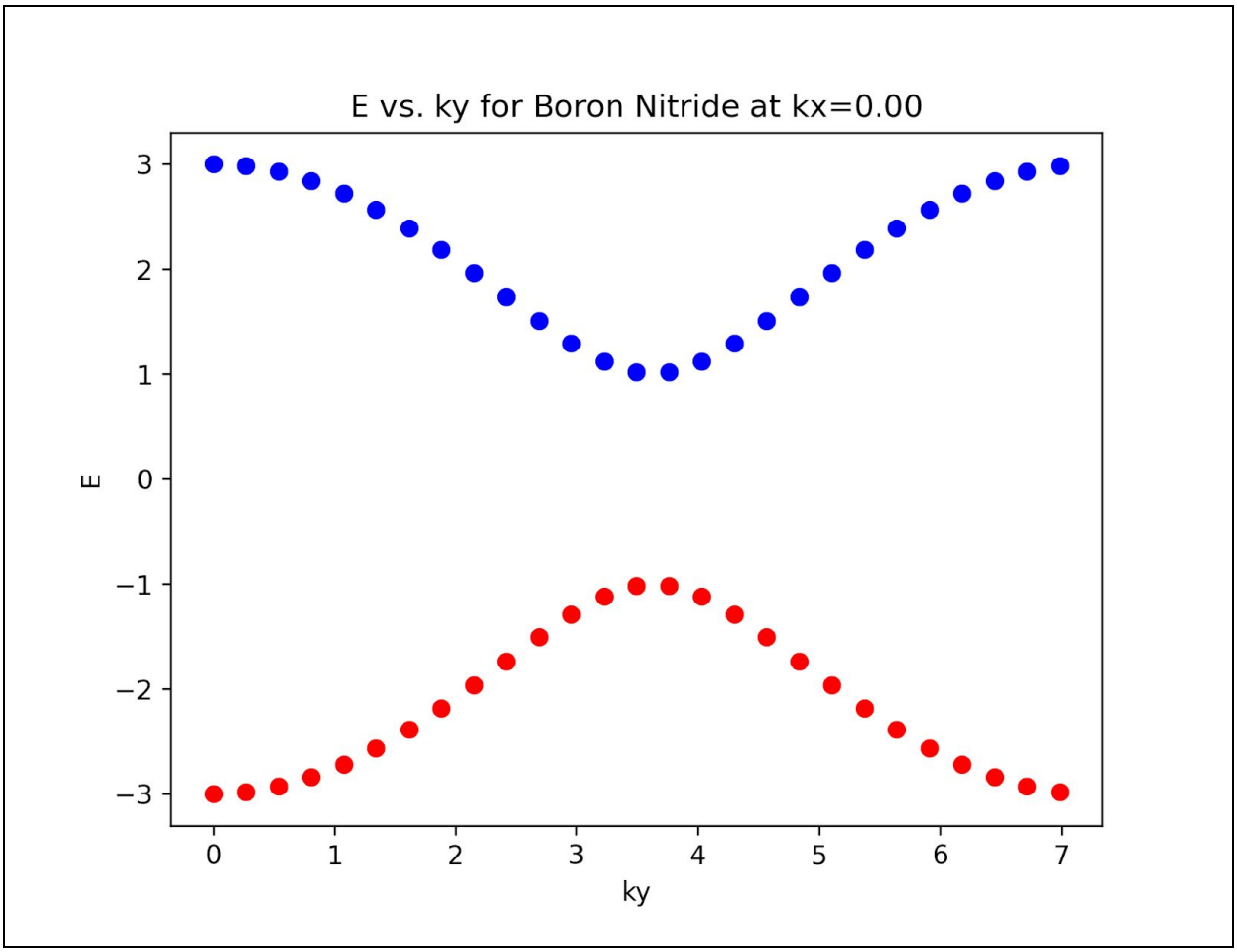

E vs. ky for graphene at kx=4.19
E
ky
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2
−1
0
1
2
3
4

