PythTB for (topological) tight-binding models

Jennifer Cano

Stony Brook University

FLATIRON INSTITUTE

PythTB is based at: http://physics.rutgers.edu/pythtb/

Download Python codes here: http://samos.martech.fsu.edu/TWS/default.htm

What is PythTB?

- PythTB is a software package providing a Python implementation for tight-binding models.
- Developed by Sinisa Coh and David Vanderbilt

PythTB is based at: http://physics.rutgers.edu/pythtb/

Making tight-binding models is easy. Why should I use PythTB?

- Only work in real space.
- Easily compute band structure and get eigenvectors.
- Easily create slab, cube, or other finite boundary conditions.
- Easily compute Berry phase or plot Wilson loop eigenvalues.

PythTB is based at: http://physics.rutgers.edu/pythtb/

Goals in PythTB

- Plot band structures
- Verify topological phases by
  - Visualizing topological surface states
  - Plotting Berry phase

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Tight-binding degrees of freedom

Atoms located at positions in unit cell: $\mathbf{r}_\alpha$

Each atom has orbitals labelled by j = 1, …, n

An atom has infinitely many orbitals — to model a physical system, need to decide which atoms/orbitals are relevant!

$$\phi_{\mathbf{R},\alpha,j}(\mathbf{r}) = \varphi_{\alpha,j}(\mathbf{r} - \mathbf{R} - \mathbf{r}_\alpha)$$

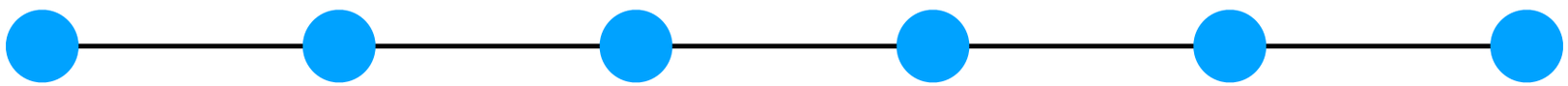
unit cell atom orbital

assume orthonormality: $\langle \phi_{\mathbf{R},\alpha,j} | \phi_{\mathbf{R}',\beta,i} \rangle = \delta_{R,\mathbf{R}'} \delta_{\alpha,\beta} \delta_{ij}$

Hamiltonian consists of "hopping terms"

$$H_{\alpha i,\beta j}(\mathbf{R}) \equiv \langle \phi_{\mathbf{R}',\alpha i} | H | \phi_{\mathbf{R}'+\mathbf{R},\beta j} \rangle = \langle \phi_{\mathbf{0},\alpha i} | H | \phi_{\mathbf{R},\beta j} \rangle$$

Example 1: atoms in 1d

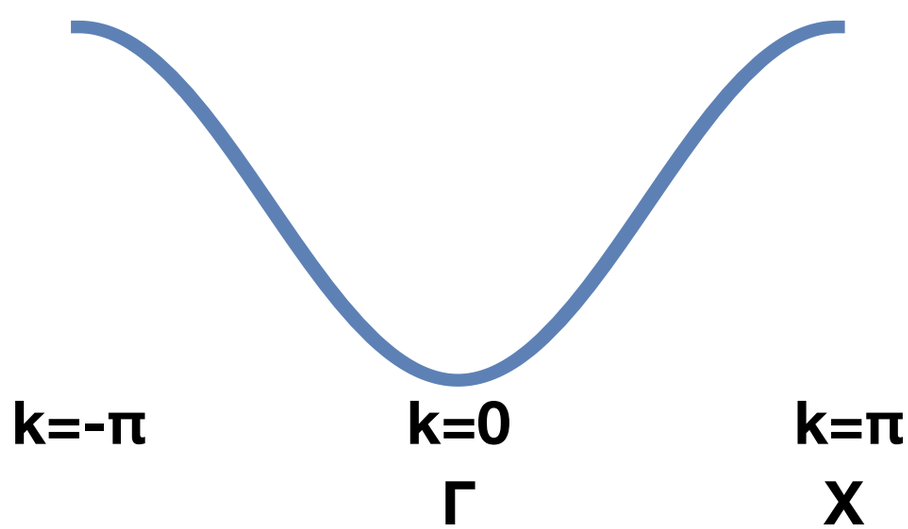


1 orbital/site ⇒ trivial subscripts: $\mathbf{r}_\alpha = \mathbf{r}_1 = \mathbf{0} \quad i = 1$

$$H(\mathbf{R} = \pm\hat{x}) = -t$$

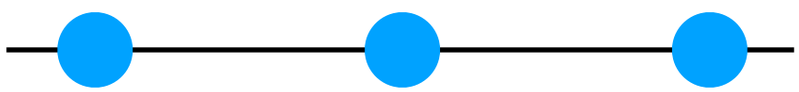
$$H(\mathbf{R} \neq \pm\hat{x}) = 0$$

$$H^{\mathbf{k}} = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} H(\mathbf{R}) = -t(e^{i\mathbf{k}\cdot\hat{x}} + e^{-i\mathbf{k}\cdot\hat{x}}) = -2t\cos k$$



$$H(\mathbf{R} = \pm\hat{x}) = -t$$

$$H(\mathbf{R} \neq \pm\hat{x}) = 0$$



Example 1: atoms in 1d
How to define model

```
# adaptation from "simple example"
# at http://physics.rutgers.edu/pythtb/examples.html
```

Lattice vectors (we only have one)

Orbitals in units of lattice vecs (we only have one)

Define model: (dim k space, dim real space, lattice vecs, orbital vecs)

Hopping term: (amplitude, iα, jβ, **R**)

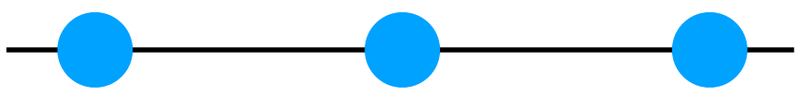
```
# specify model
# lattice vectors
lat=[[1.0]]
# positions of orbitals
orb=[[0.0]]

# define the model
my_model=tb_model(1,1,lat,orb)
# assign hopping terms
my_model.set_hop(-1., 0, 0, [1])
```

PythTB is based at: http://physics.rutgers.edu/pythtb/

Example 1: atoms in 1d
How to plot

$$H(\mathbf{R} = \pm\hat{x}) = -t$$

$$H(\mathbf{R} \neq \pm\hat{x}) = 0$$



k path to plot in units of reciprocal lattice vecs (-π to π)

Labels of k-points on path

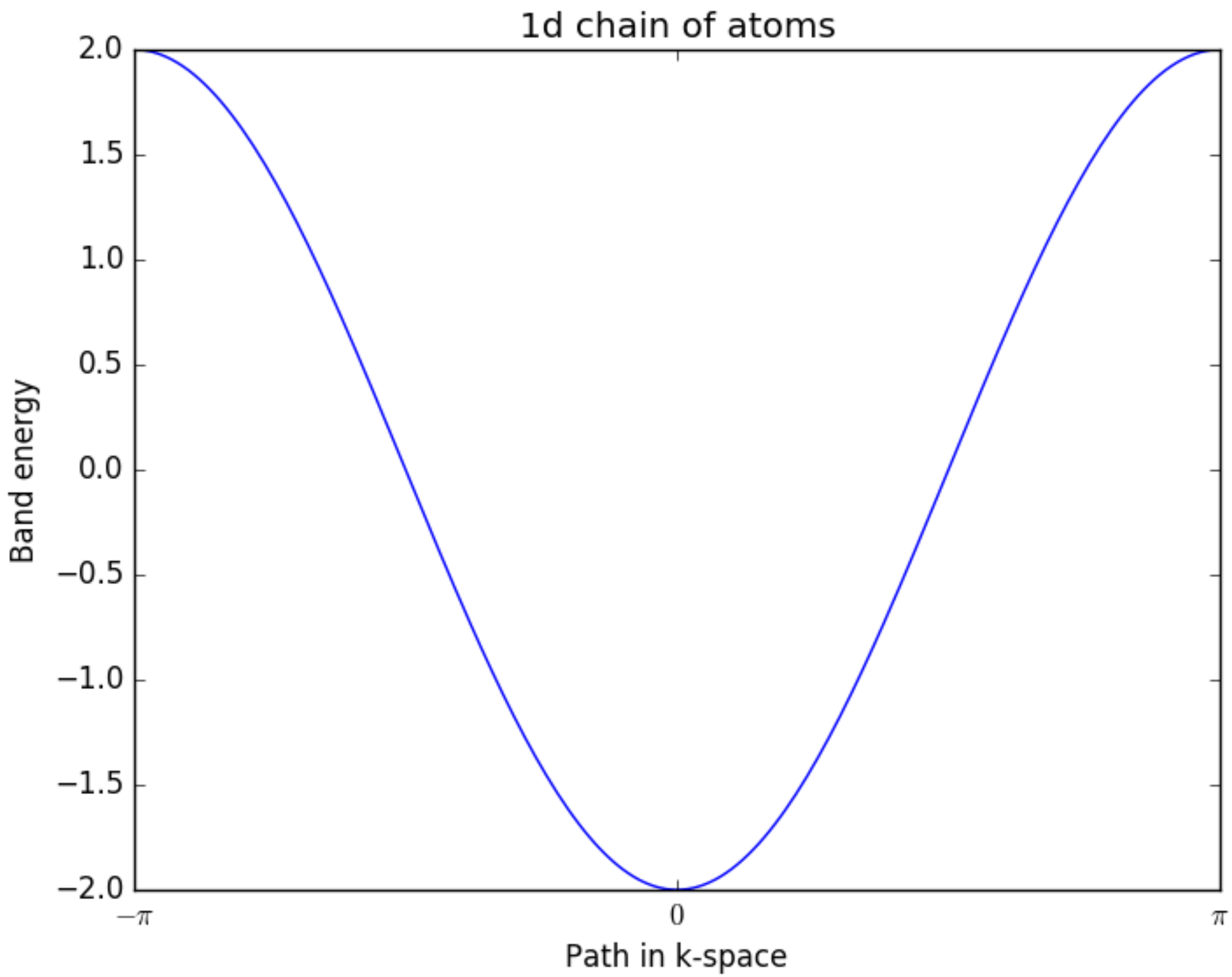
Repeat this line for more bands, up to evals[n]

Where to put ticks (from path and numsteps)

```
# define a path in k-space to plot
path=[[-.5],[0],[.5]]
# label k points
label=(r'$-\pi$',r'$0$',r'$\pi $')
# number of steps between points
numsteps=100
kpts=k_path(path,numsteps)

# solve model
evals=my_model.solve_all(kpts)

# make a figure object
fig=pl.figure()
# plot bands
pl.plot(evals[0])
# put title on top
pl.title("1d chain of atoms")
pl.xlabel("Path in k-space")
pl.ylabel("Band energy")
pl.xticks([0,100,200],label)
```

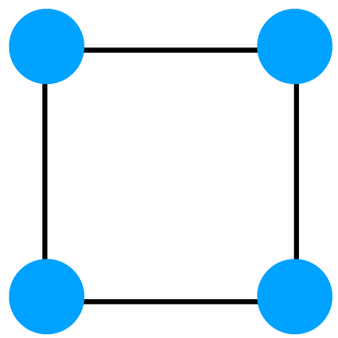
PythTB is based at: http://physics.rutgers.edu/pythtb/

