PythTB for (topological) tight-binding models Part 2

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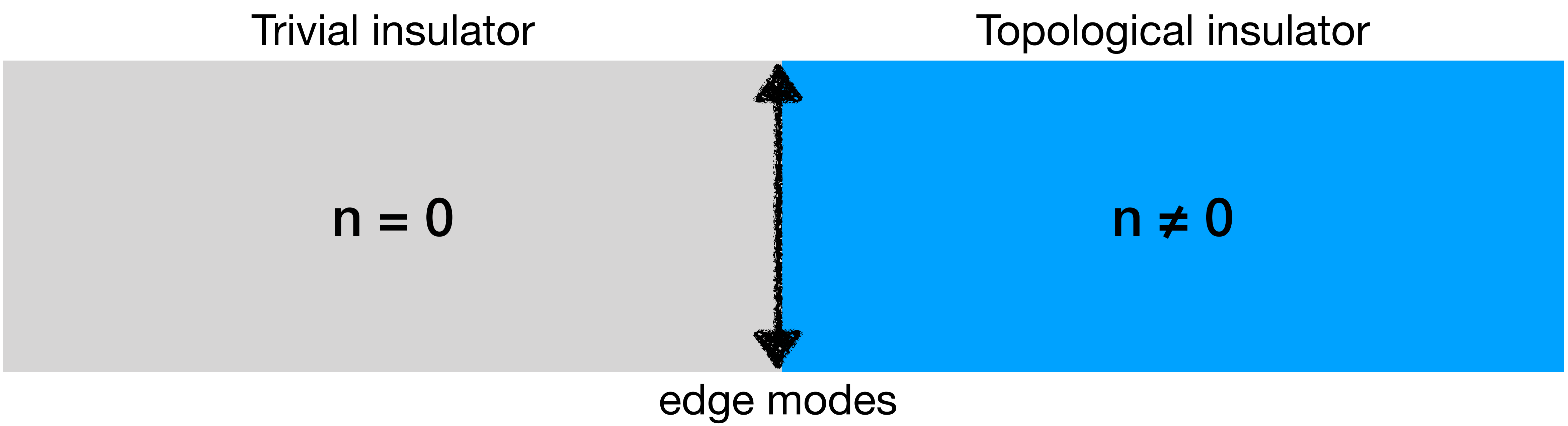
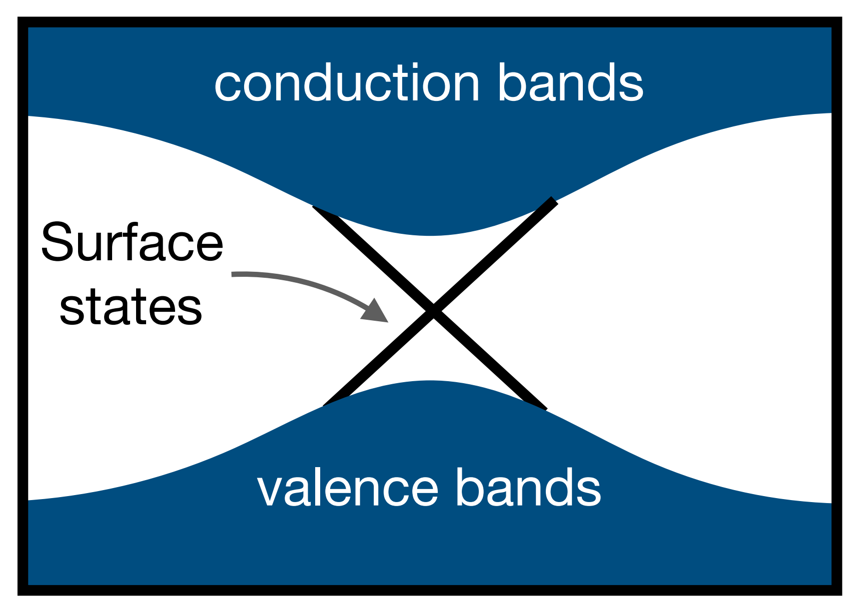
PythTB is based at: http://physics.rutgers.edu/pythtb/

Bulk-boundary correspondence



Quantized topological invariant

⇒ gapless edge states

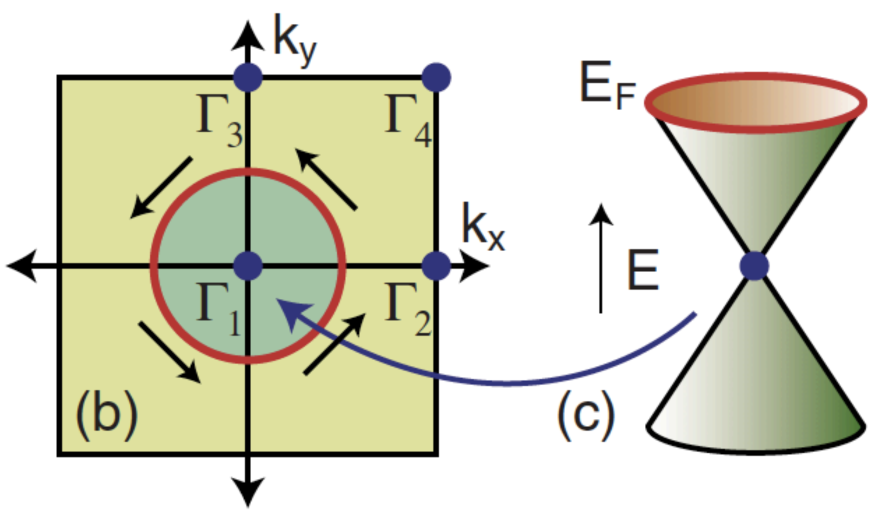


Slab band structure

Bulk-boundary correspondence in 3d

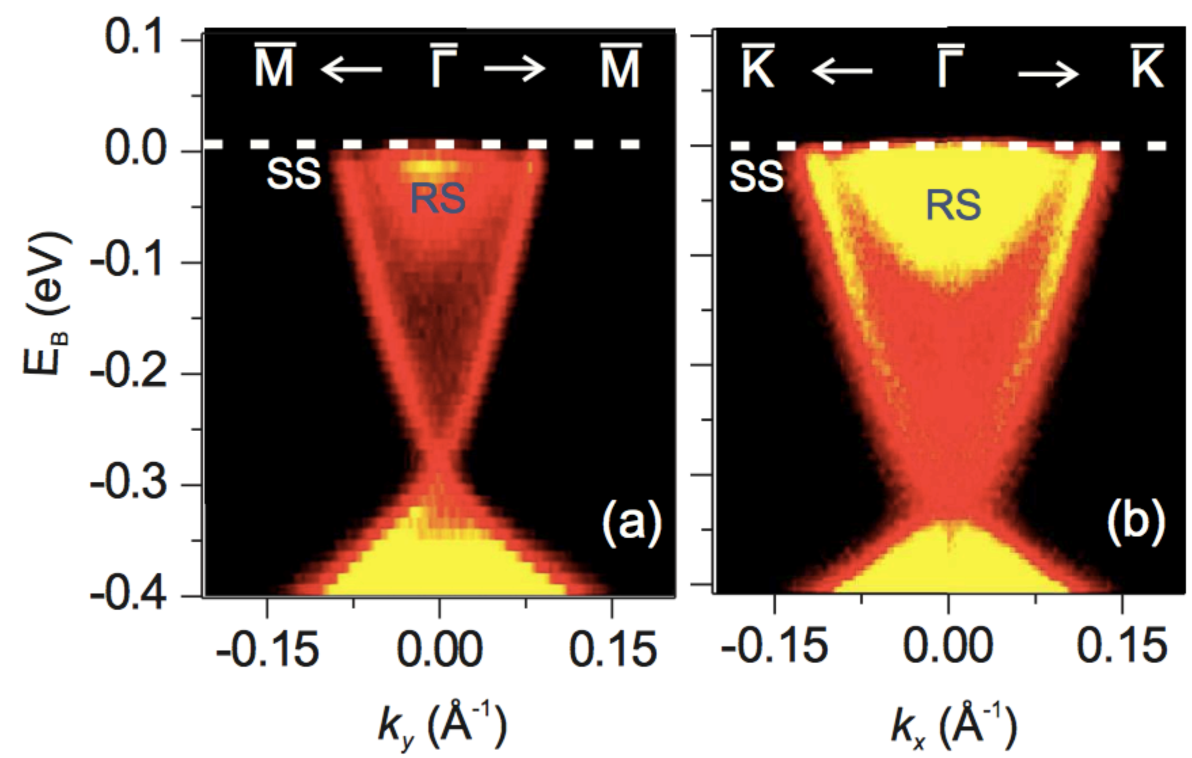
- Surface states are “Dirac cones:” gapless and disperse in two directions