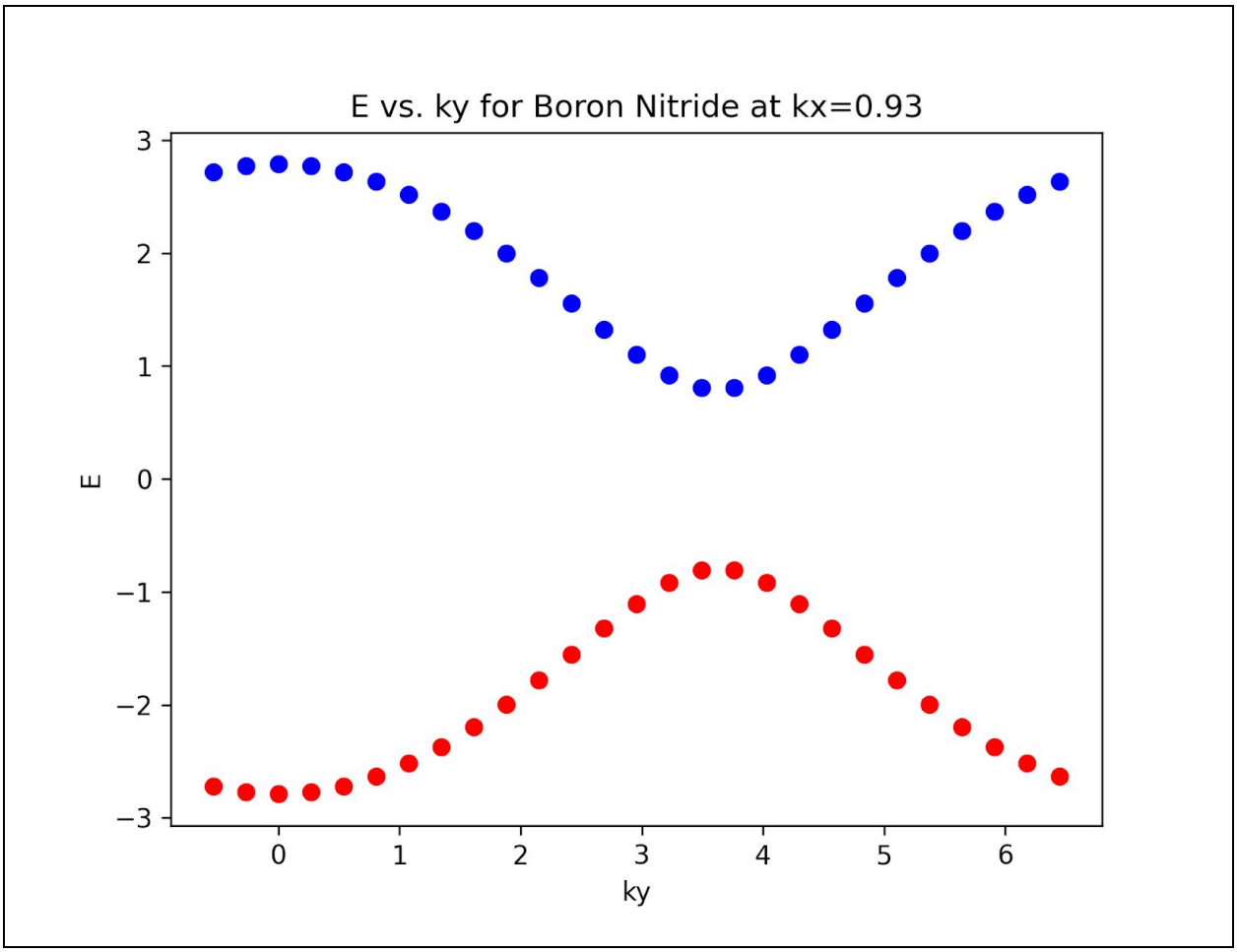


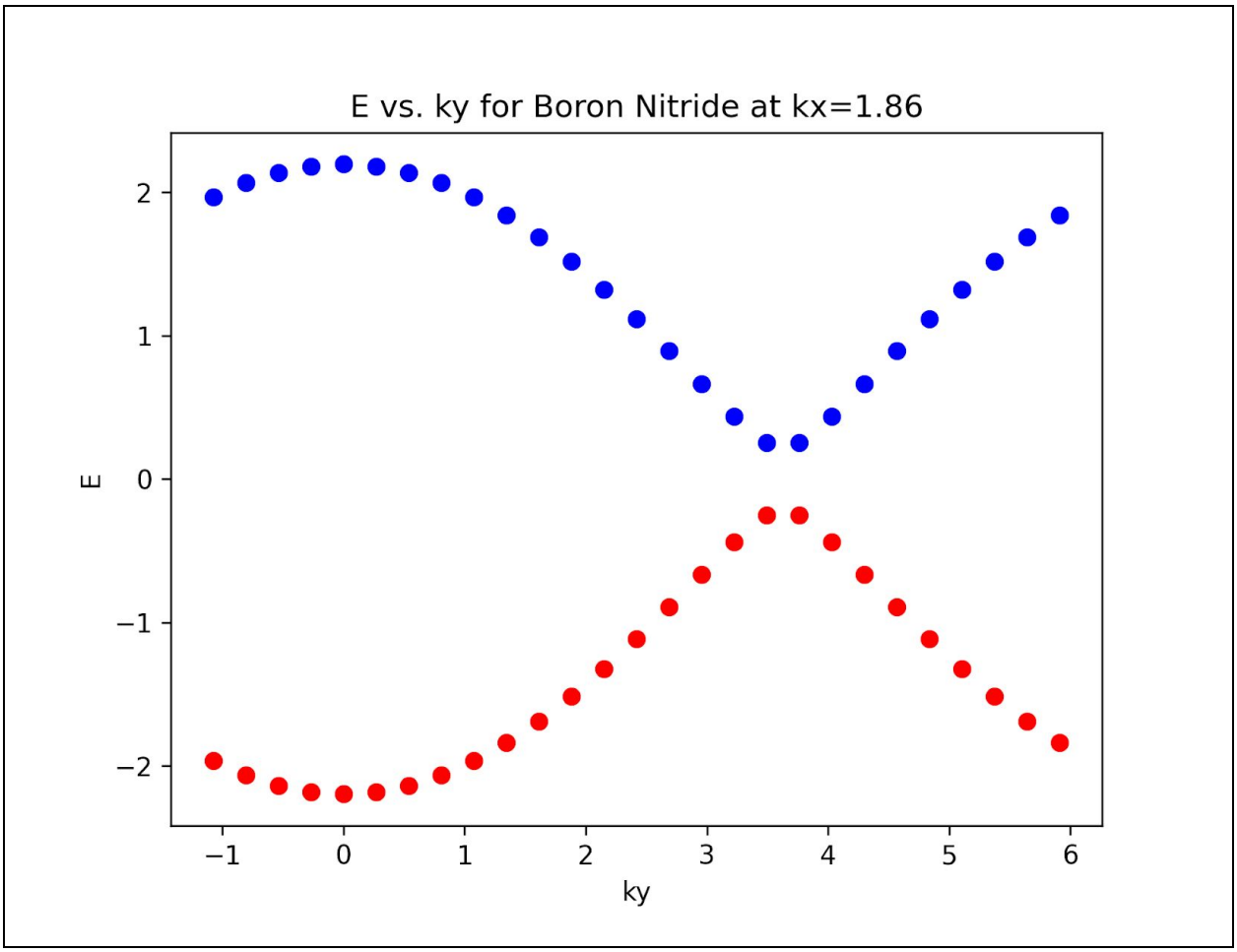
Hamiltonian IV: Boron nitride

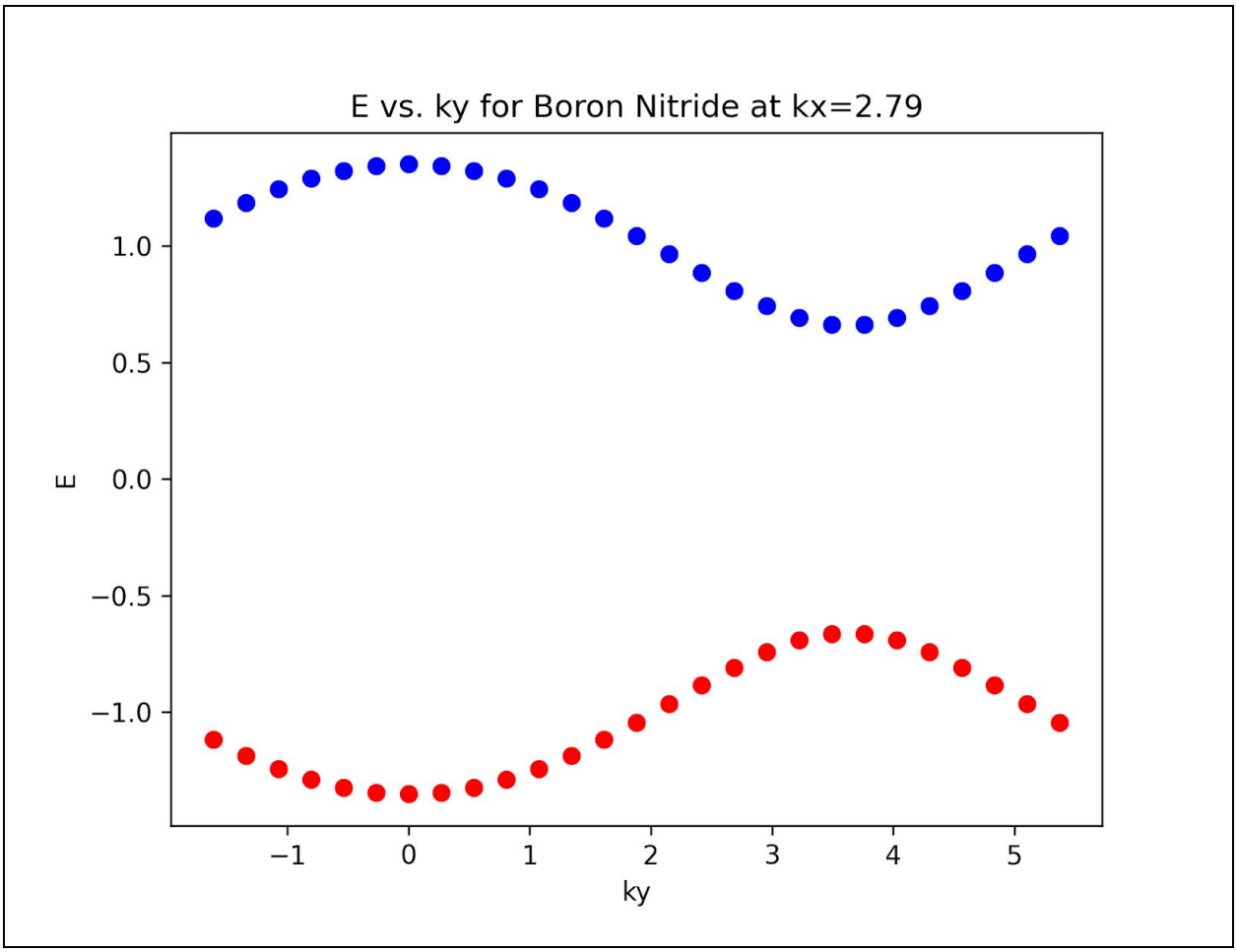
Plot E(k_x, k_y) vs. k_x, k_y on a 27 x 27 lattice for the E>0 and E<0 bands. Make a 3d plot or many 2d plots (or both).