Example 1: atoms in 1d



PythTB is based at: http://physics.rutgers.edu/pythtb/

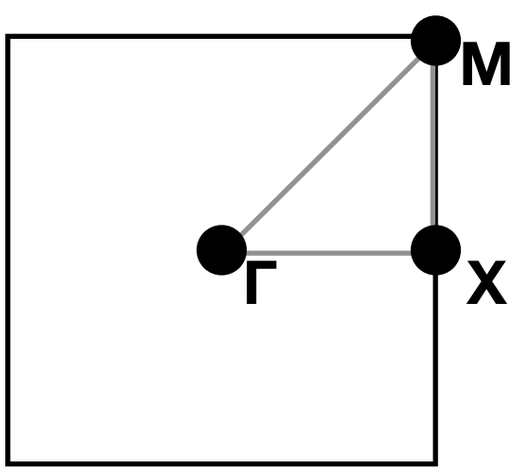
Example 2: square lattice

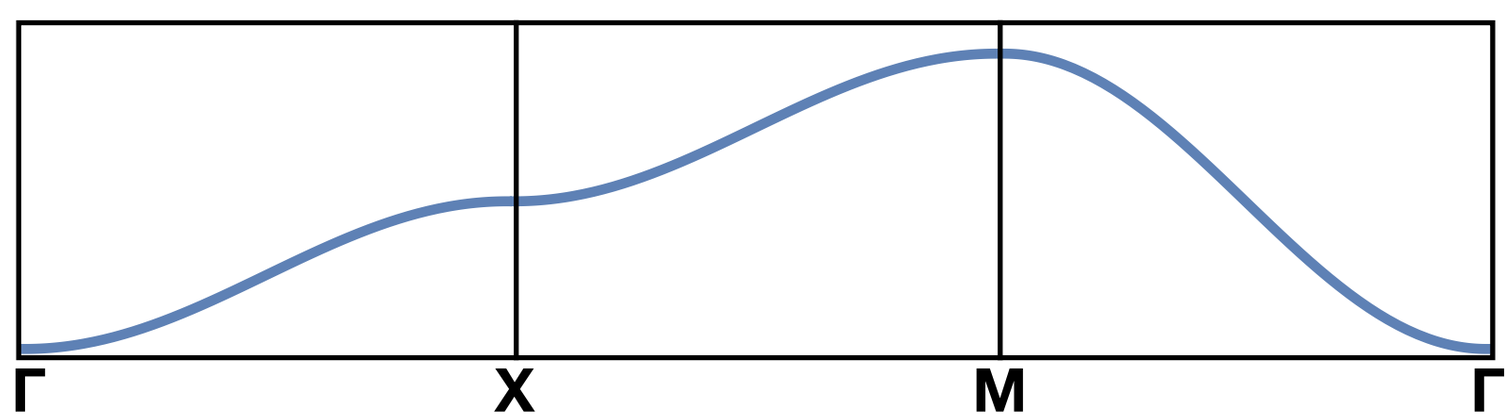


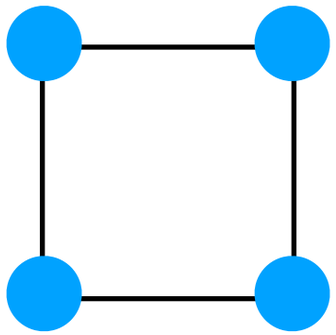
$$H(\mathbf{R}) = \begin{cases} -t & \text{if } \mathbf{R} = \pm\hat{x}, \pm\hat{y} \\ 0 & \text{else} \end{cases}$$

$$H^{\mathbf{k}} = -2t(\cos k_x + \cos k_y)$$

How to plot 2d spectrum? identify high-symmetry path







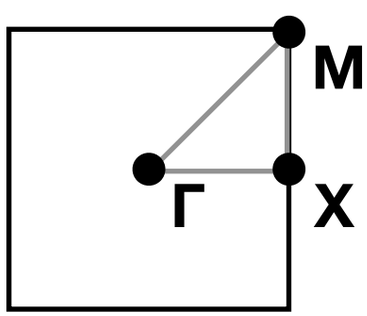
Example 2: square lattice

$$H(\mathbf{R}) = \begin{cases} -t & \text{if } \mathbf{R} = \pm\hat{x}, \pm\hat{y} \\ 0 & \text{else} \end{cases}$$

Two two-component lattice vecs

Still one orbital;
two components

```
# specify model
# lattice vectors
lat=[[1.0,0.0],[0.0,1.0]]
# positions of orbitals
orb=[[0.0,0.0]]

# define the model
my_model=tb_model(2,2,lat,orb)
# assign hopping terms
# x-hopping
my_model.set_hop(-1., 0, 0, [1.0,0])
# y-hopping
my_model.set_hop(-1., 0, 0, [0,1.0])

# define a path in k-space to plot
path=[[0.0,0.0],[.5,0],[.5,.5],[0.0,0.0]]
```

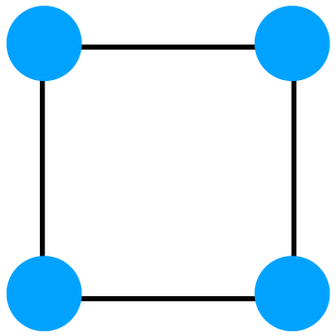


k path: Γ, X, M, Γ

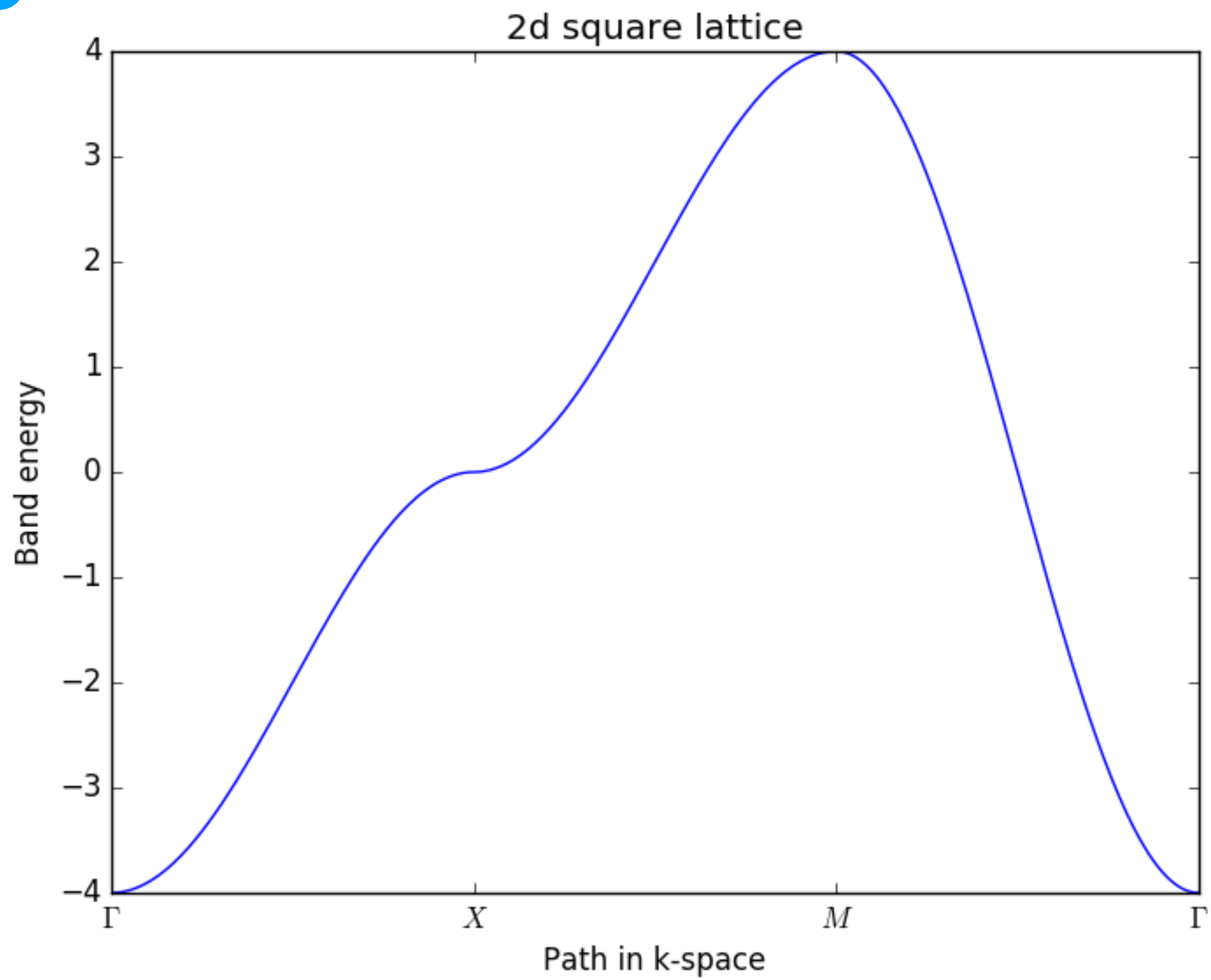
Another tick because more k pts

```
pl.xticks([0,100,200,300],label)
```

PythTB is based at: http://physics.rutgers.edu/pythtb/

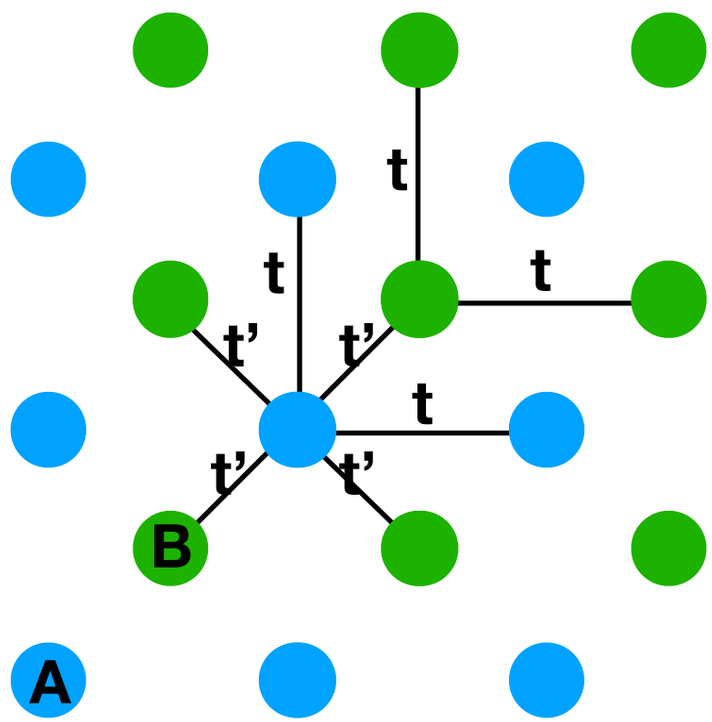


Example 2: square lattice



PythTB is based at: http://physics.rutgers.edu/pythtb/

Example 3: interpenetrating square lattices



$$\mathbf{r}_A = (0,0)$$

$$\mathbf{r}_B = (1/2, 1/2)$$

only one orbital/site ⇒ i = 1

$$H_{AA}(\mathbf{0}) = \mu_A$$

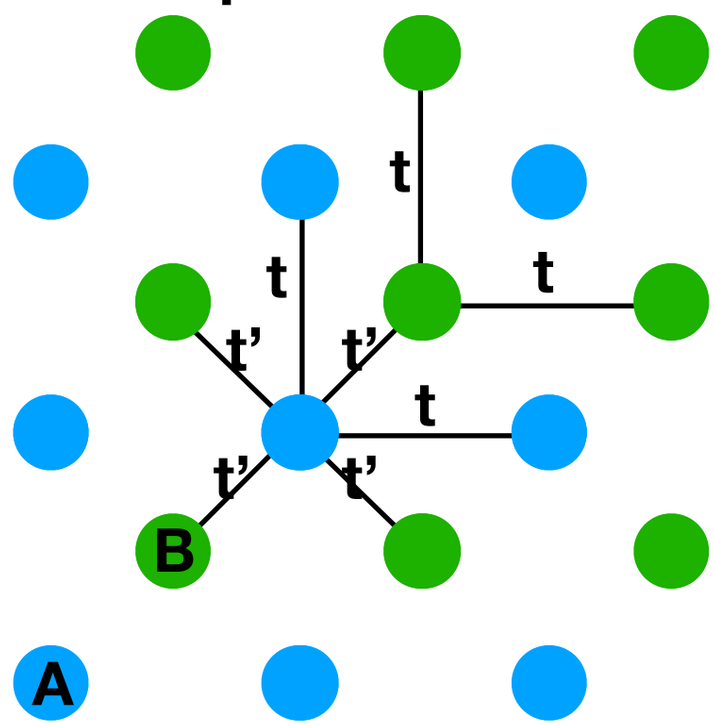
$$H_{BB}(\mathbf{0}) = \mu_B$$

$$H_{AA}(\pm\hat{x}) = H_{AA}(\pm\hat{y}) = H_{BB}(\pm\hat{x}) = H_{BB}(\pm\hat{y}) = -t$$