“Strong” topological insulator has odd number of surface Dirac cones



Recommended review article:
Kane and Hasan, RMP **82**, 3045 (2010)

Surface Dirac cone in Bi_2Se_3

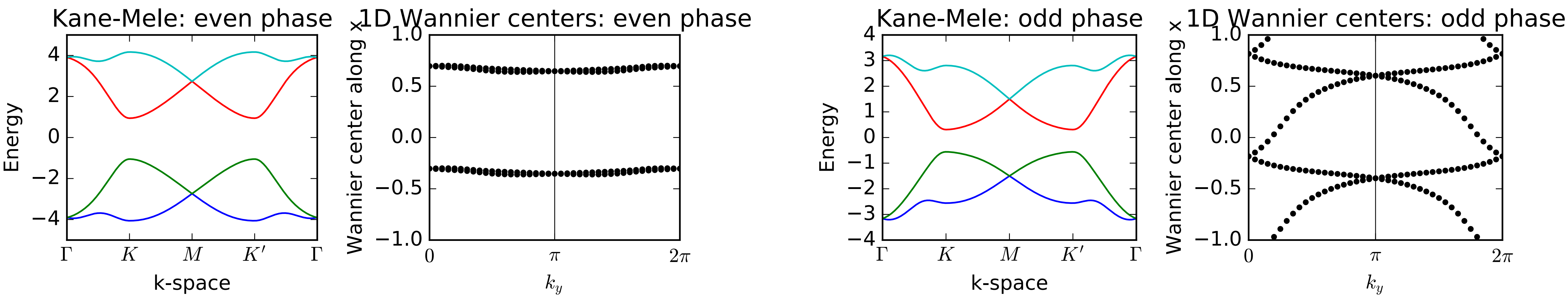


Xia et al, *Nat. Phys.* 5, 398–402 (2009)

Kane-Mele model

- Recall Barry's lecture: 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

Output:



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Kane-Mele model: edge states

New attribute: cut_piece
Arguments: 1. # layers in slab,
2. real space lattice vector that is finite in slab,
3. do (not) glue edges

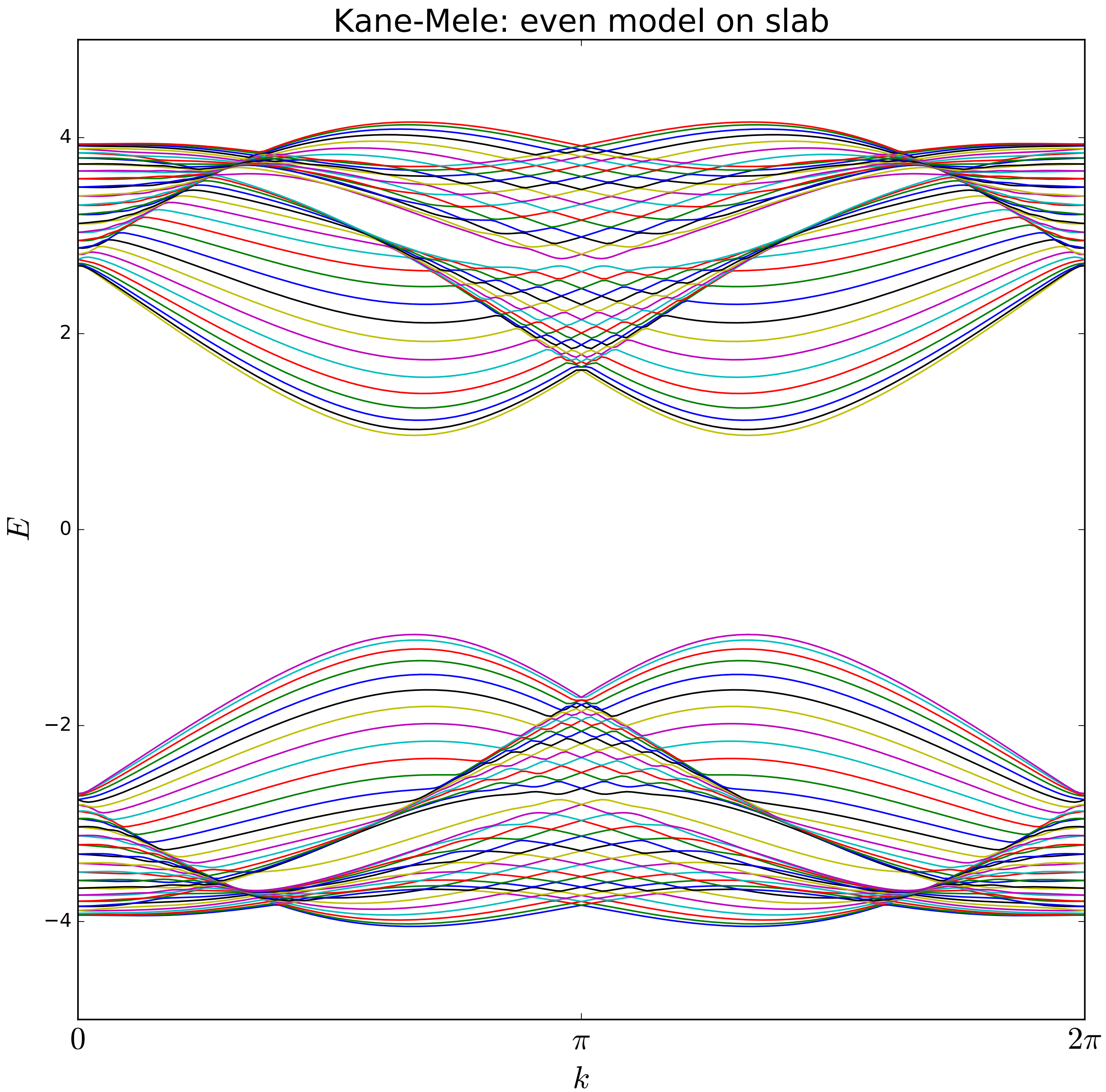
Then plot in **surface BZ**
(slab has only one periodic direction)

