

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.



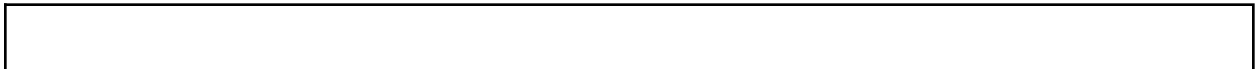
Hamiltonian II: Distorted hydrogen chain

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



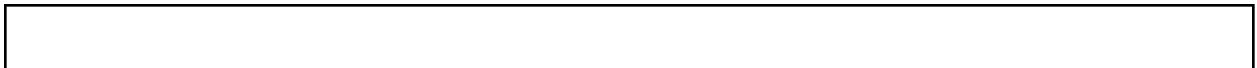
Hamiltonian III: graphene

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

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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?

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

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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 edge modes at $M=0.2$ and not at $M=2.0$

M=0.2	M=2.0
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