$$H_{AB}(\mathbf{0}) = H_{AB}(-\hat{x}) = H_{AB}(-\hat{x}-\hat{y}) = H_{AB}(-\hat{y}) = -t'$$

label by **R** (unit cell),
not $\mathbf{r}_{AB}$

Example 3: interpenetrating square lattices




```python
# specify model
# lattice vectors
lat=[[1.0,0.0],[0.0,1.0]]
# positions of orbitals
orb=[[0.0,0.0],[.5,.5]]

# define the model
my_model=tb_model(2,2,lat,orb)

# assign onsite energy
my_model.set_onsite([1.0,-1.0])

# assign hopping terms
t=1.0
t2=1.0
# x-hopping within sublattice of orbital "0"
my_model.set_hop(-t, 0, 0, [1.0,0])
# y-hopping within sublattice of orbital "0"
my_model.set_hop(-t, 0, 0, [0,1.0])
# x-hopping within sublattice of orbital "1"
my_model.set_hop(-t, 1, 1, [1.0,0])
# y-hopping within sublattice of orbital "1"
my_model.set_hop(-t, 1, 1, [0,1.0])
# four inter-sublattice hopping terms, from "0" to "1"
my_model.set_hop(-t2, 0, 1, [0.0,0.0])
my_model.set_hop(-t2, 0, 1, [-1.0,0.0])
my_model.set_hop(-t2, 0, 1, [-1.0,-1.0])
my_model.set_hop(-t2, 0, 1, [0.0,-1.0])
```

Two orbitals!

Onsite energy for each orbital

A sublattice hopping

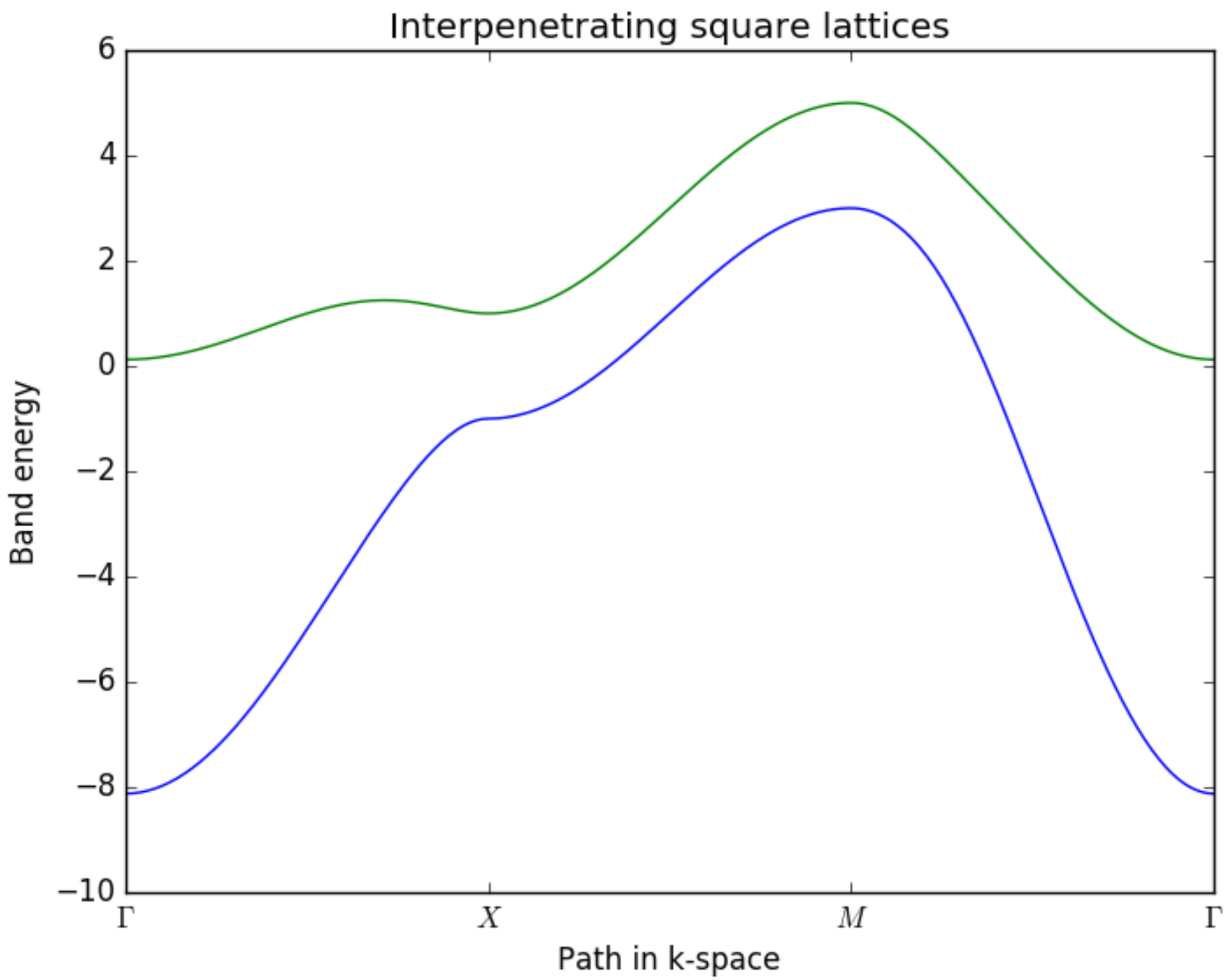
B sublattice hopping

Inter-sublattice hopping (last term is R)

Now plotting two bands

```python
# plot bands
pl.plot(evals[0])
pl.plot(evals[1])
```

Example 3: interpenetrating square lattices



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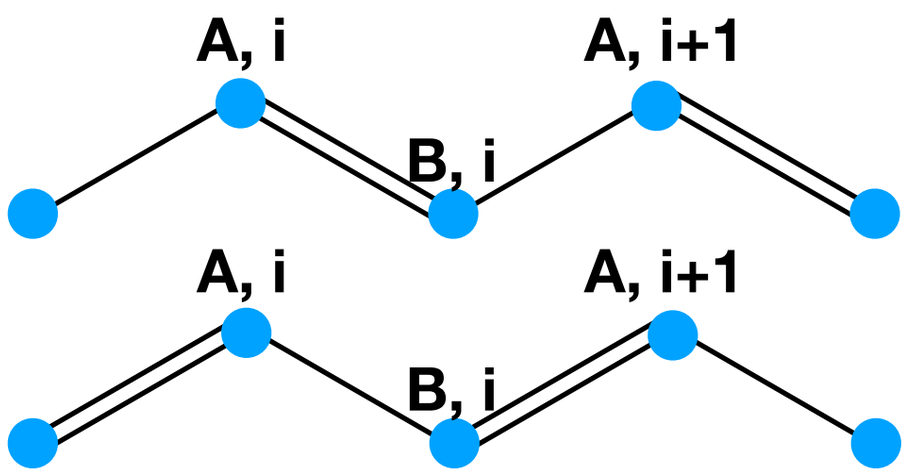
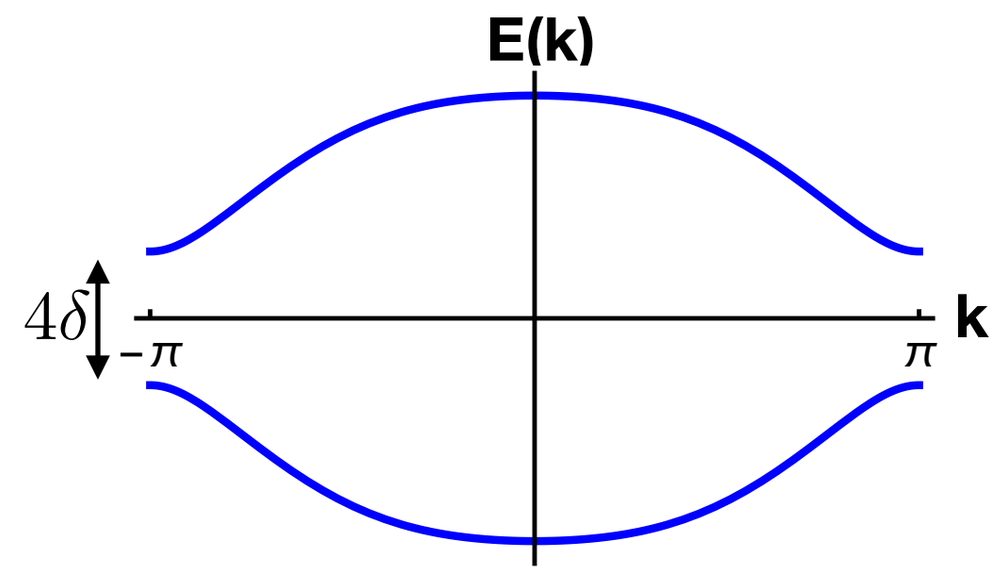
Exercise 1: Implement SSH model

$$H = \sum_i (t+\delta) c^\dagger_{A,i} c_{B,i} + (t-\delta) c^\dagger_{A,i+1} c_{B,i} + \text{h.c.}$$

$\delta > 0$

$\delta < 0$





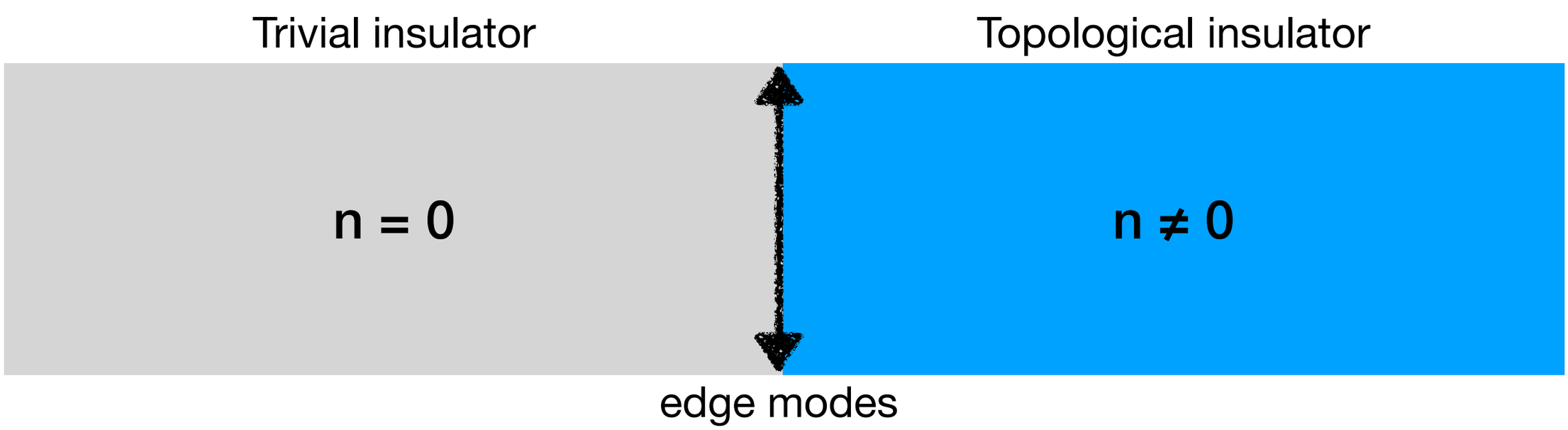
a) reproduce band structure

b) verify Berry phase differs by π when δ changes sign

Berry phase code snippet:

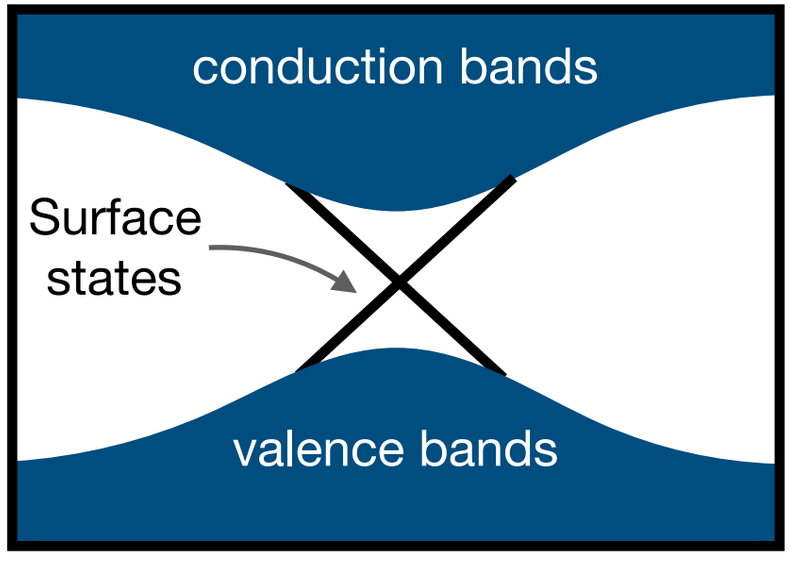
```
# Construct wf_array
# capable of storing 11 wavefunctions
wf = wf_array(my_model, [11])
# populate this wf_array with regular
# grid of points in BZ cenetered at 0.0
wf.solve_on_grid([0.0])
# compute Berry phase of lowest band
pha = wf.berry_phase([0])
```

Bulk-boundary correspondence



Quantized topological invariant

⇒ gapless edge states



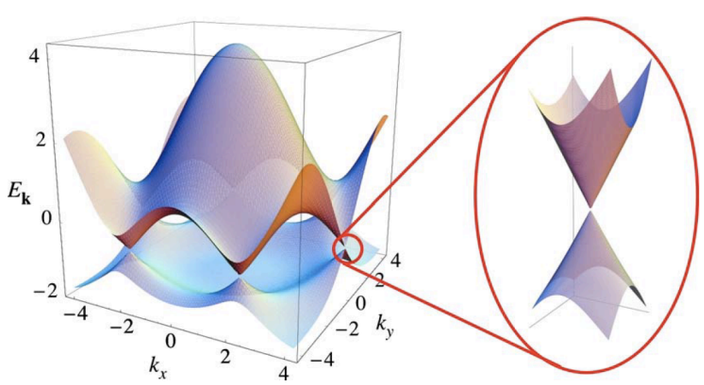
Slab band structure

Kane-Mele model

- Recall: the Kane-Mele model is an example of a 2D topological phase protected by time-reversal symmetry (ref: Kane and Mele, PRL 95, 146802 (2005), Eq. (1))

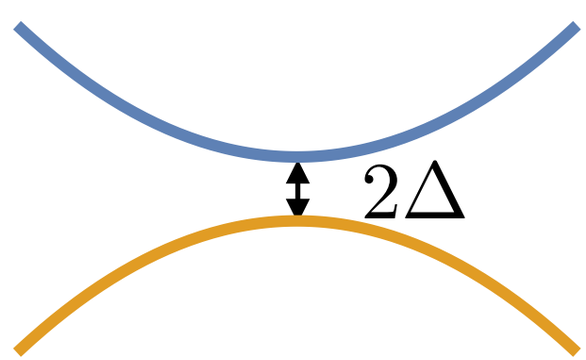
- Sample file: http://physics.rutgers.edu/pythtb/examples.html

- We will verify topological nature by plotting surface states



$$\mathcal{H}_0 = -i\hbar v_F \psi^\dagger (\sigma_x \tau_z \partial_x + \sigma_y \partial_y)\psi$$

$$\sigma_z = \text{sublattice} \quad \tau_z = \text{valley} \quad s_z = \text{spin}$$



open gap:

$$\Delta_{\text{SOC}} \sigma_z \tau_z s_z$$

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Kane-Mele model: edge states

New features:

```
# cut into a slab
fin_model=my_model.cut_piece(numbands,0,glue_edgs=False)
```

 # layers

real space direction that is finite in slab

```
# path in surface BZ
fin_path=k_path([[0.],[.5],[1.0]],numpoints)
```

Number of bands is (# orbitals) x (# layers)

```
for i in range(4*numbands): ## 4 is the number of orbitals
    pl.plot(fin_evals[i],linewidth=1.0)
```

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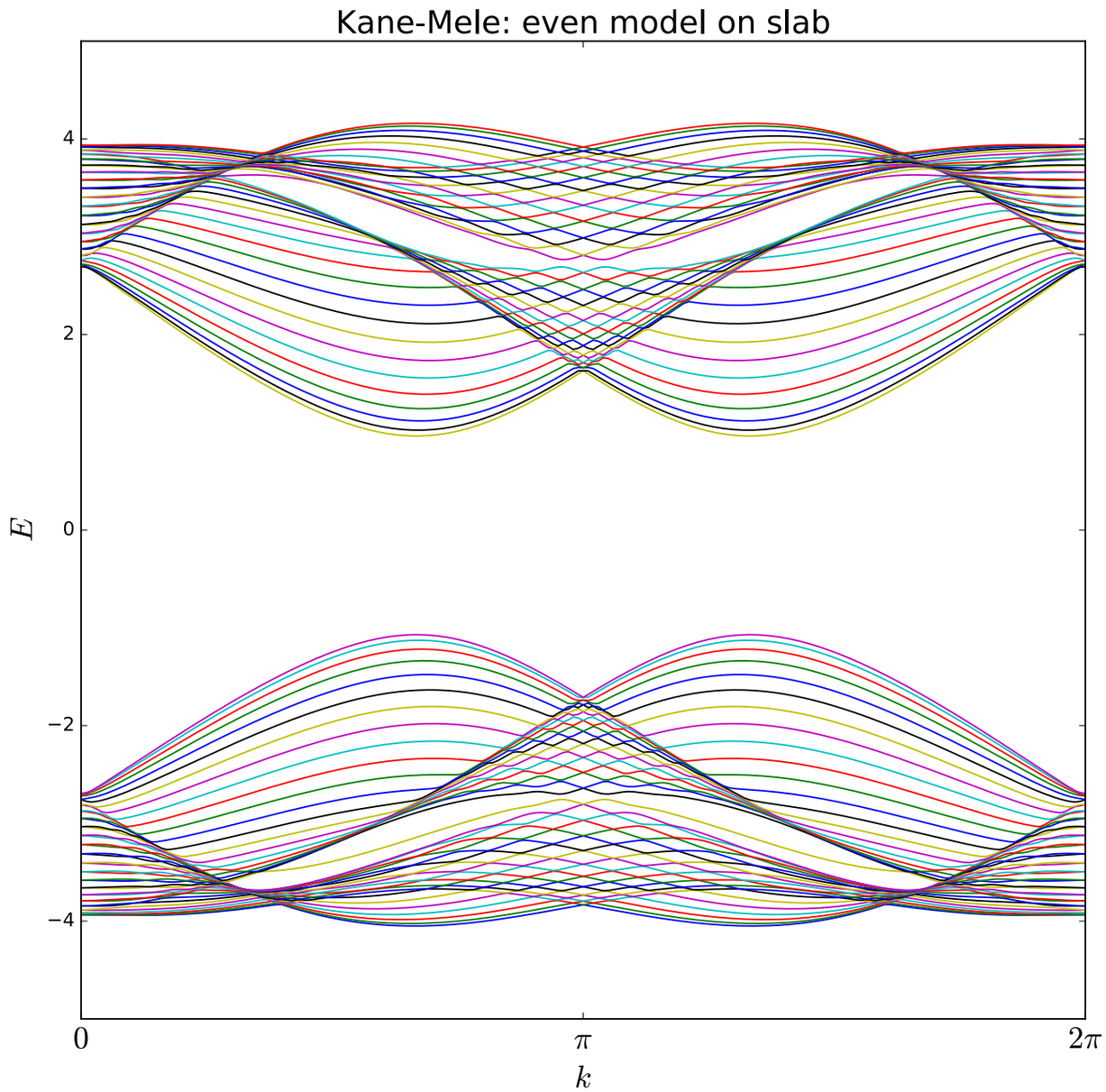
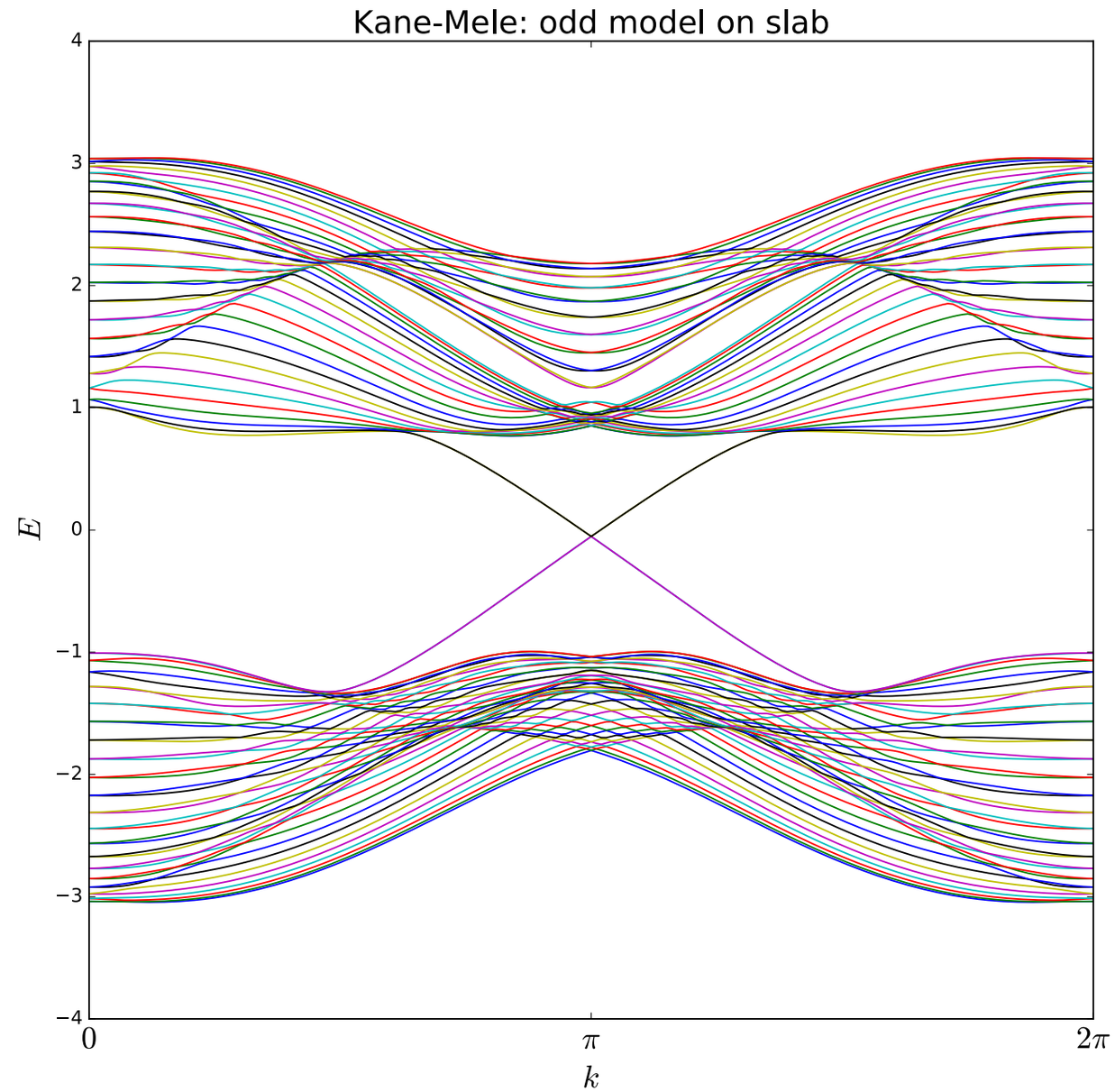
Kane-Mele model: edge states