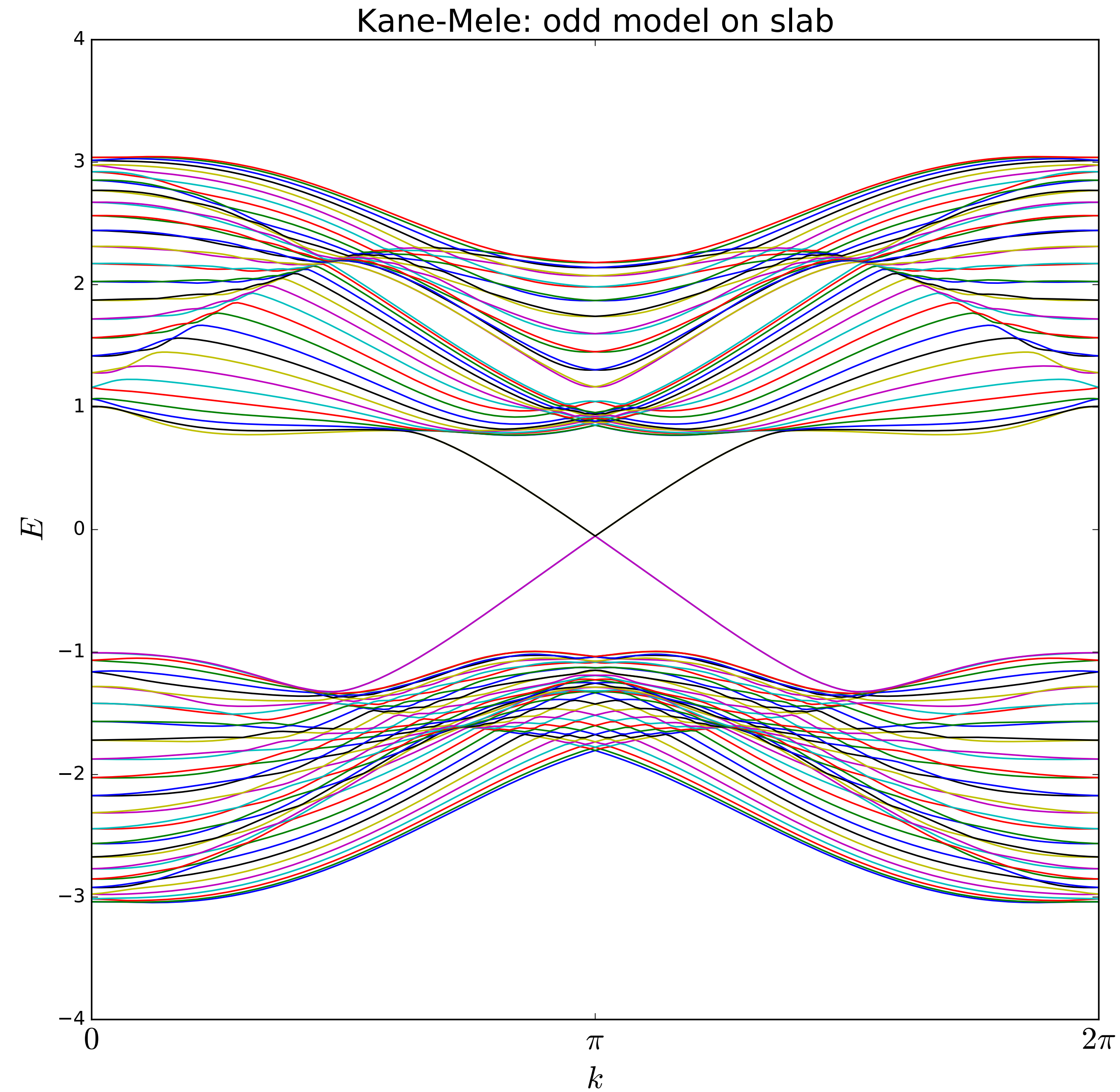
```
# now plot the edge states
for top_index in ["even","odd"]:

    # number of layers in slab
    numbands=20

    # get model (topo or trivial)
    my_model=get_kane_mele(top_index)

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

    # number of kpts between high-symmetry points
    numpoints=100

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

    #get evals
    fin_evals=fin_model.solve_all(fin_path)

    #plot
    fin_fig=pl.figure(figsize=(10,10))
    for i in range(4*numbands): ## 4 is the number of orbitals
        pl.plot(fin_evals[i],linewidth=1.0)
    pl.xticks([0,numpoints,2*numpoints],[r'$0$',r'$\pi$',r'$2\pi $',]
    pl.xlabel(r'$k$',fontsize=20)
    pl.ylabel(r'$E$',fontsize=20)
    pl.title("Kane-Mele: "+top_index+" model on slab",fontsize=20)

    fin_fig.tight_layout()
    fin_fig.savefig("kane_mele_"+top_index+"_edge.pdf")
```

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

Kane-Mele model: edge states

Output:





Would get same result for any slab termination

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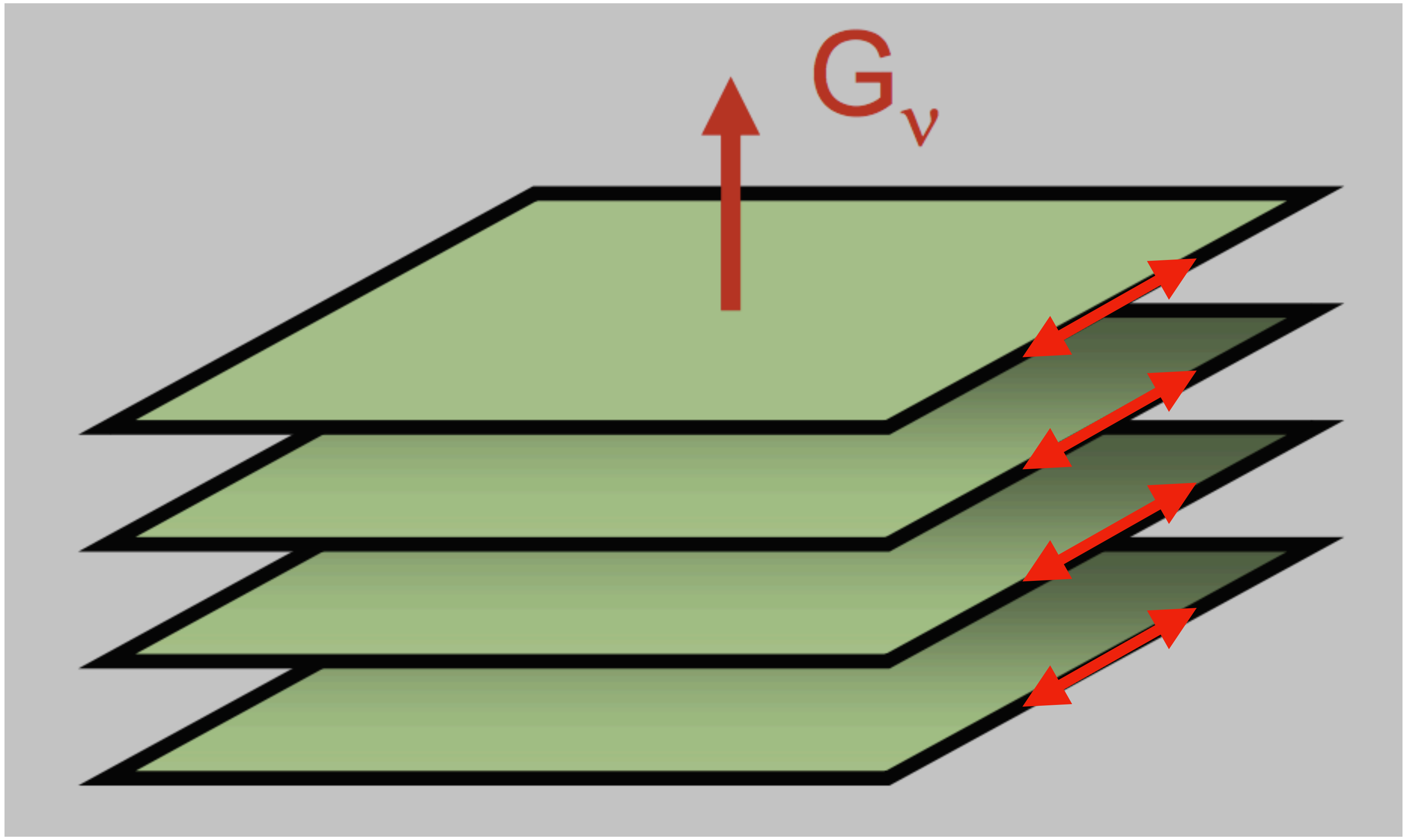
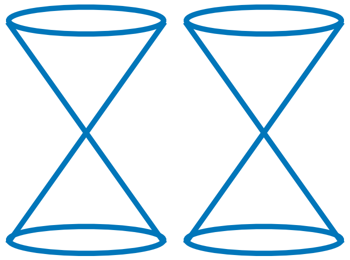
“Weak” topological insulator from stack of 2D TIs