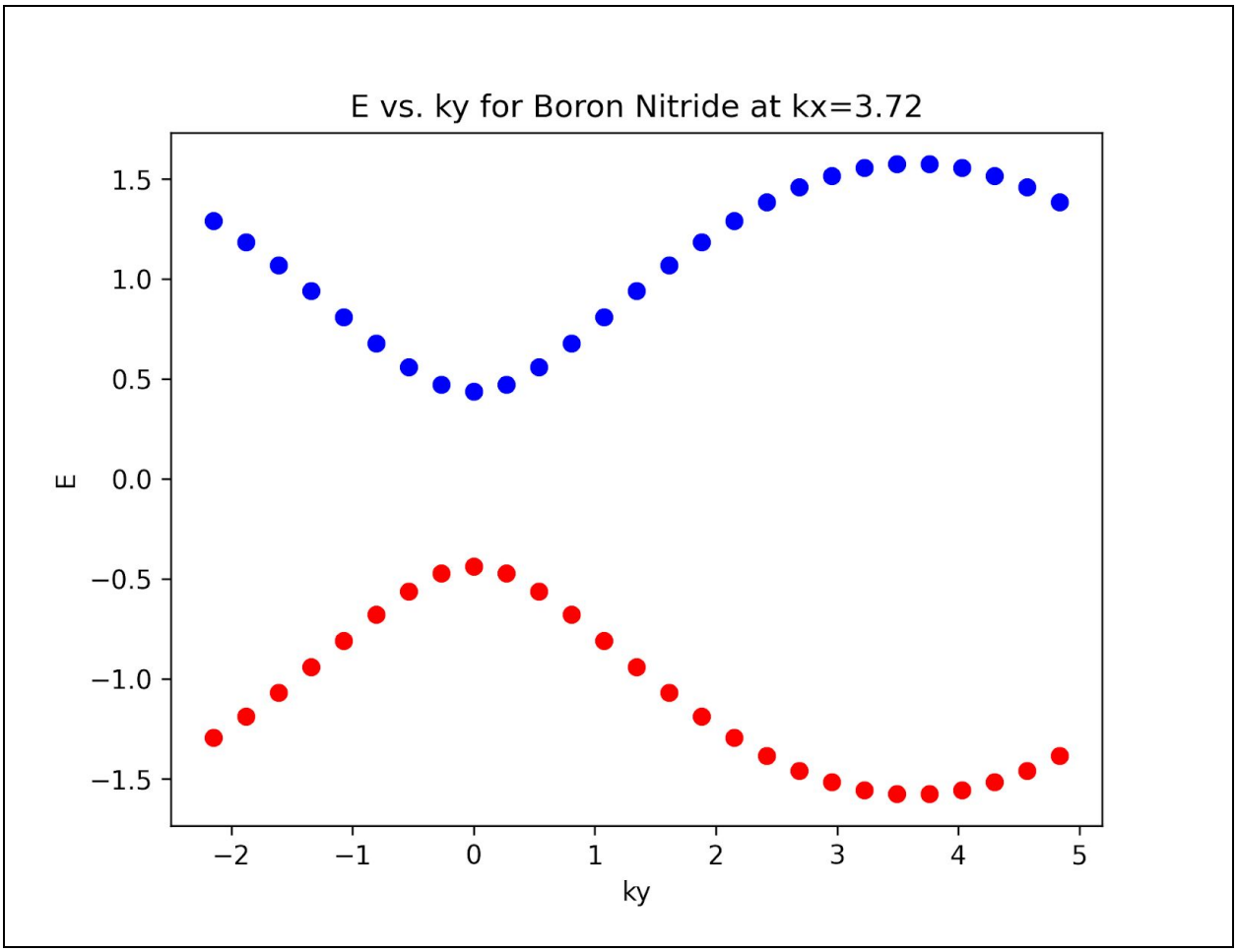

E vs. (kx,ky) for Boron Nitride
E
3
2
1
0
−1
−2
−3
−4
−2
0
2
4
6
k_y
0
1
2
3
4
5
6
k_x