Output:

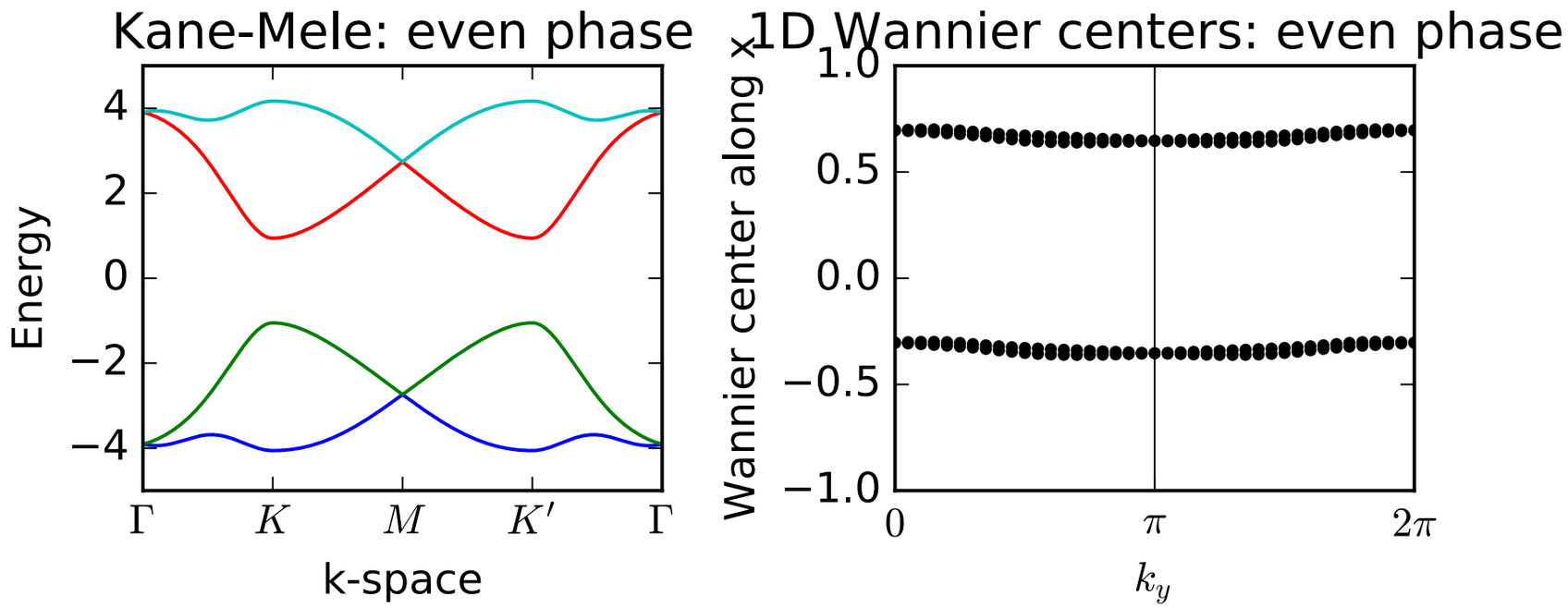


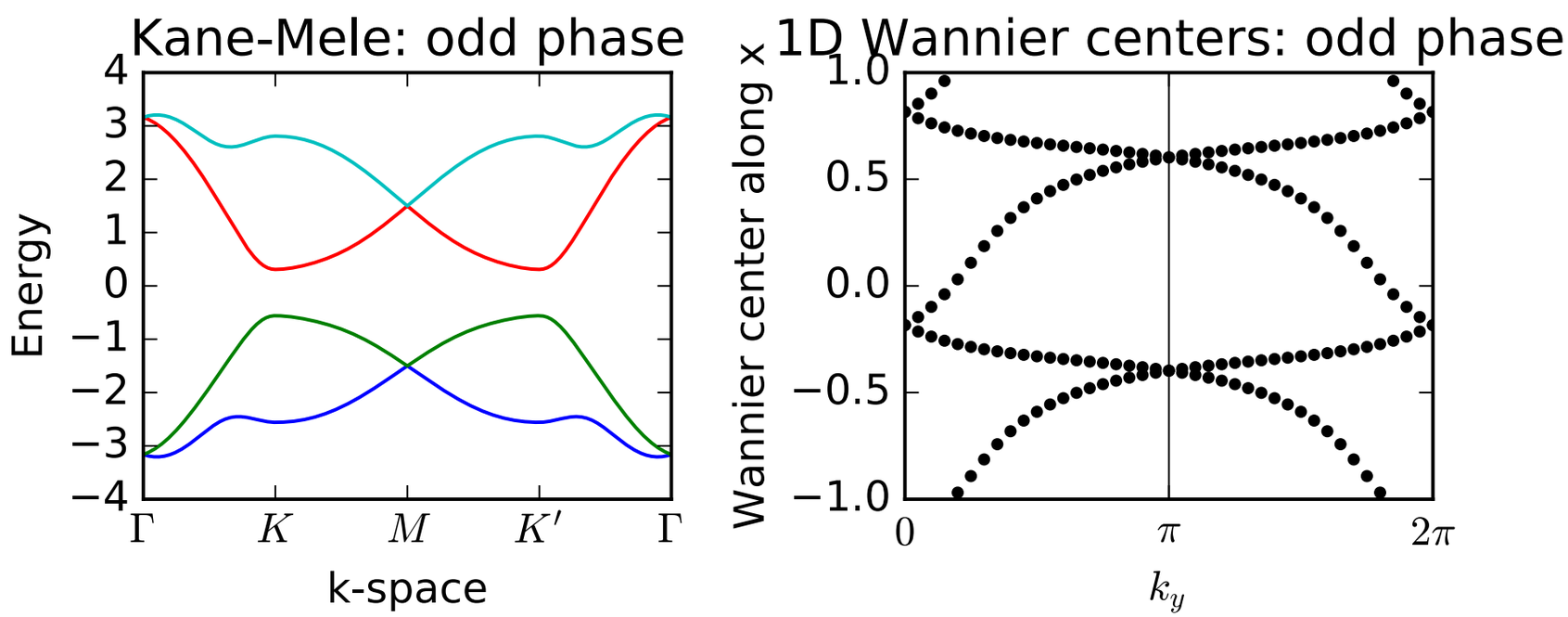


Would get same result for any slab termination

PythTB is based at: http://physics.rutgers.edu/pythtb/

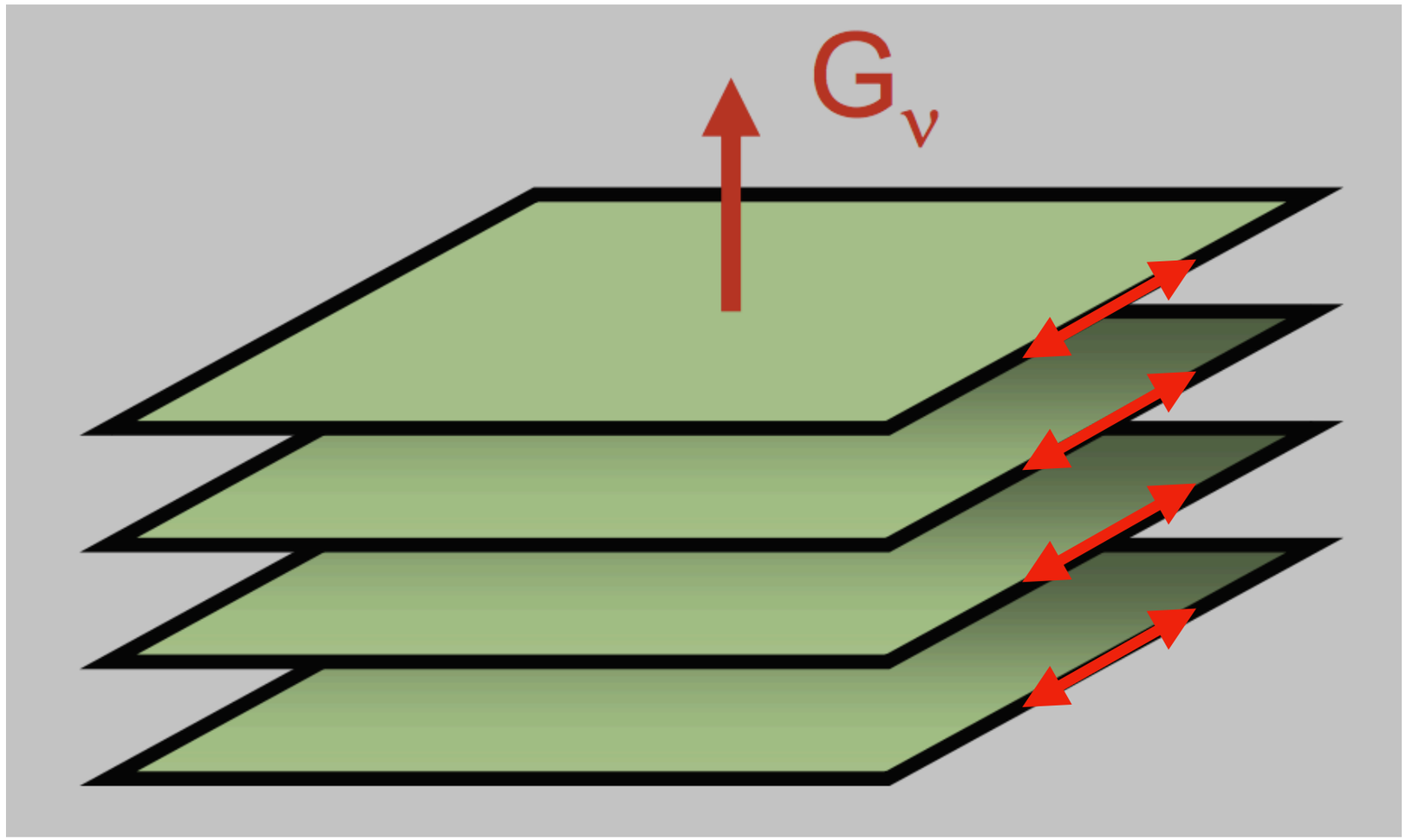
Kane-Mele model: winding Berry phase

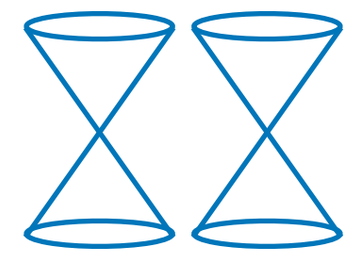




“Weak” topological insulator from stack of 2D TIs

Ref: Fu, Kane, Mele Phys. Rev. Lett. 98, 106803 (2007)





2 Dirac cones on side surfaces

Figure: Charlie Kane’s, Windsor Summer School slides:
http://www.physics.upenn.edu/~kane/

Stacked Kane-Mele

- Add a third dimension (all vectors get a third component!)
- Couple layers (otherwise bands are flat)
- Many ways to couple the layers: I recommend the following coupling term that breaks spin conservation:

```
# add coupling in z direction
zhop=.1*0
zsoc=.3*spin_orb
ret_model.set_hop(-j*zsoc*sigma_z, 0, 0, [ 0., 0., 1.])
ret_model.set_hop(j*zsoc*sigma_z, 1, 1, [ 0., 0., 1.])
```

(A real term preserves an anti-unitary symmetry that flattens the Dirac cones; details: ArXiv: 1410.4440)