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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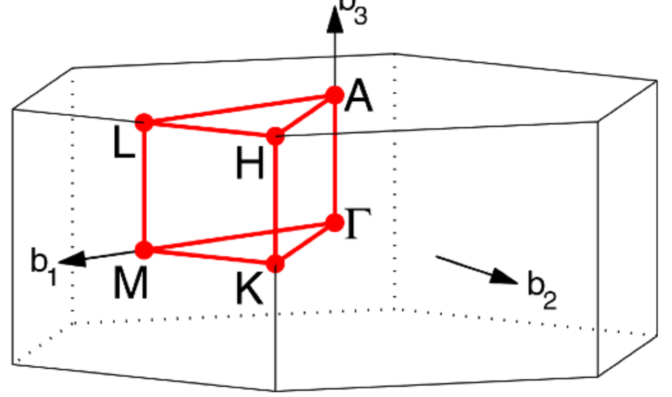
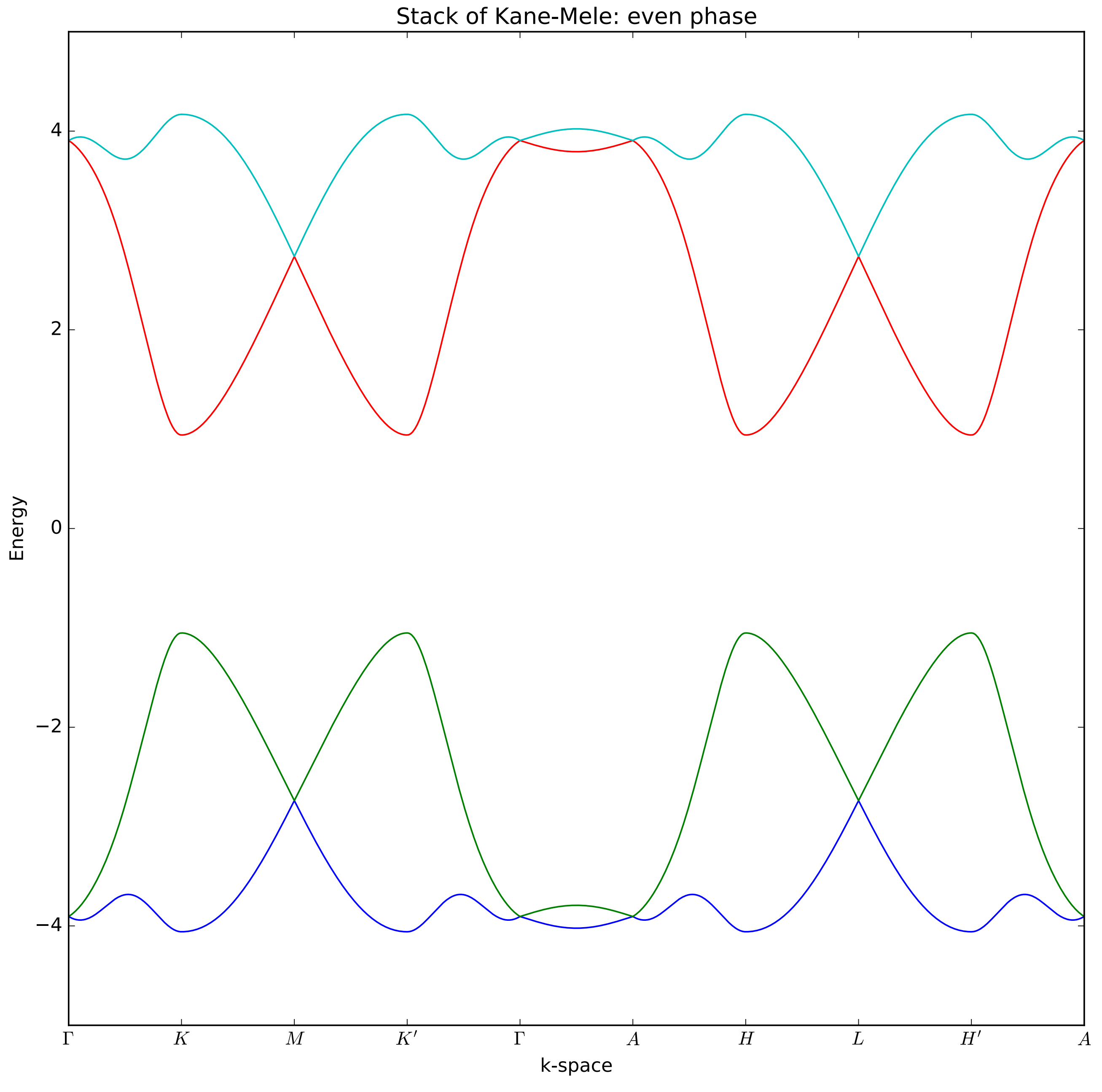
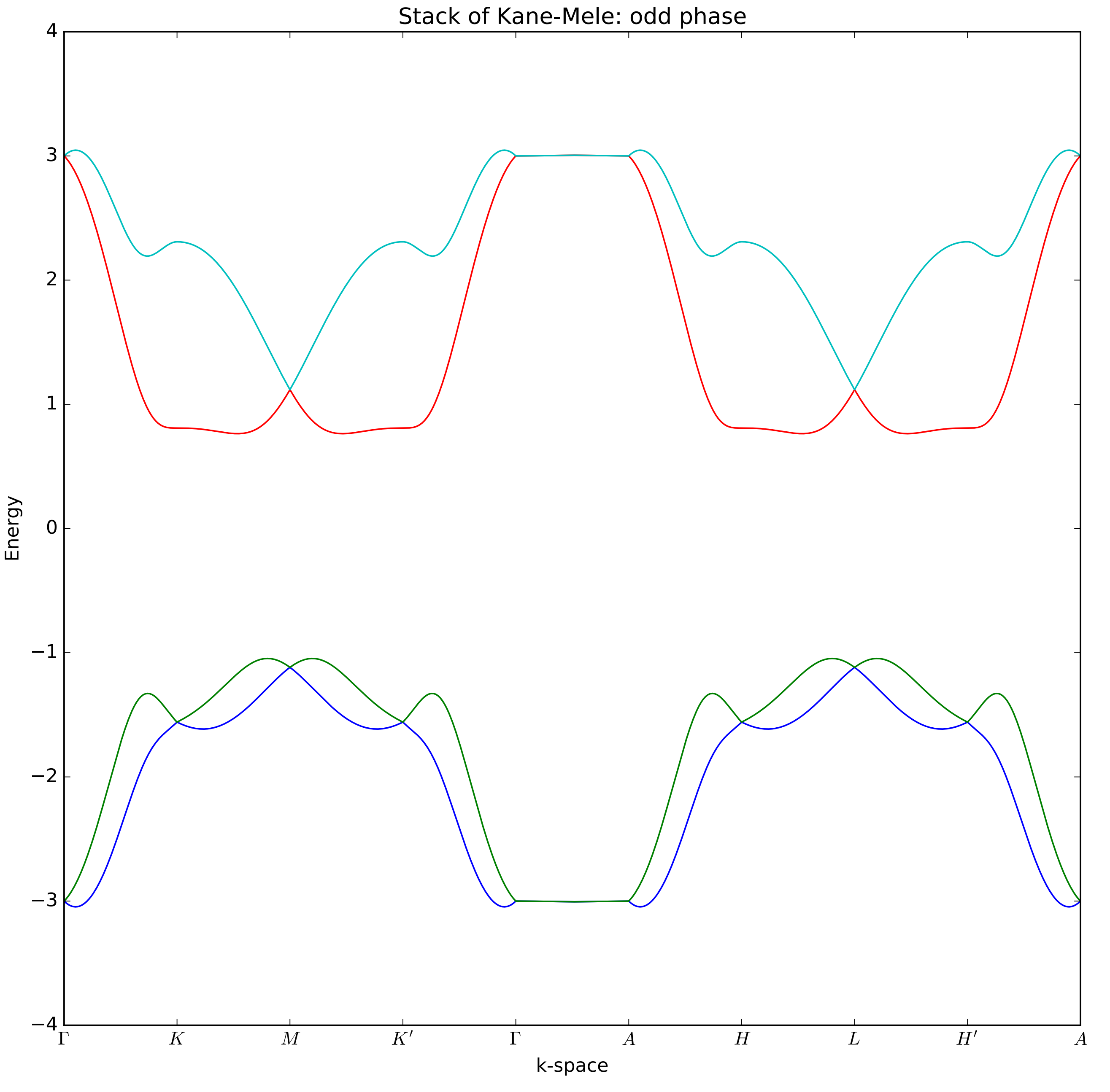