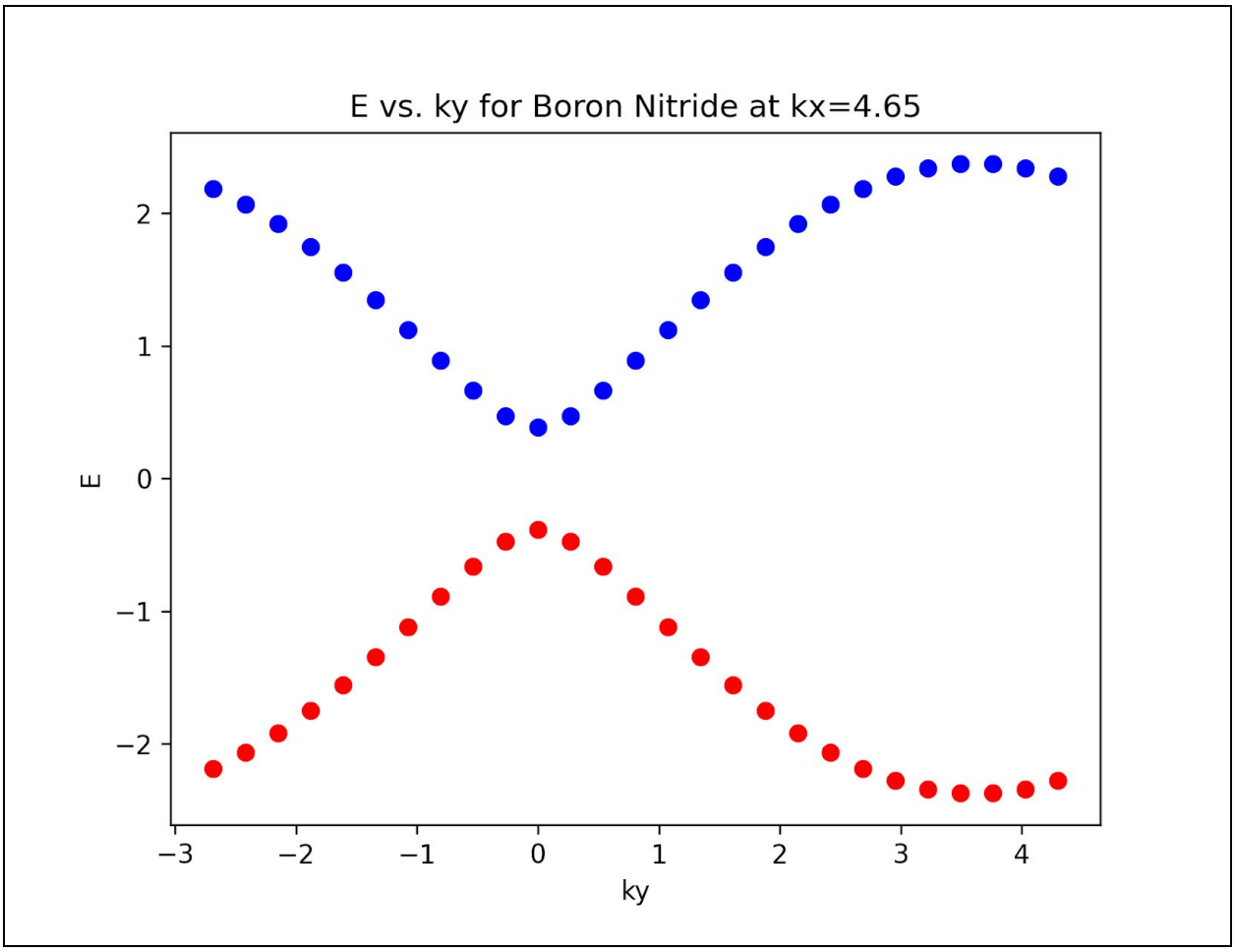

E vs. ky for Boron Nitride at kx=0.00
E
ky
3
2
1
0
−1
−2
−3
0
1
2
3
4
5
6
7

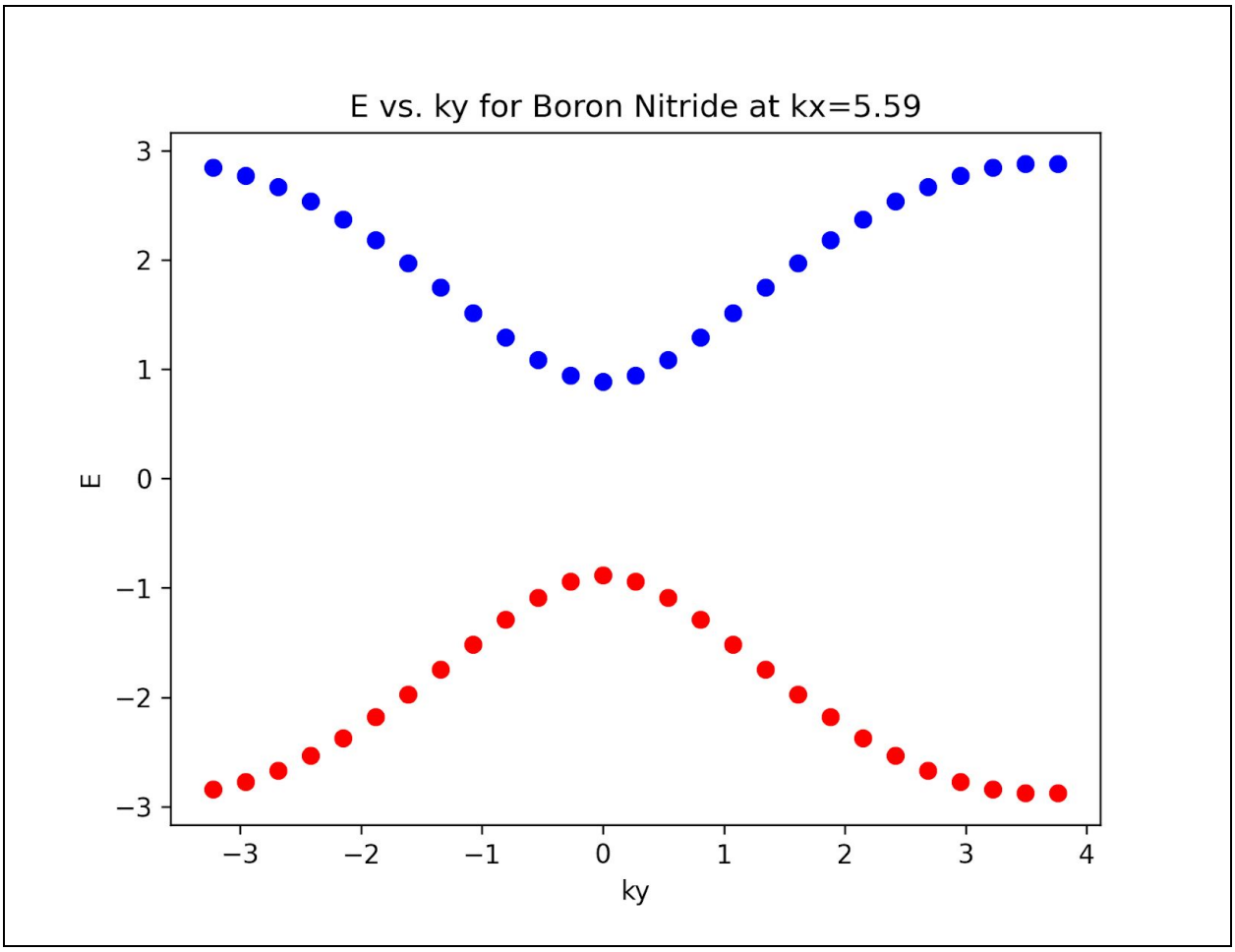

E vs. ky for Boron Nitride at kx=0.93
E
ky
3
2
1
0
−1
−2
−3
0
1
2
3
4
5
6


E vs. ky for Boron Nitride at kx=1.86
E
ky
2
1
0
−1
−2
−1
0
1
2
3
4
5
6


E vs. ky for Boron Nitride at kx=2.79
1.0
0.5
0.0
−0.5
−1.0
E
−1
0
1
2
3
4
5
ky

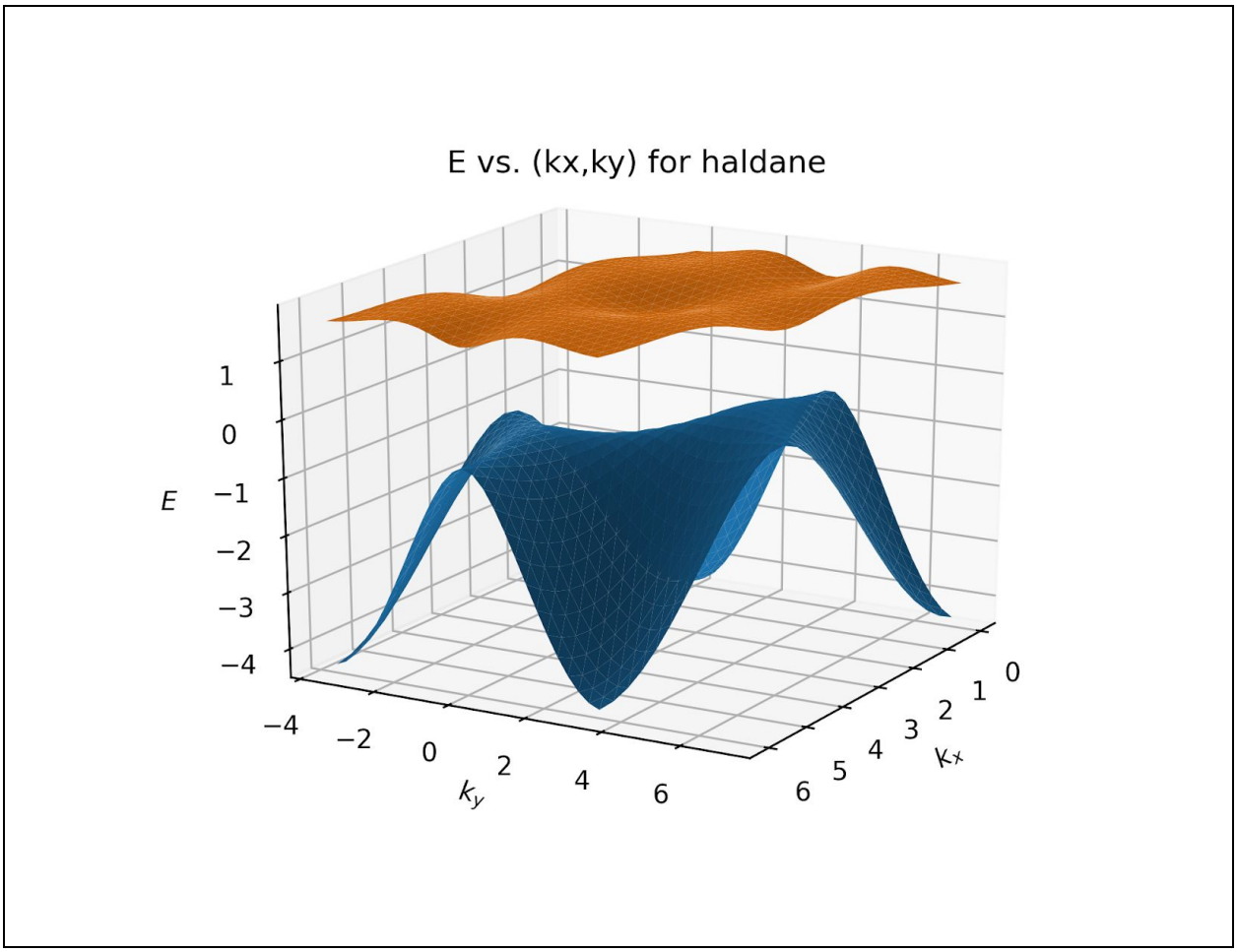

E vs. ky for Boron Nitride at kx=3.72
E
ky
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2
−1
0
1
2
3
4
5