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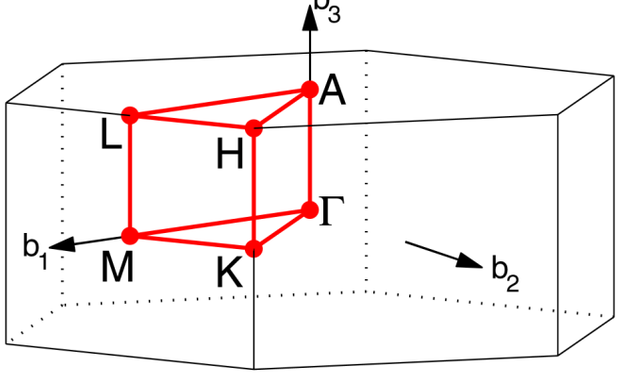
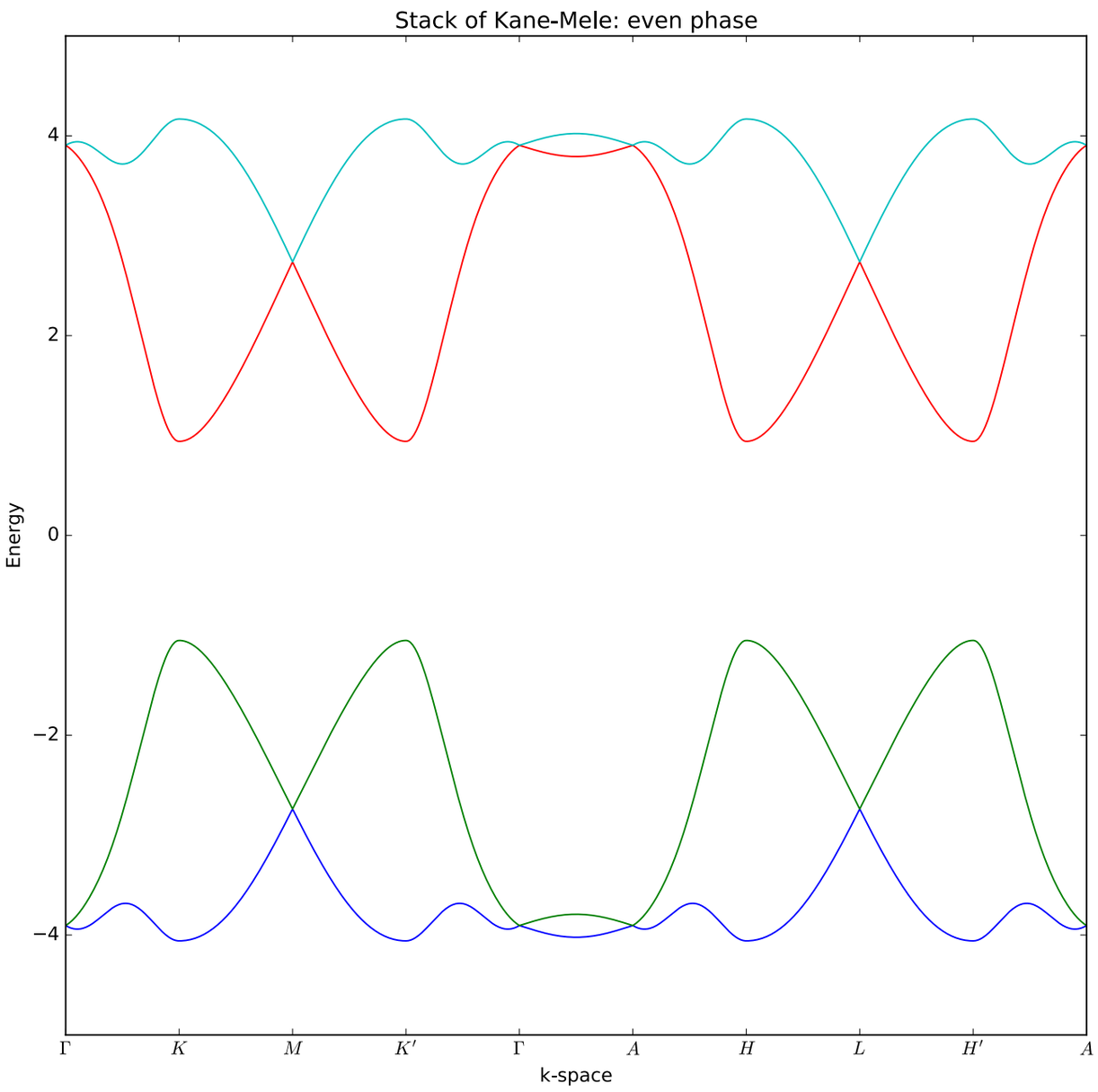
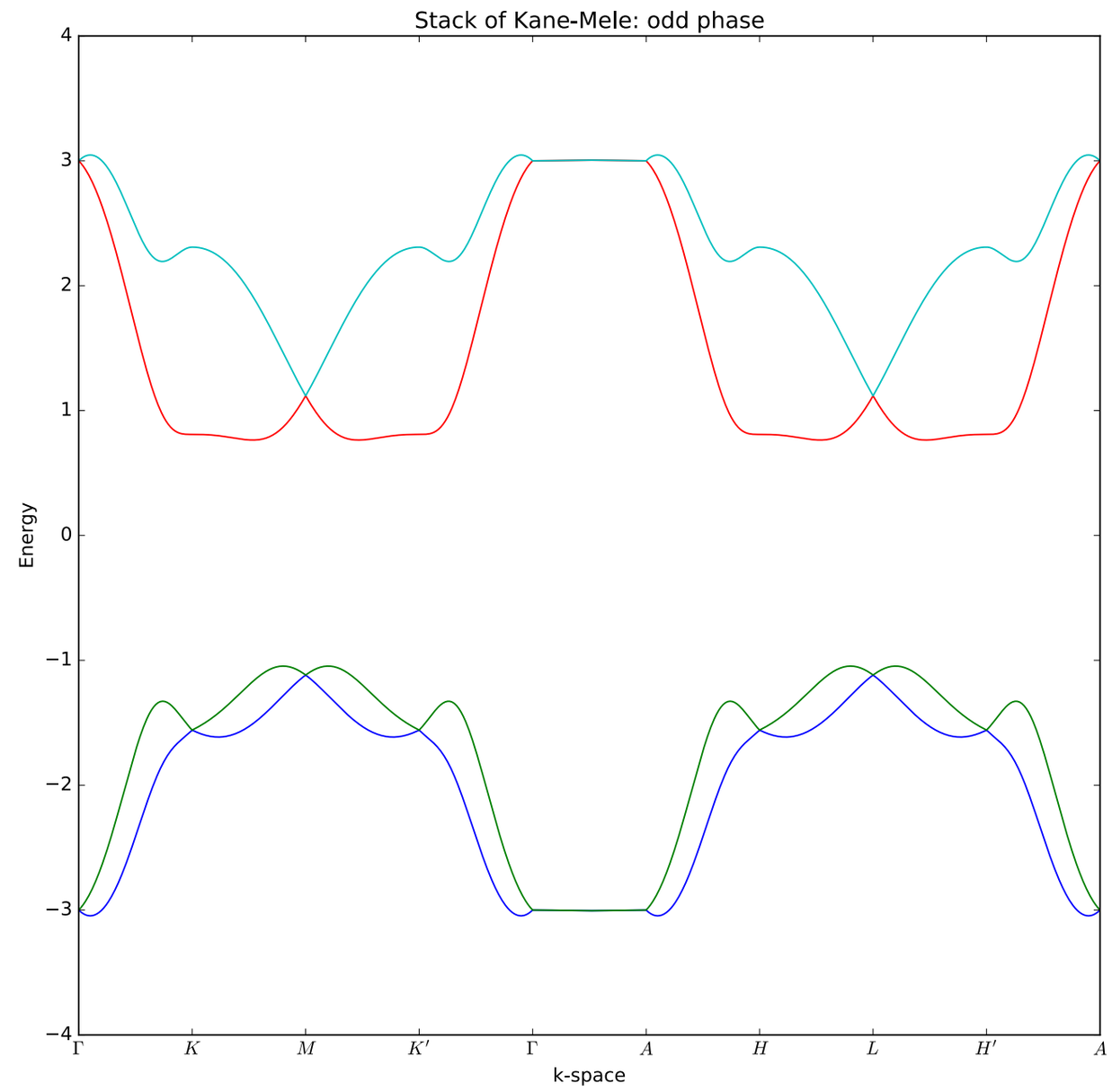


Stacked Kane-Mele

HEX path: Γ-M-K-Γ-A-L-H-A|L-M|K-H

[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]