Stacked Kane-Mele

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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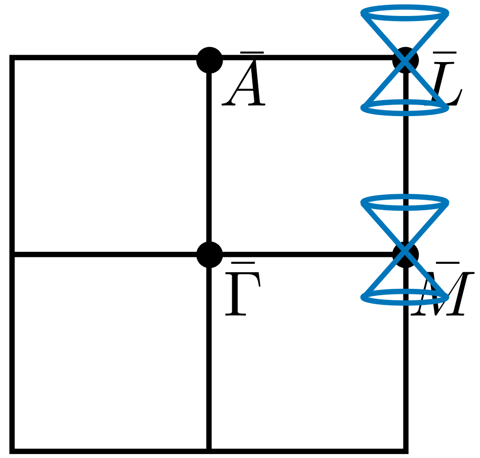
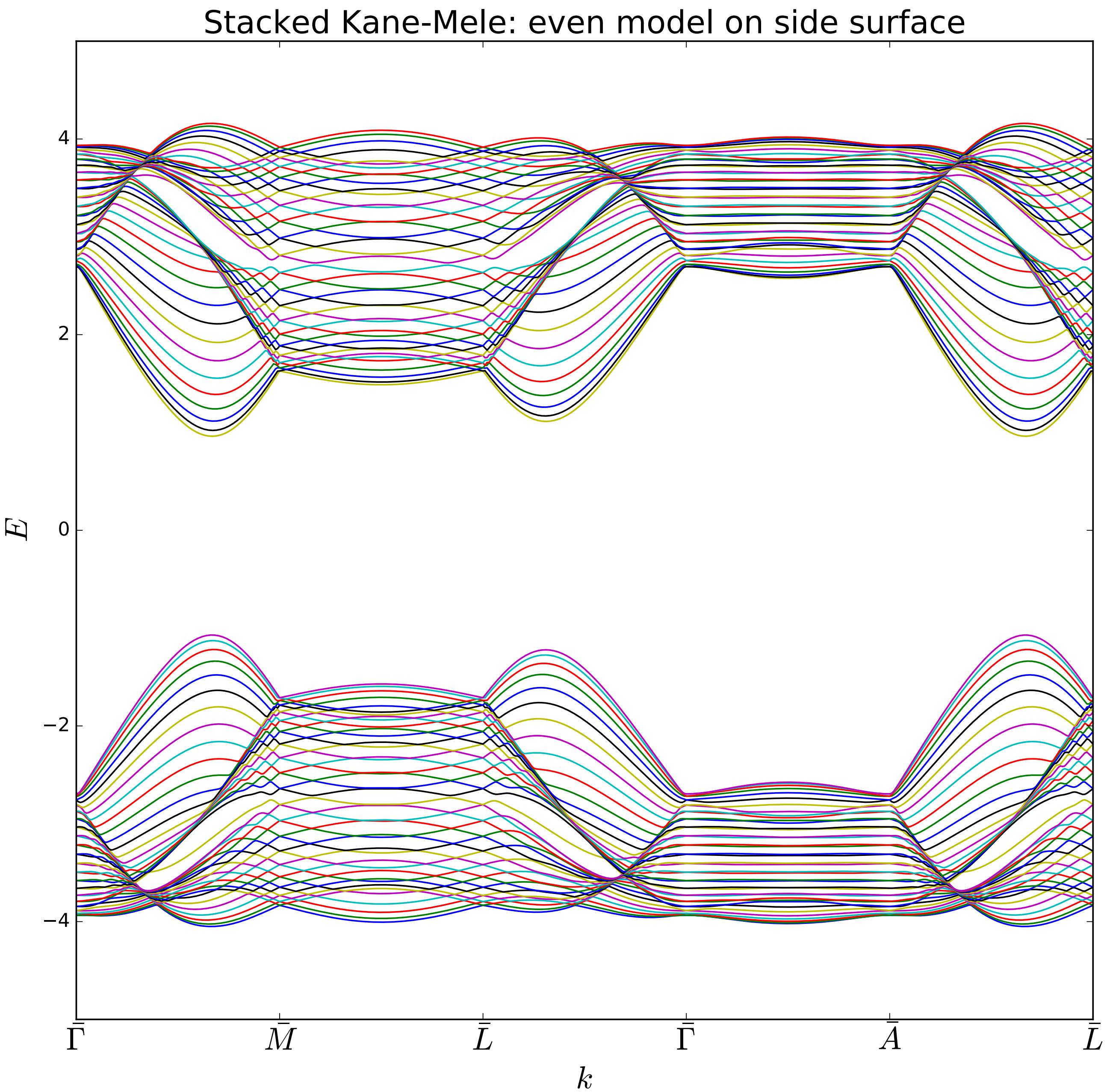
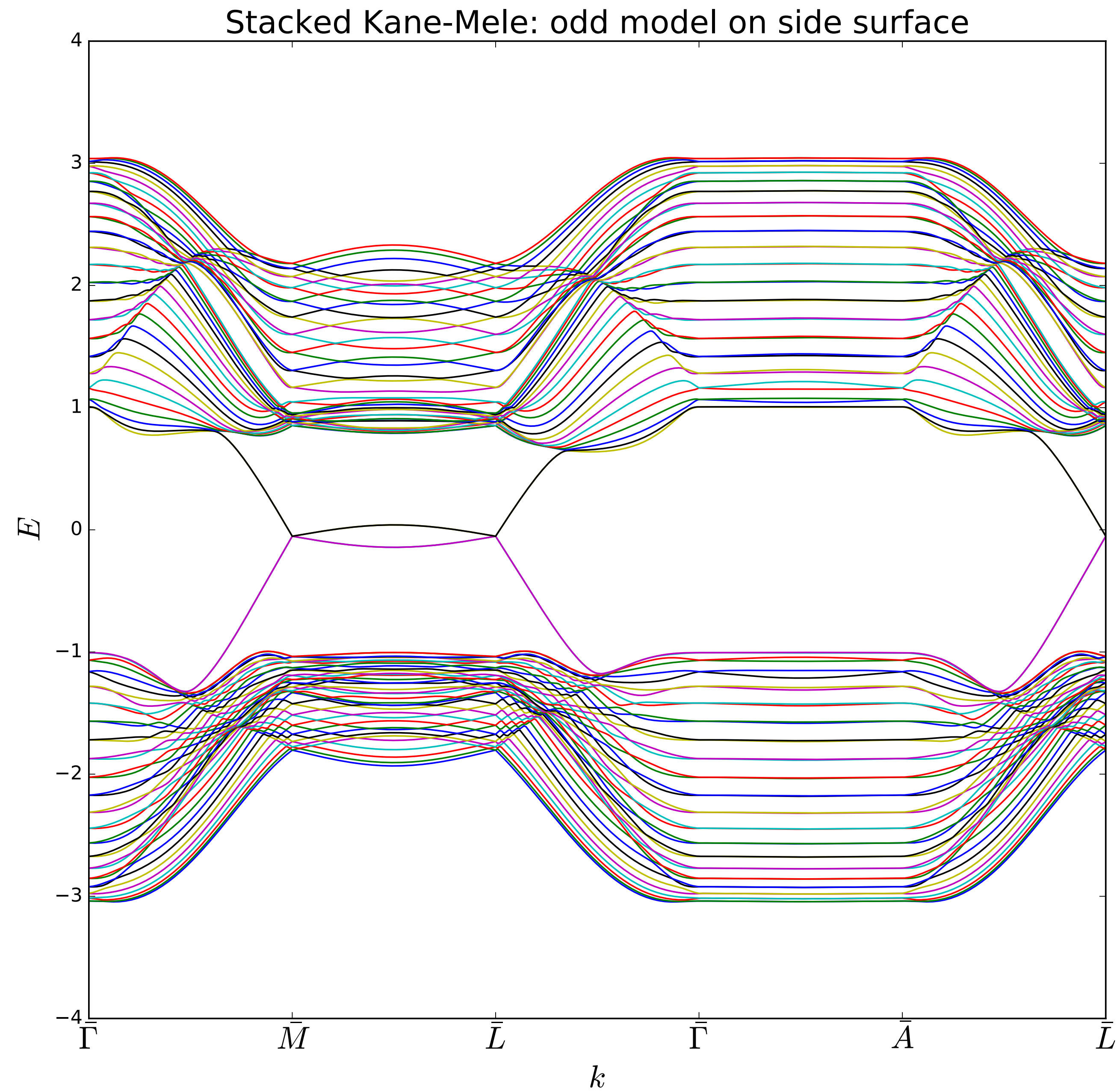