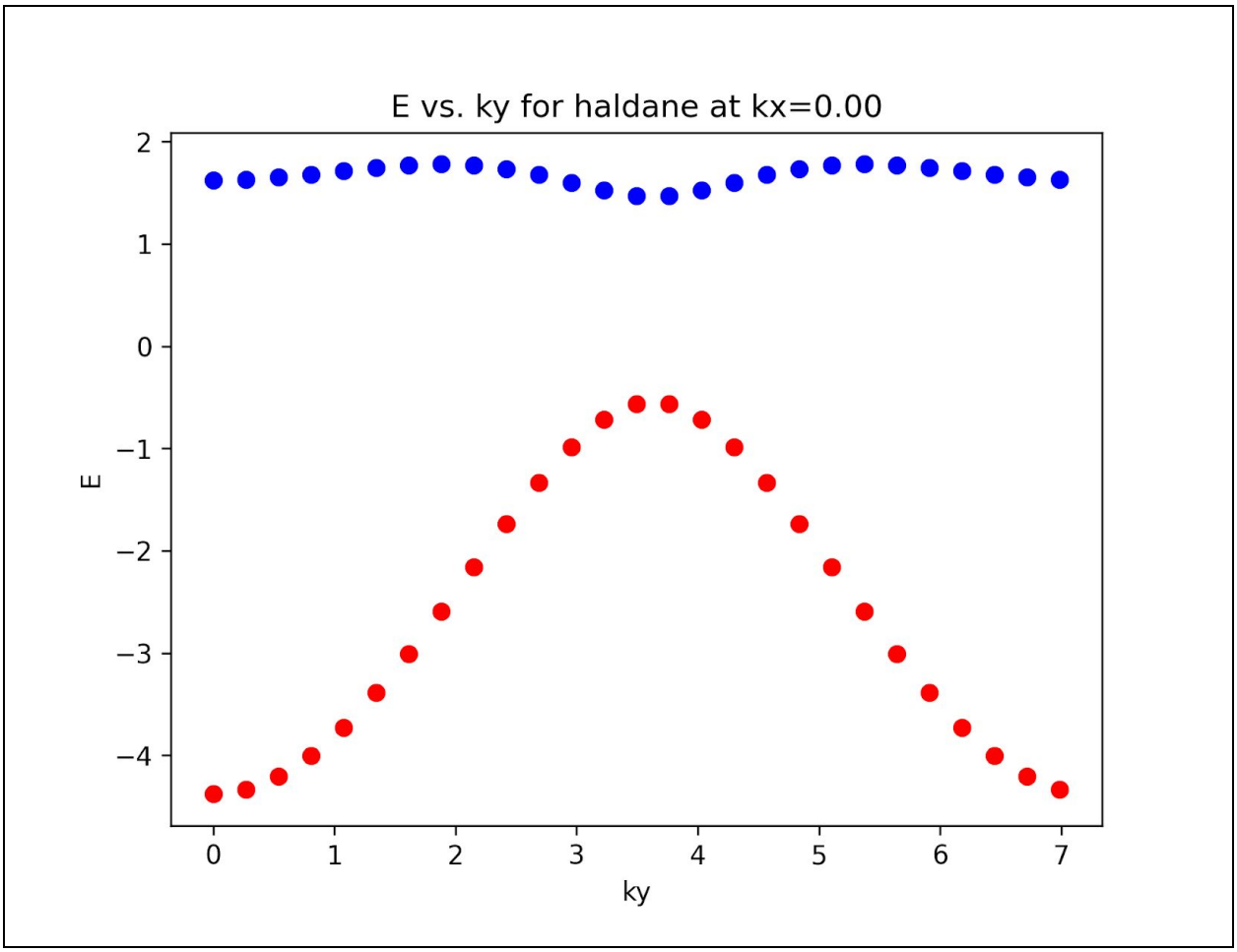

E vs. ky for Boron Nitride at kx=4.65
E
ky
2
1
0
−1
−2
−3
−2
−1
0
1
2
3
4

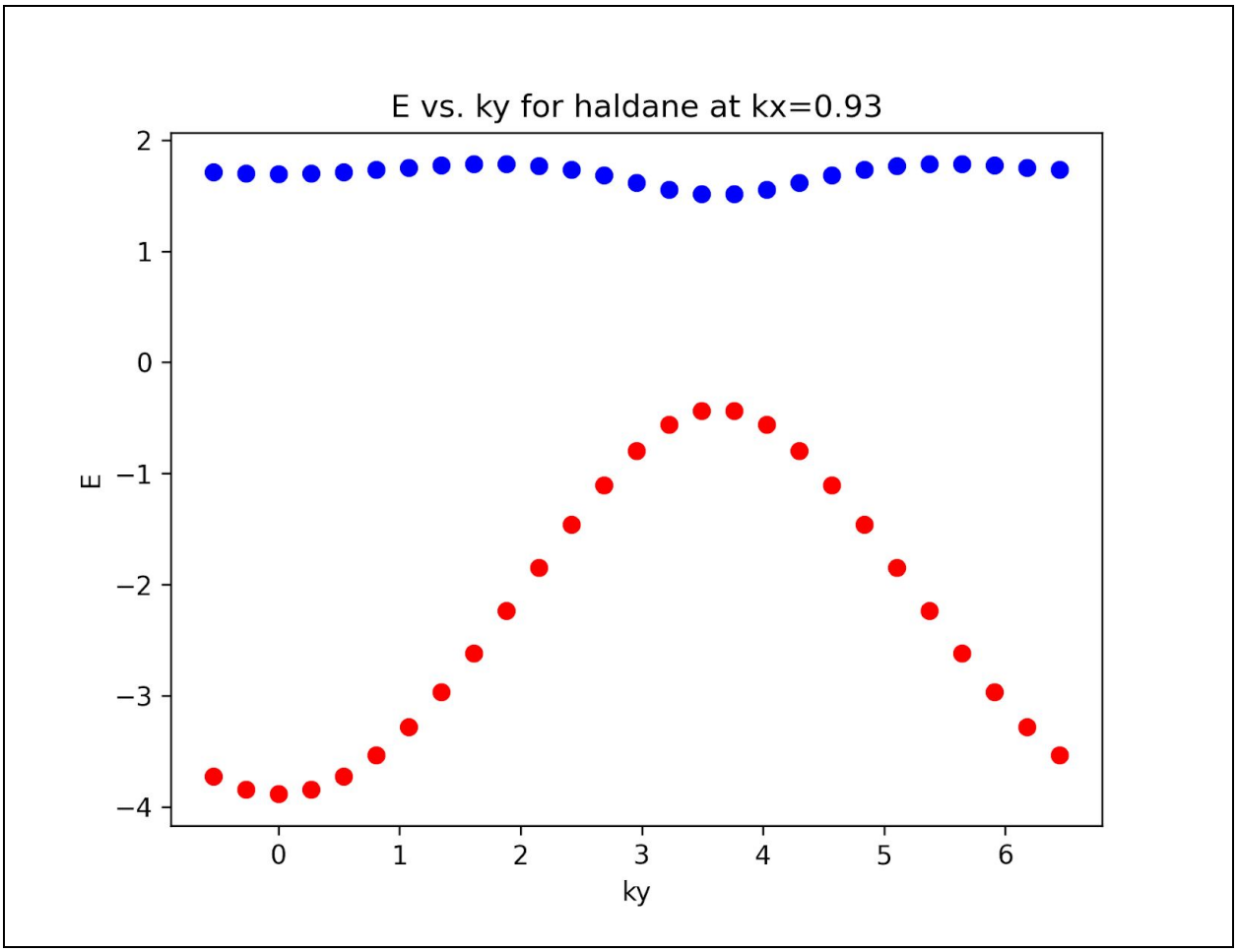


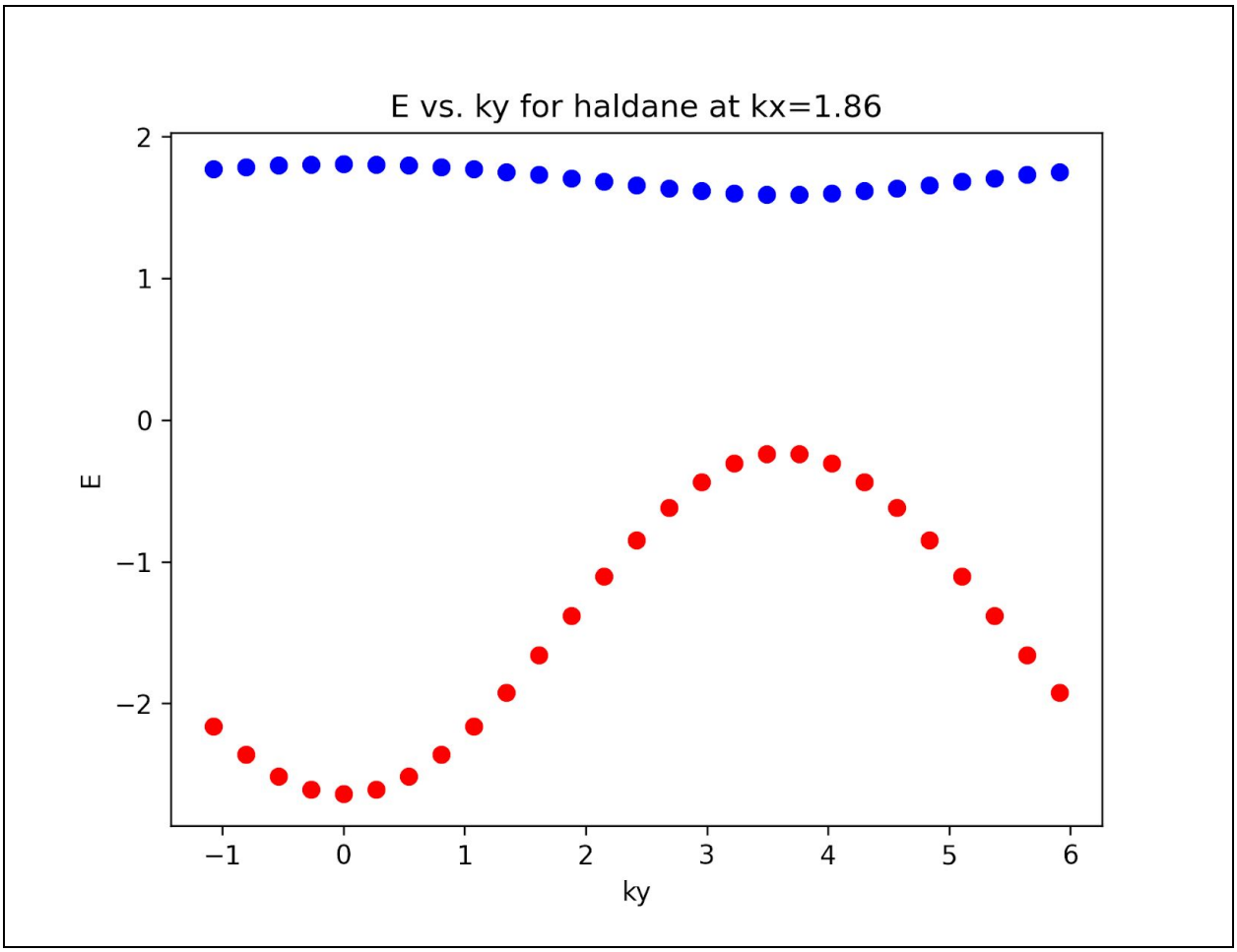