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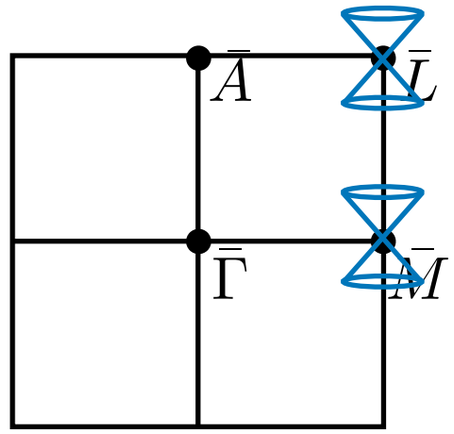
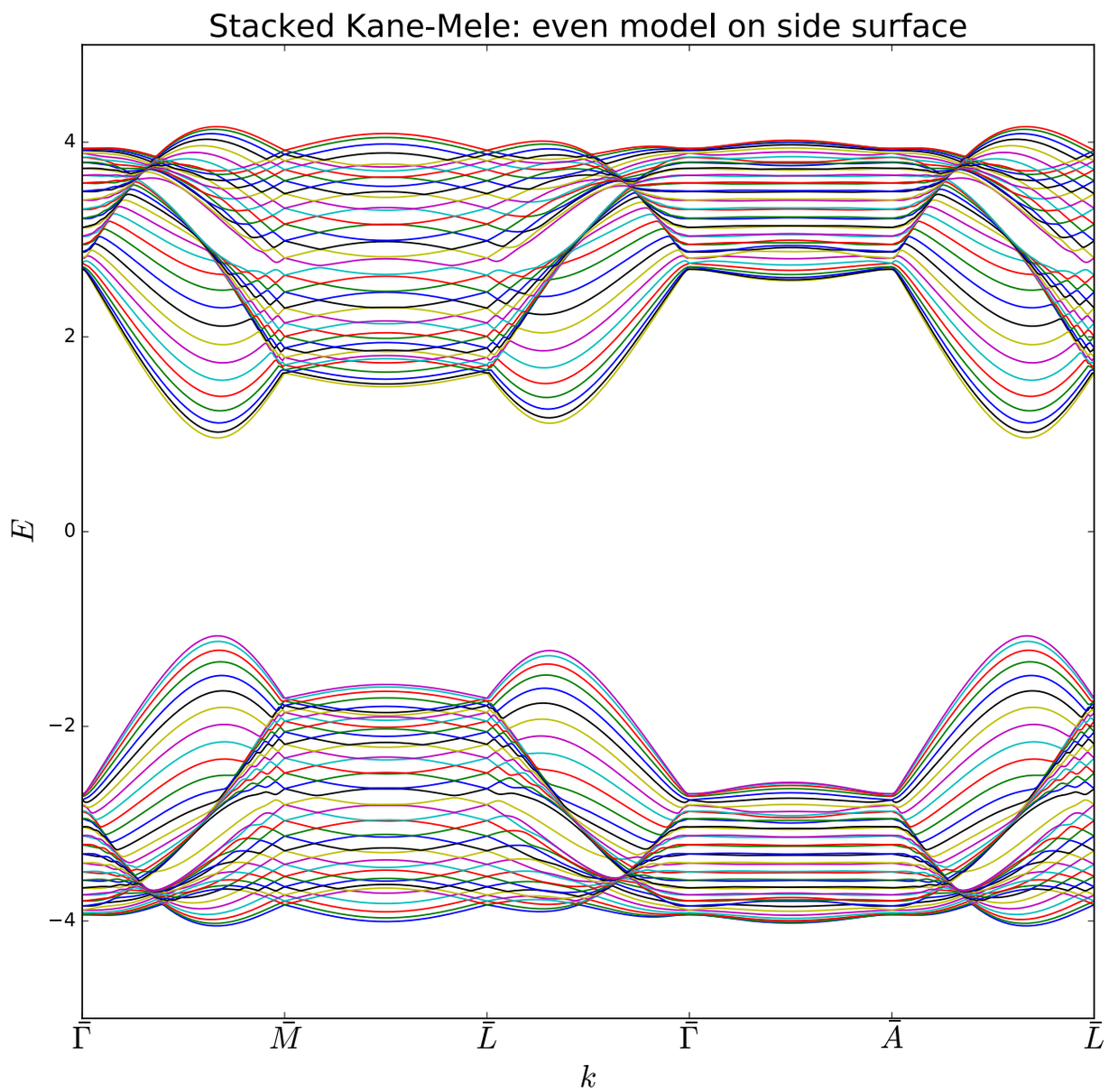
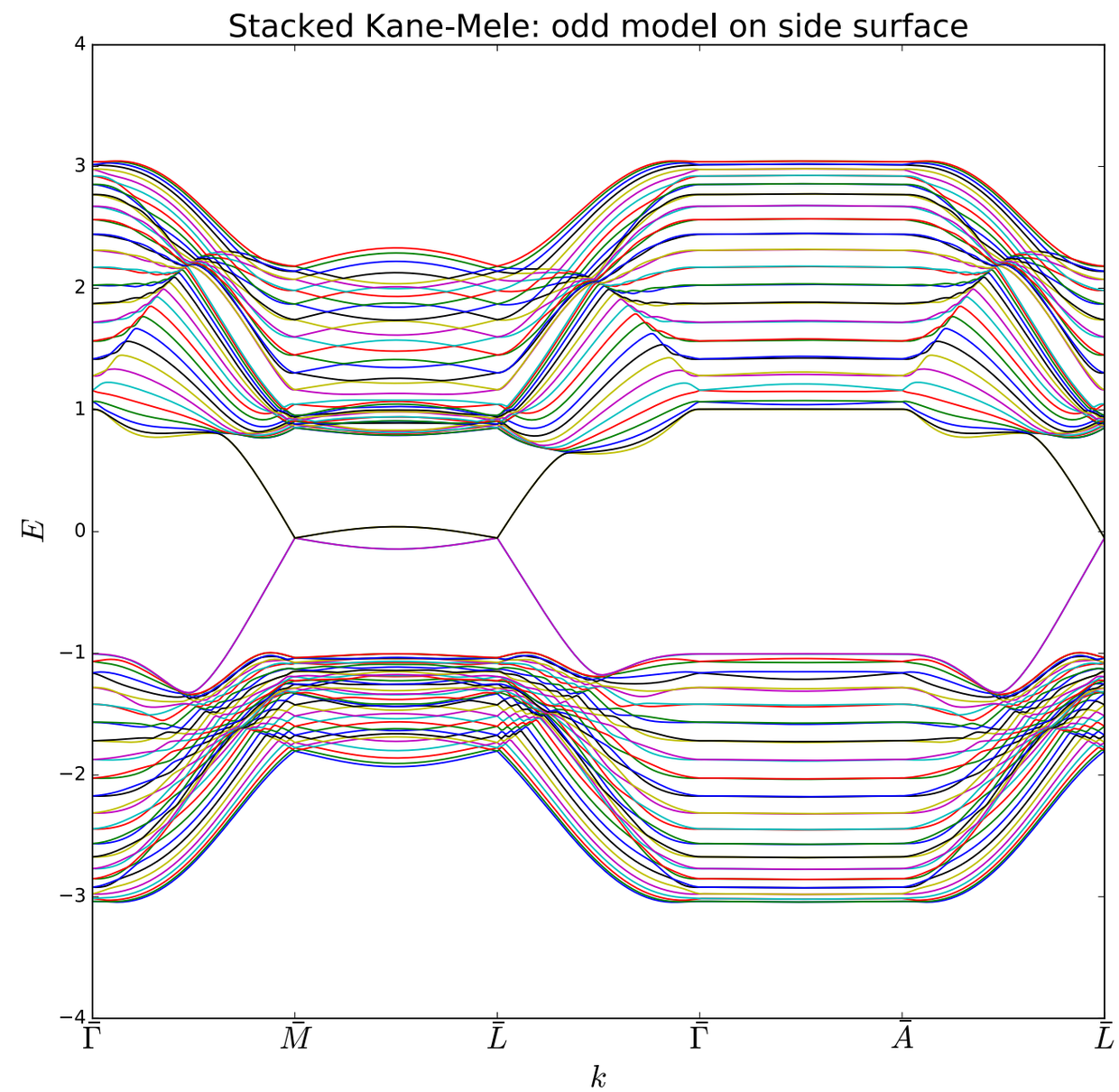


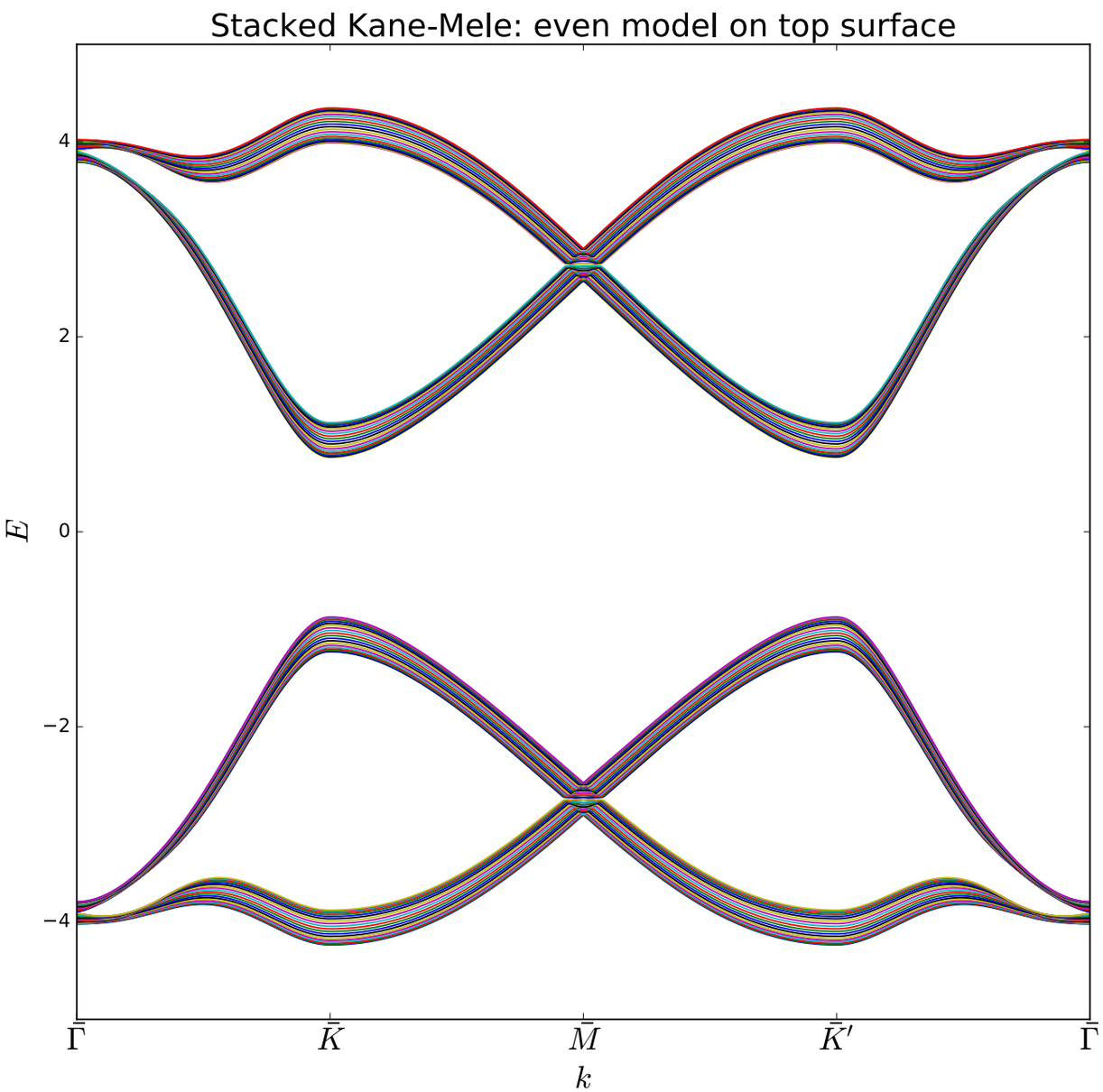
Stacked Kane-Mele: side surfaces have two Dirac cones