Stacked Kane-Mele: side surfaces have two Dirac cones





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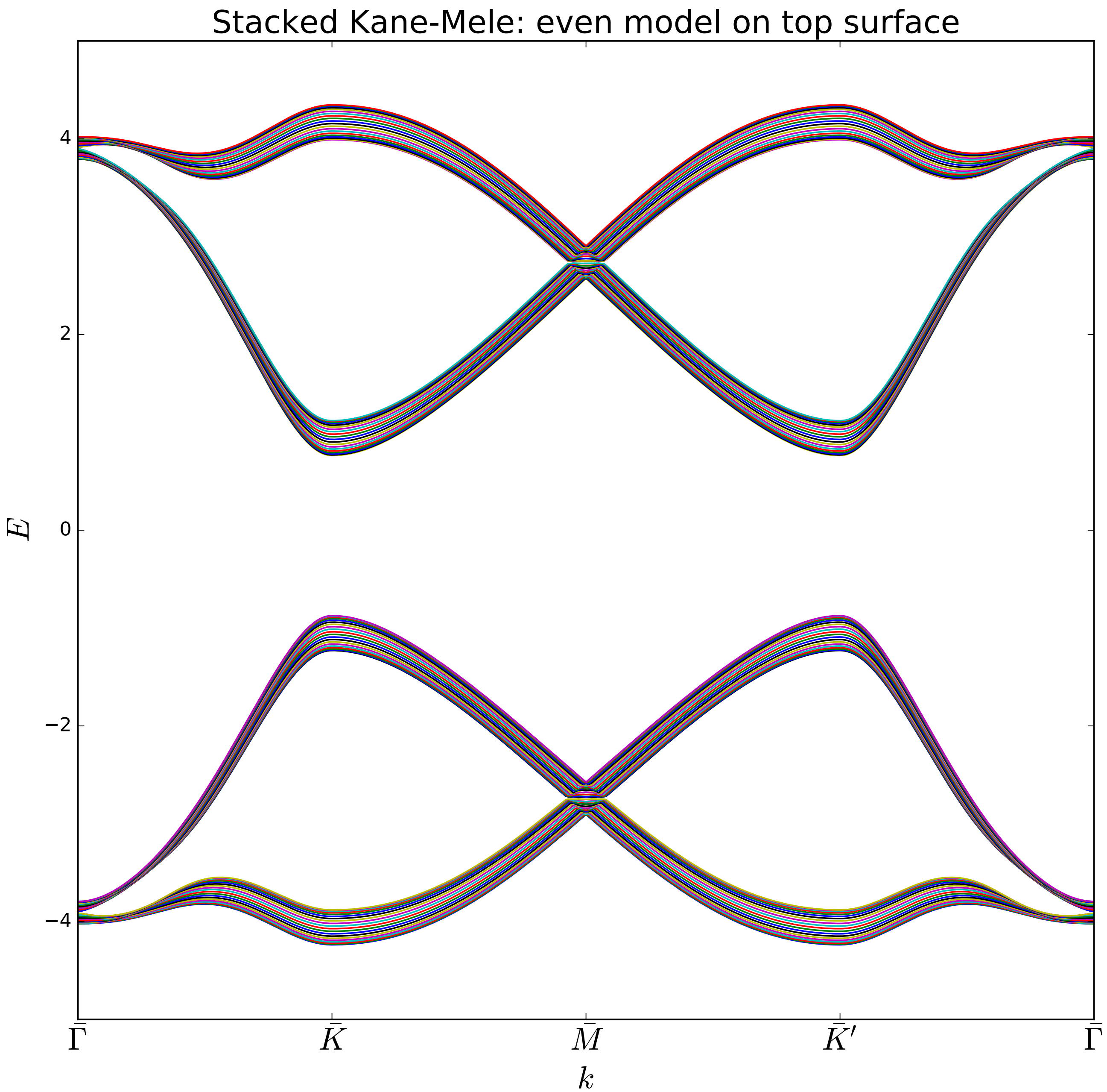
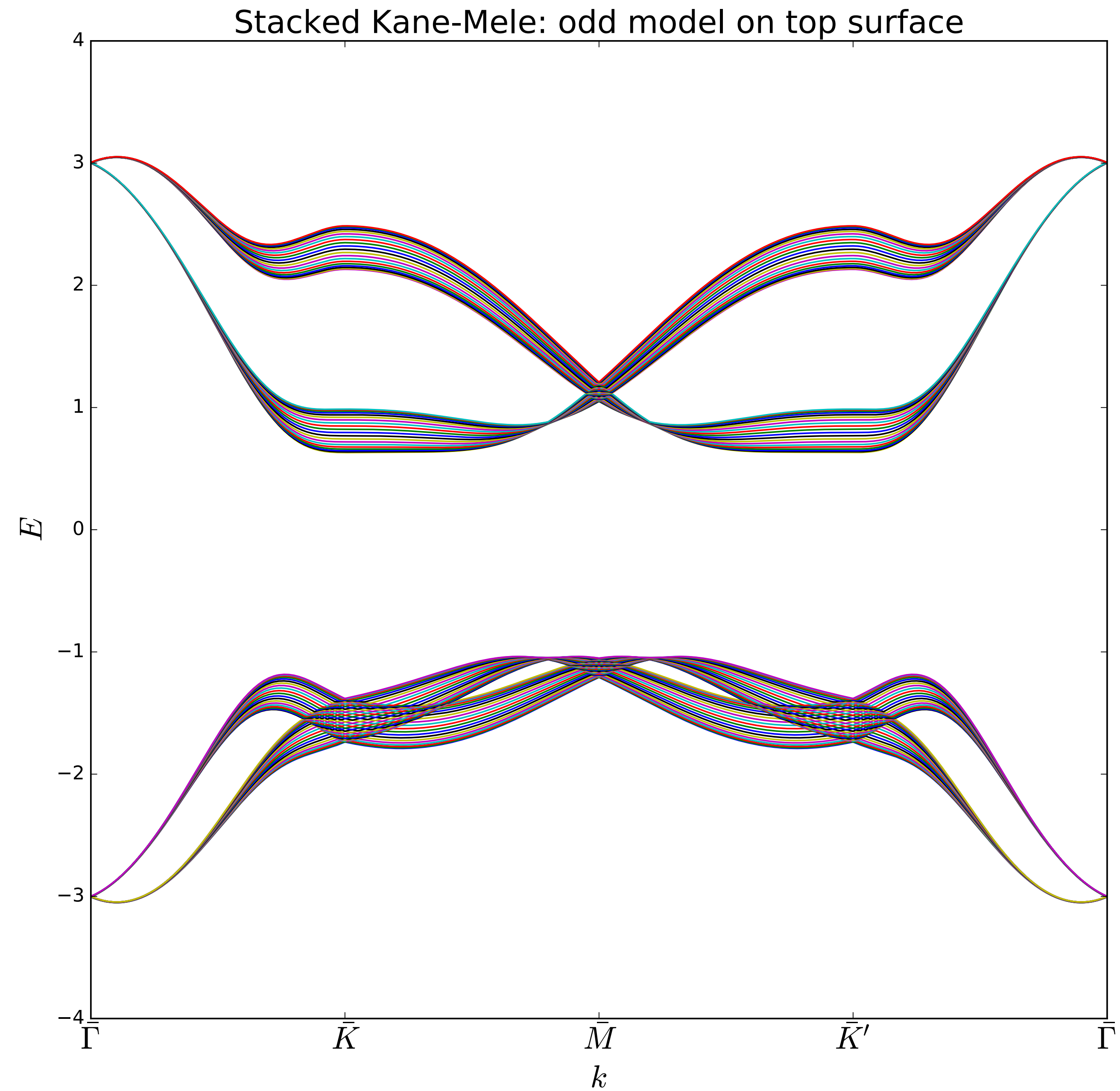