Hamiltonian V: Haldane honeycomb model

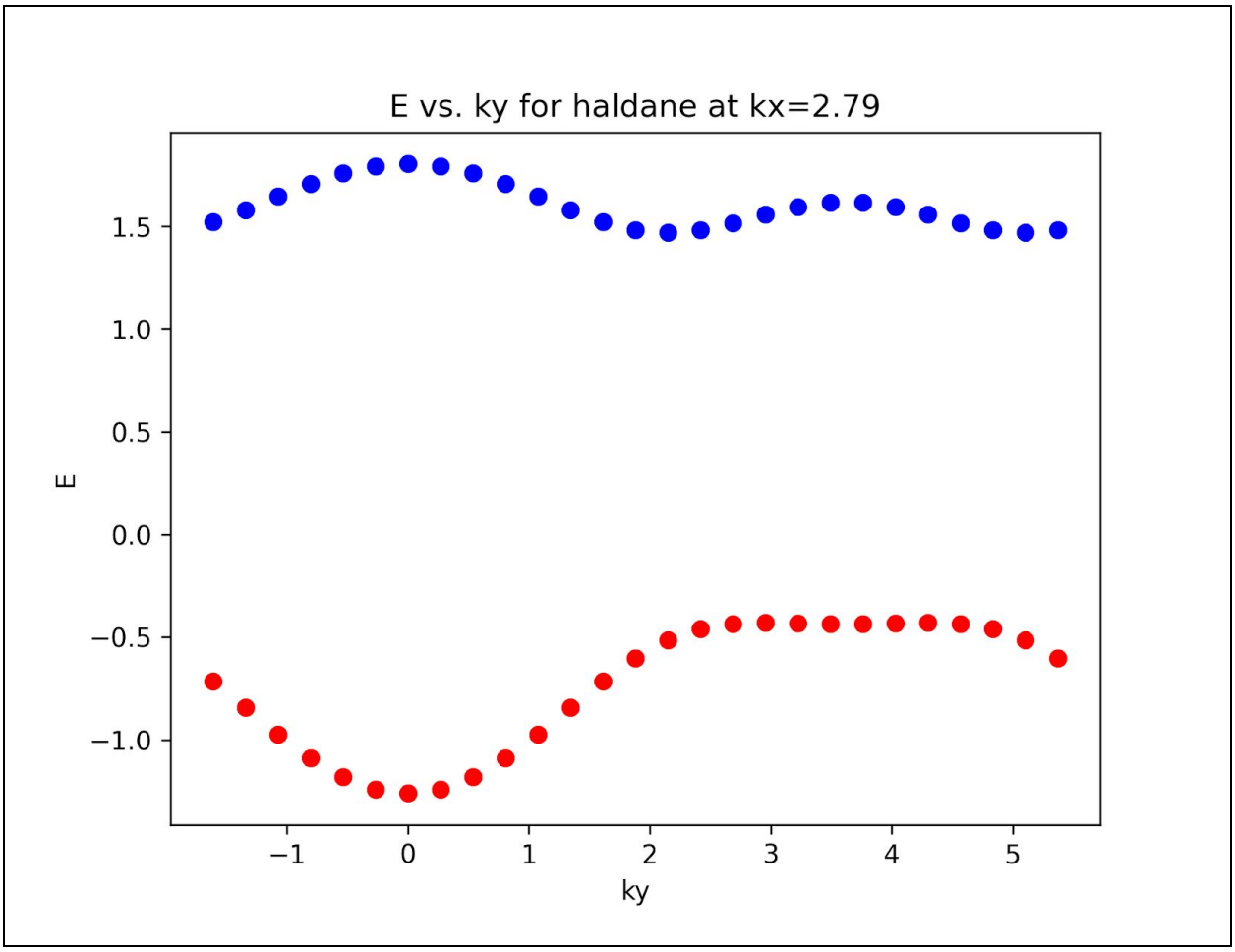
For t'=0.3, theta=0.7, M=0.1, plot E(k_x, k_y) vs. k_x, k_y on a 27 x 27 lattice for the E>0 and E<0 bands. Make a 3d plot or many 2d plots (or both).