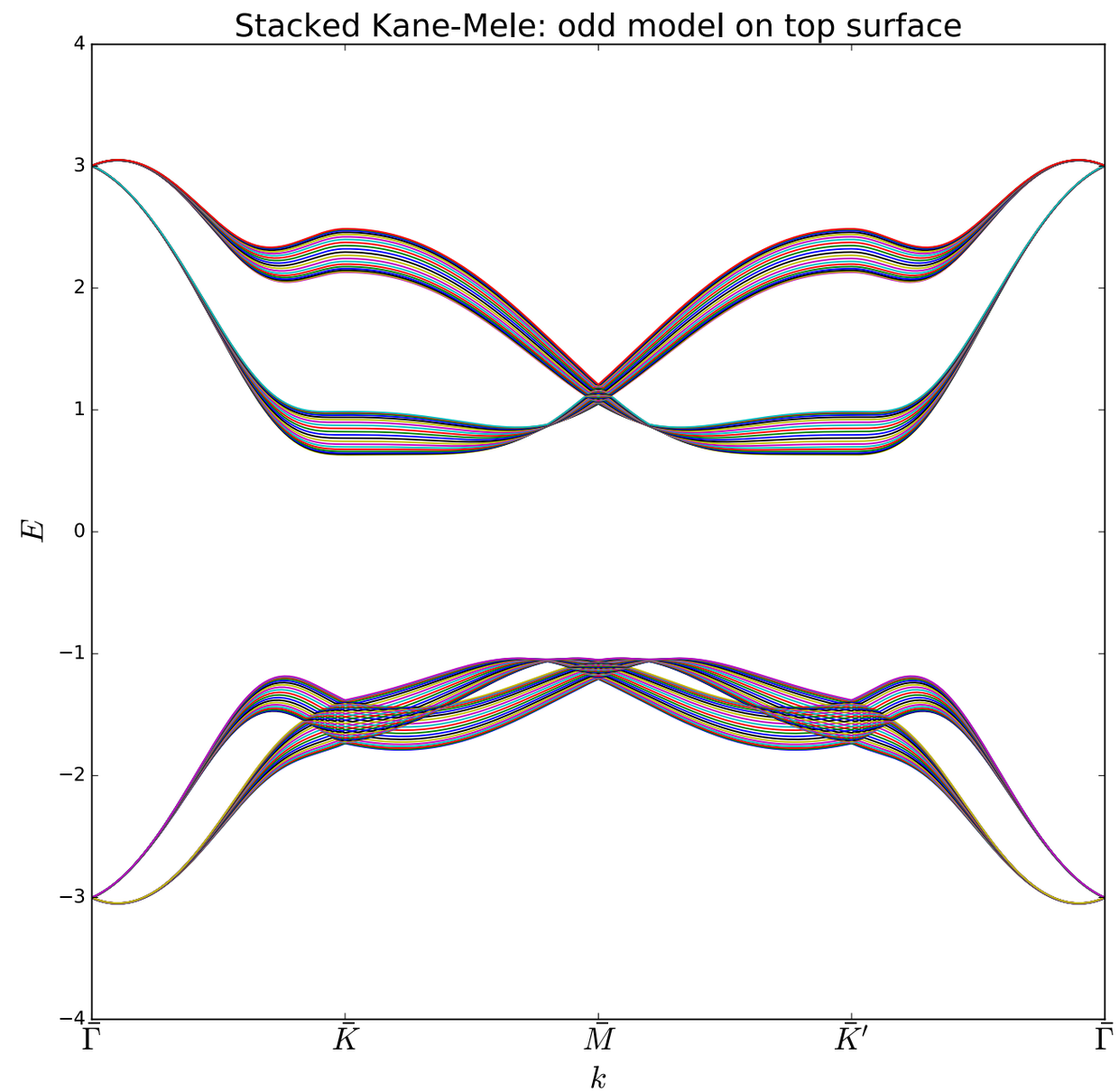




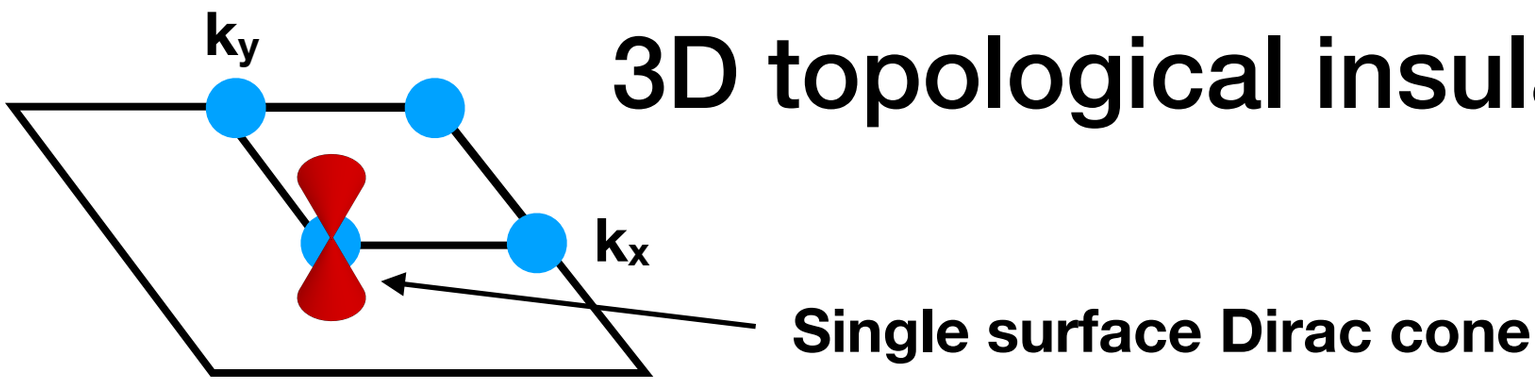
PythTB is based at: http://physics.rutgers.edu/pythtb/

Stacked Kane-Mele: top surface is gapped





PythTB is based at: http://physics.rutgers.edu/pythtb/

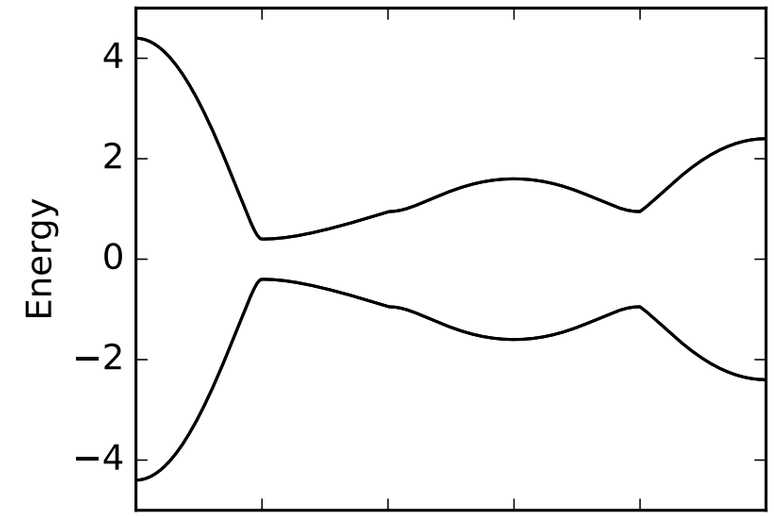


3D topological insulator

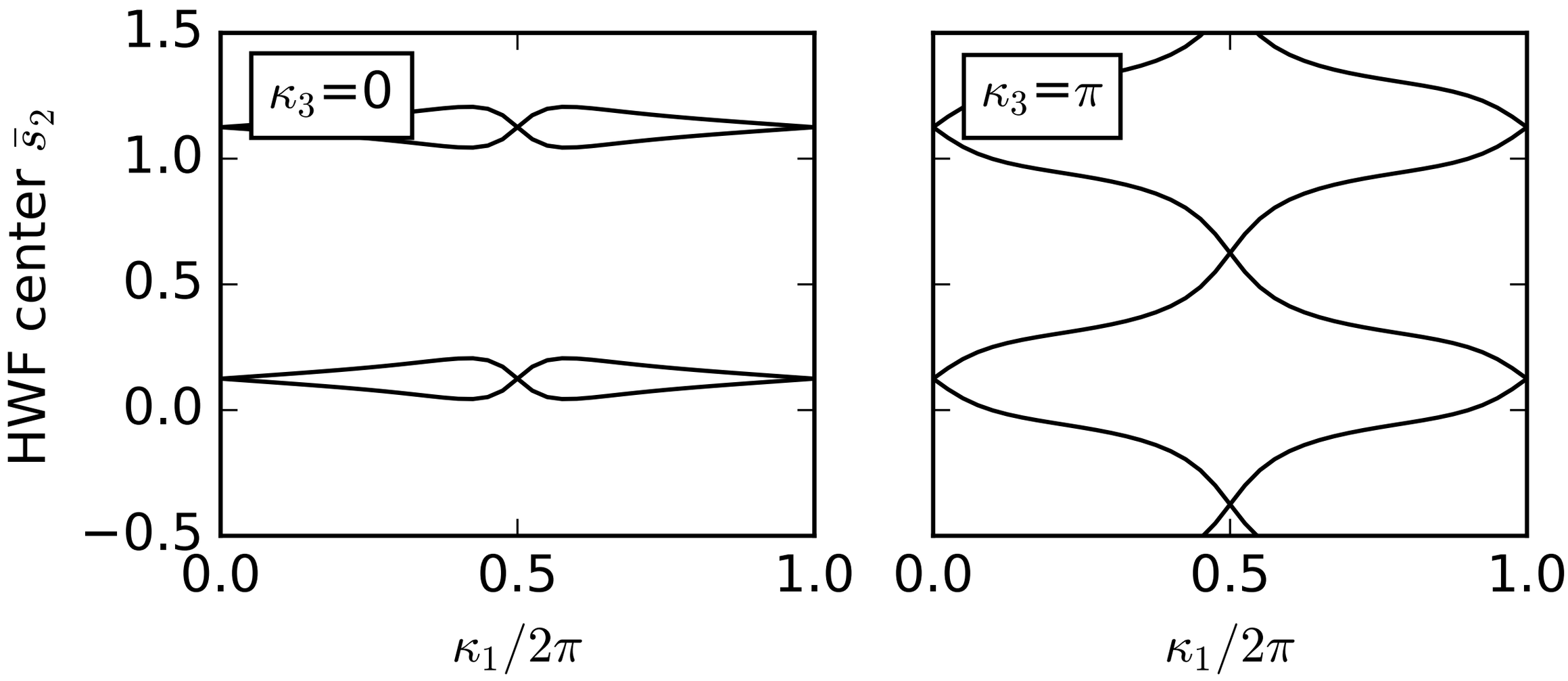
- Fu-Kane-Mele model: Phys. Rev. Lett. 98, 106803 (2007)
- PythTB code, fkm.py, available by David Vanderbilt at: http://physics.rutgers.edu/~dhv/pythtb-book-examples/ptb_samples.html

PythTB is based at: http://physics.rutgers.edu/pythtb/

Fu-Kane-Mele model

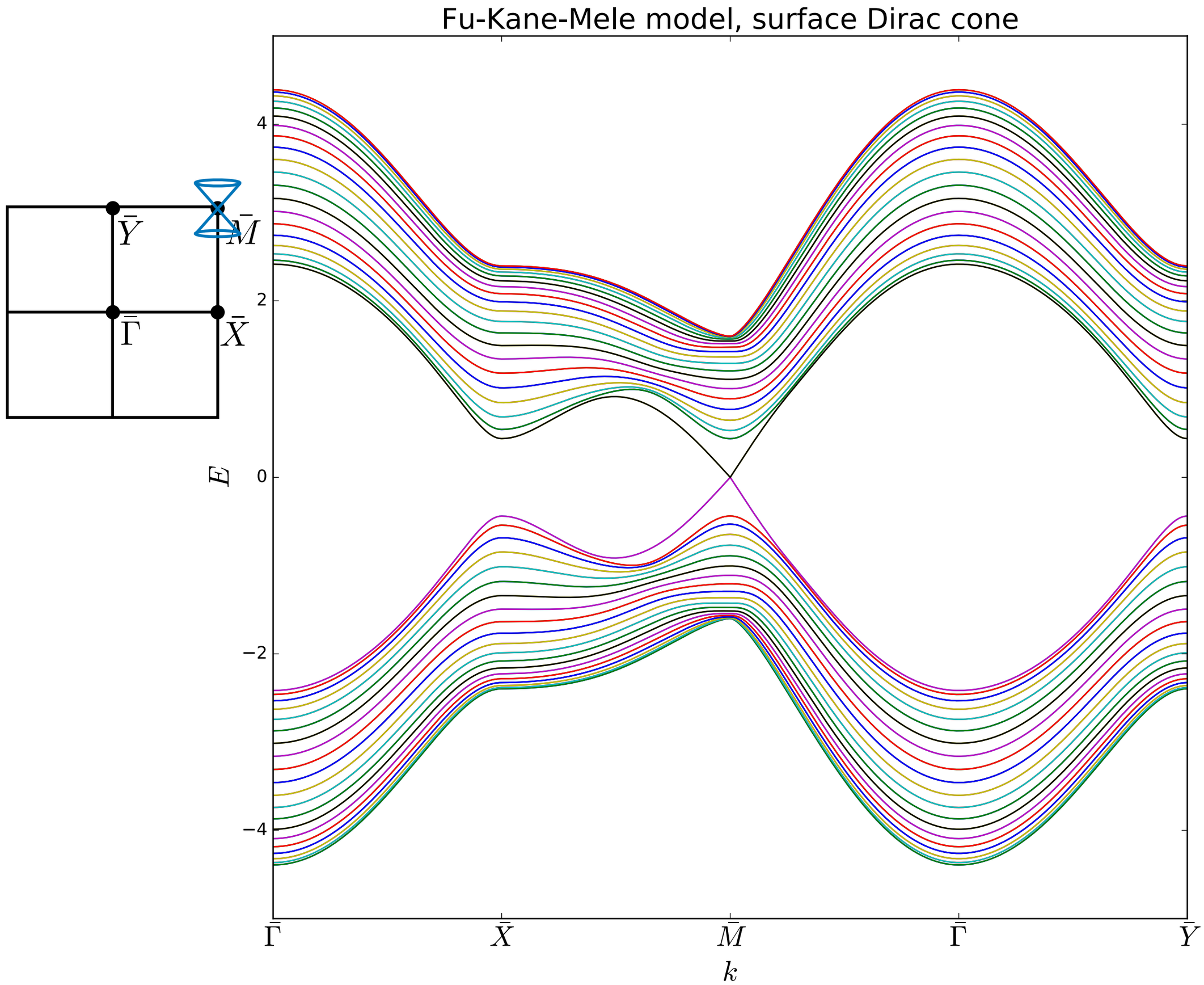


Bulk band structure is gapped



Hybrid Wannier function centers/Berry phase: wind in k3=π plane, not in k3=0

Hallmark of strong TI!!



PythTB is based at: http://physics.rutgers.edu/pythtb/

Exercises

1. Download the Kane-Mele model and plot band structure and Wannier centers. Use “cut_piece” to plot the edge band structure. In my plot I set the onsite energy to zero in the topological phase. What happens when it is non-zero?

2. Add a third dimension and implement a weak TI by stacking layers of the Kane-Mele model. Verify the side surfaces have two surface Dirac cones but the top surface is gapped. Add code to plot the Berry phase in the $k_z=0$ and $k_z=\pi$ planes.

3. Download the 3d Fu-Kane-Mele model from: http://physics.rutgers.edu/~dhv/pythtb-book-examples/ptb_samples.html. Implement the model. Cut into a finite slab to see the surface states. Notice that for a slab in any direction, there is one surface Dirac cone.

PythTB is based at: http://physics.rutgers.edu/pythtb/