Stacked Kane-Mele: top surface is gapped





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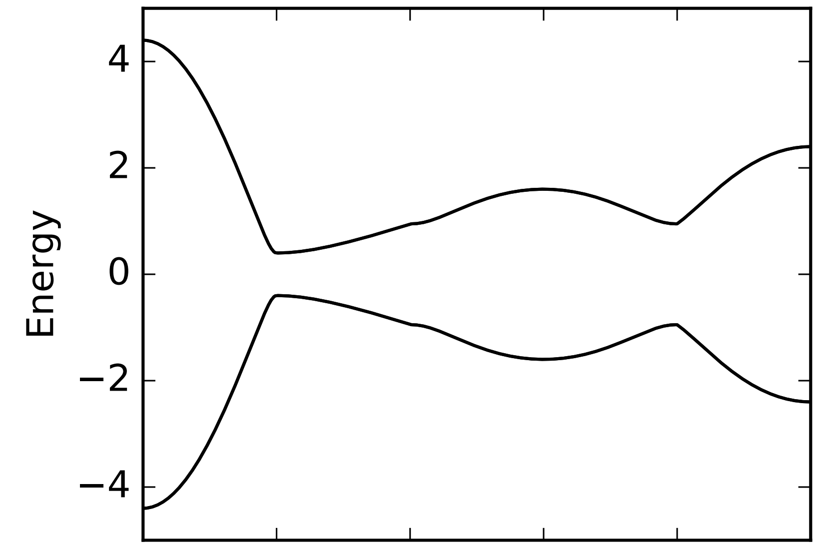
3D topological insulator