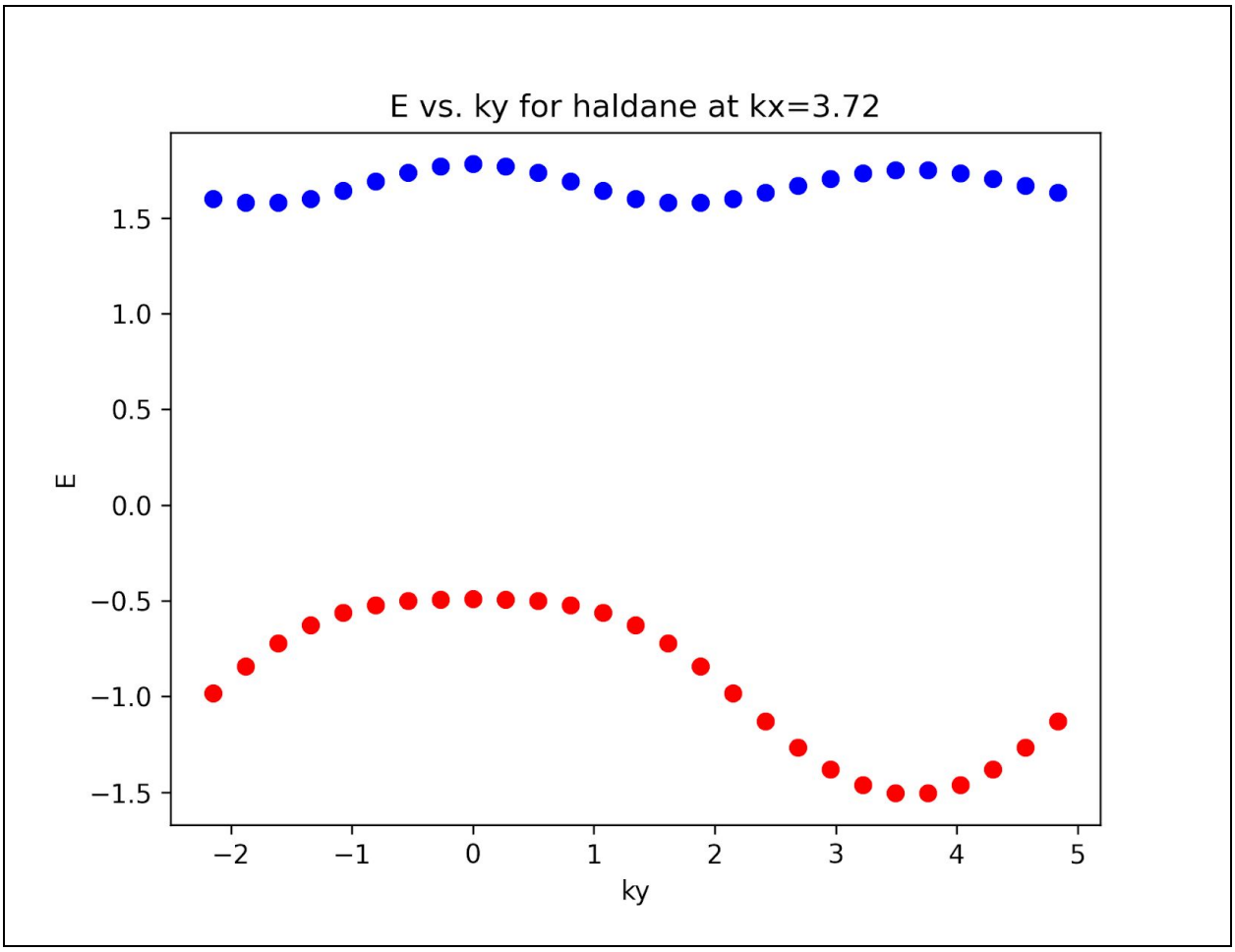

E vs. (kx,ky) for haldane
E
1
0
−1
−2
−3
−4
−4
−2
0
2
4
6
k_y
6
5
4
3
2
1
0
kx

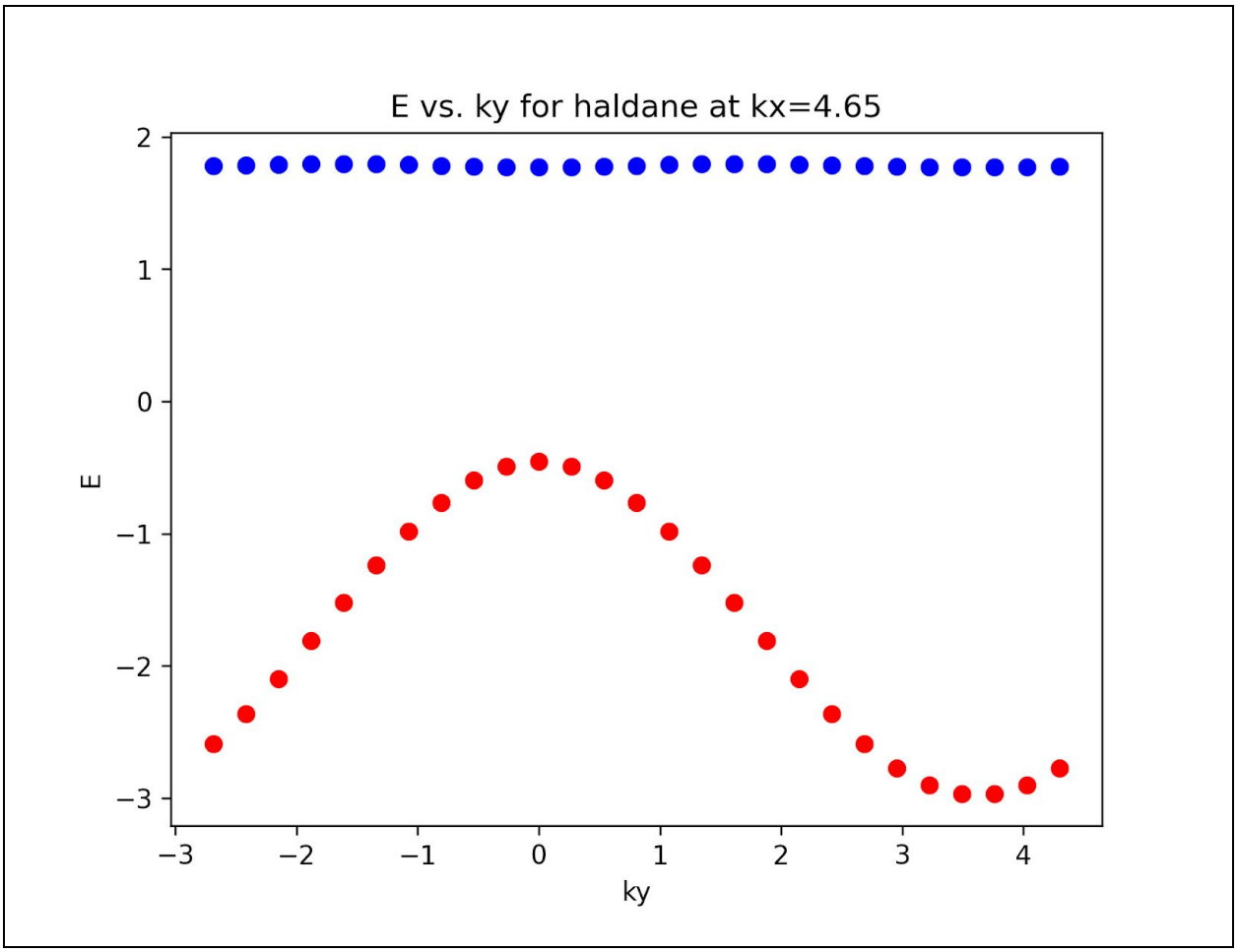

E vs. ky for haldane at kx=0.00
E
ky
2
1
0
−1
−2
−3
−4
0
1
2
3
4
5
6
7

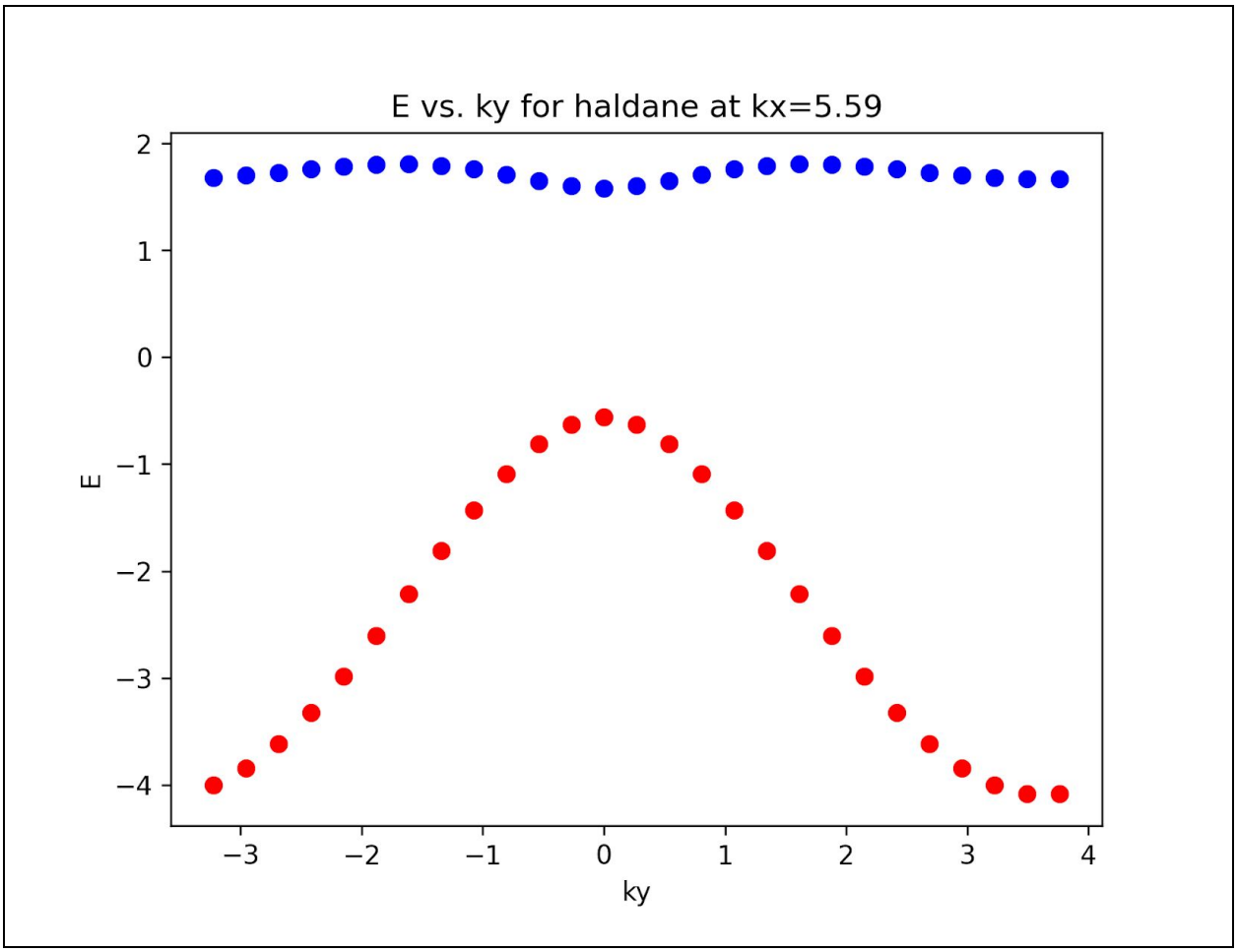

E vs. ky for haldane at kx=0.93
E
ky
2
1
0
−1
−2
−3
−4
0
1
2
3
4
5
6


E vs. ky for haldane at kx=1.86
E
ky
2
1
0
−1
−2
−1
0
1
2
3
4
5
6


E vs. ky for haldane at kx=2.79
E
ky
1.5
1.0
0.5
0.0
−0.5
−1.0
−1
0
1
2
3
4
5

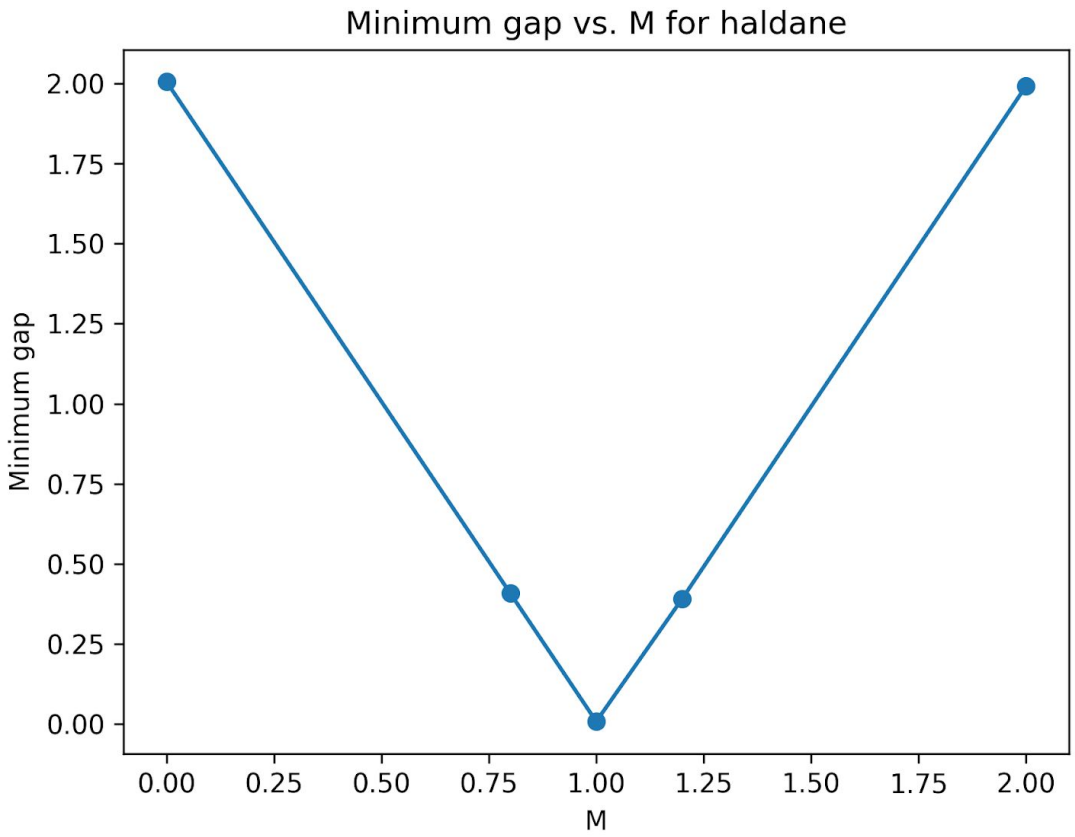

E vs. ky for haldane at kx=3.72
E
ky
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2
−1
0
1
2
3
4
5