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

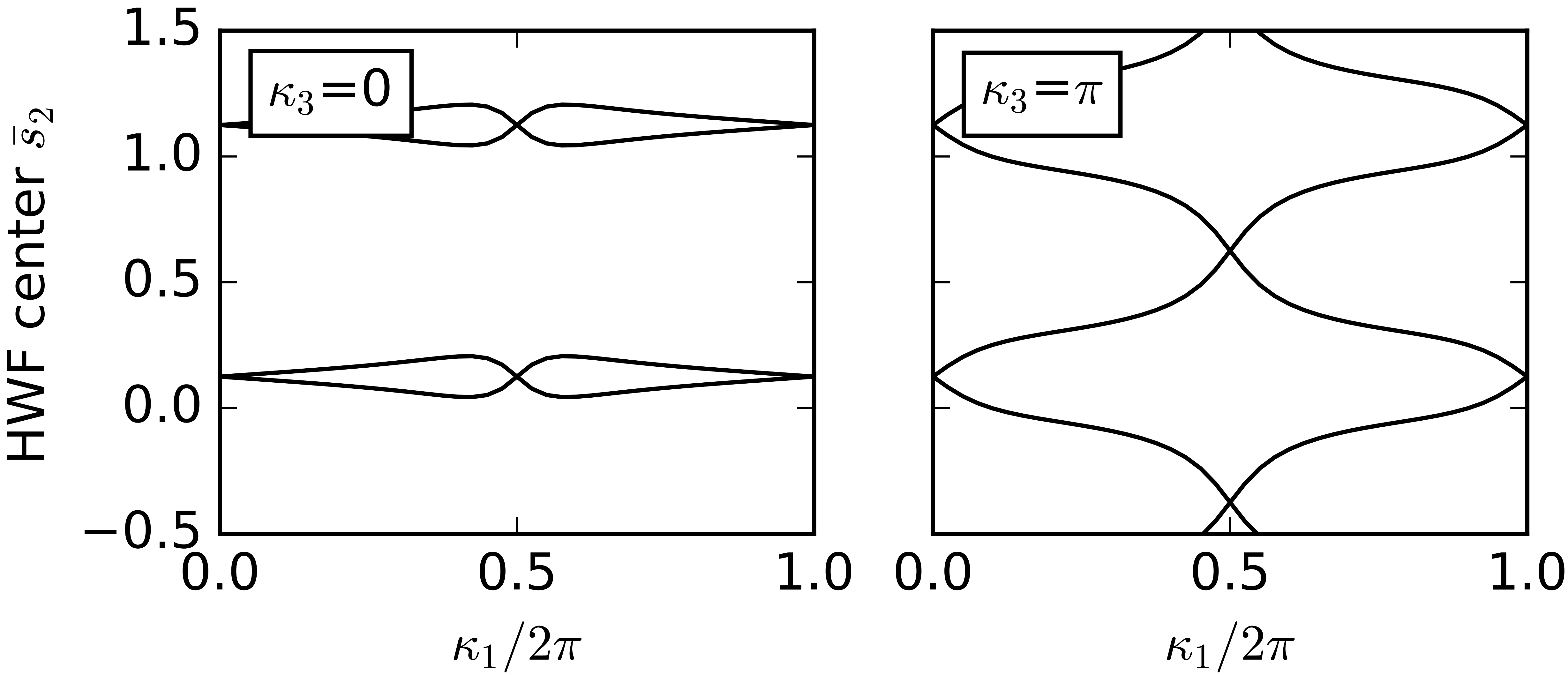
- PythTB code, fkm.py, available by David Vanderbilt at: http://physics.rutgers.edu/~dhv/pythtb-book-examples/ptb_samples.html

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

Fu-Kane-Mele model

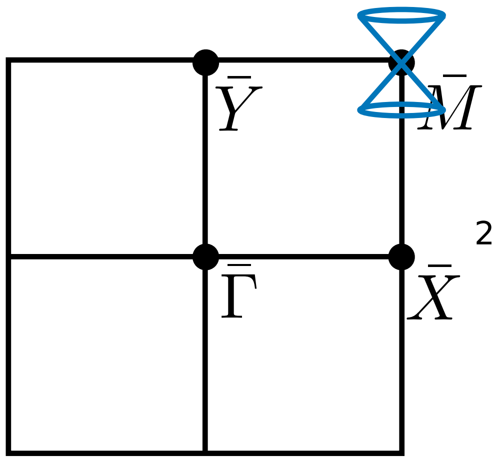


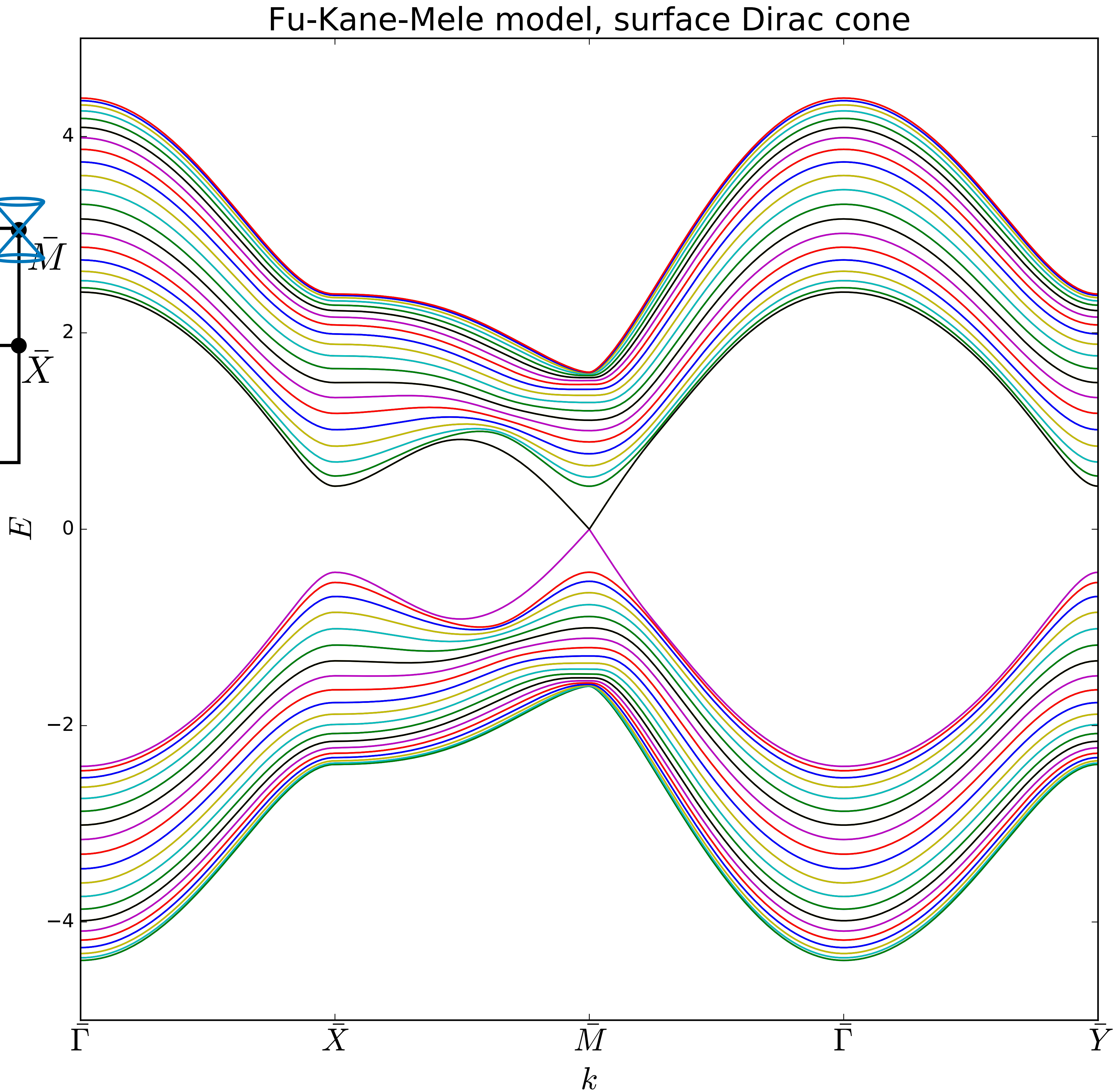
Bulk band structure is gapped



Hybrid Wannier function centers: 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 hybrid Wannier centers 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.

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