E vs. ky for haldane at kx=4.65
E
ky
2
1
0
−1
−2
−3
−3
−2
−1
0
1
2
3
4



Two forms of insulators

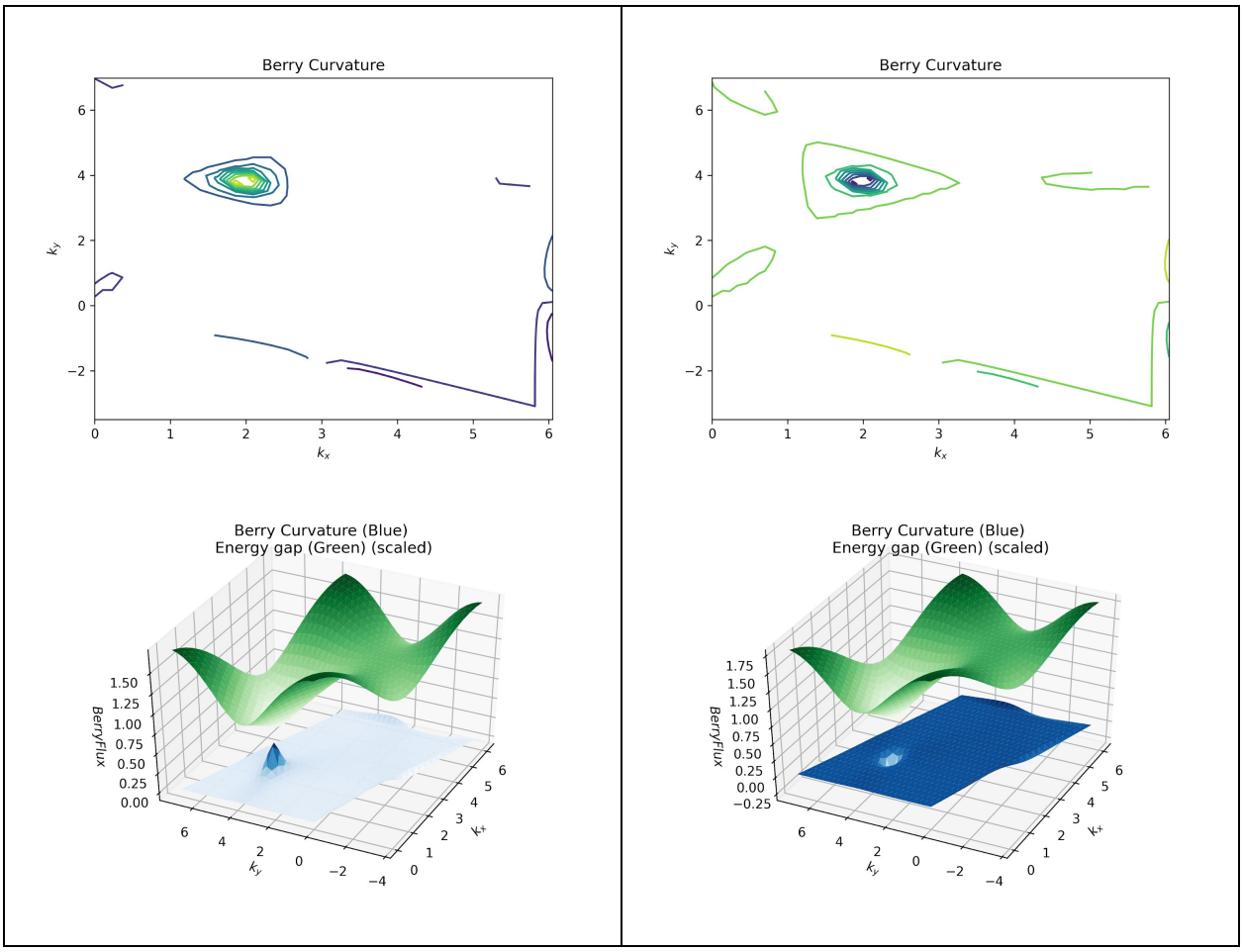
For Hamiltonian V, plot the minimum gap between the two bands as you tune M from M=0 to M=2. Do M=0, 0.8, 1.0, 1.2, 2.0. There is a transition when the gap becomes zero. At what M does this happen?



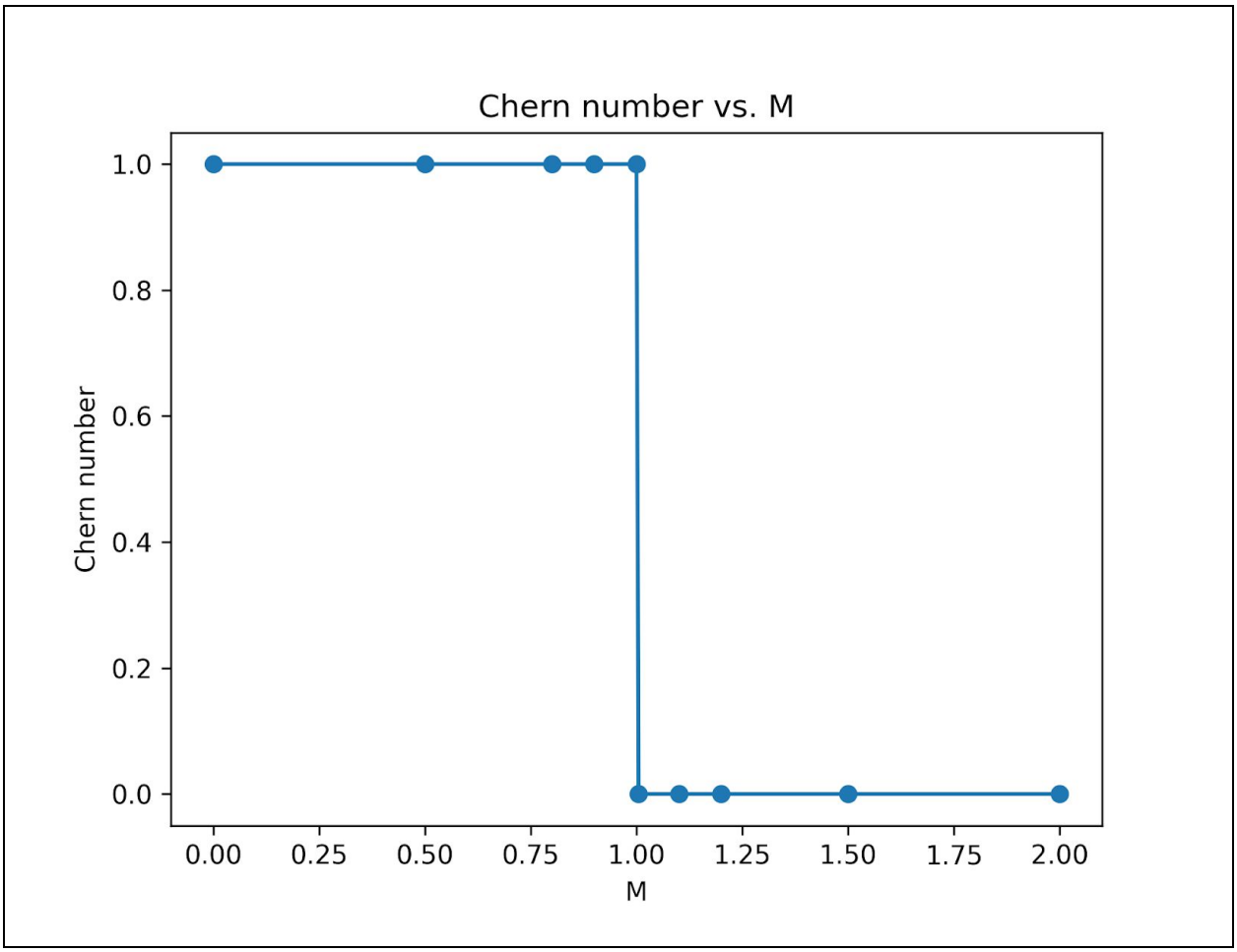
From the graph, transition happens around M=1.00. Zoomed-in iterations find that at M=1.0042, gap~1e-5.

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

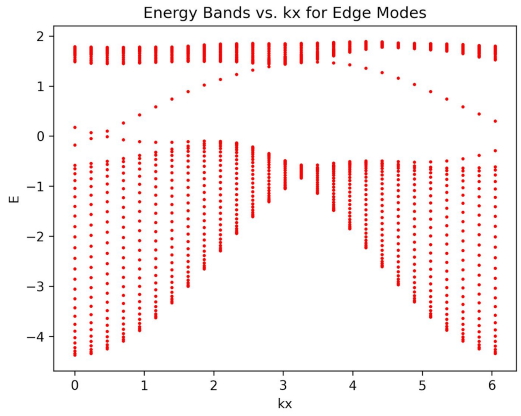


Plot the Chern number vs. M. You should see it transition between 0 and 2 at the same M that the gap became zero.



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