3D Z_2 topological insulators

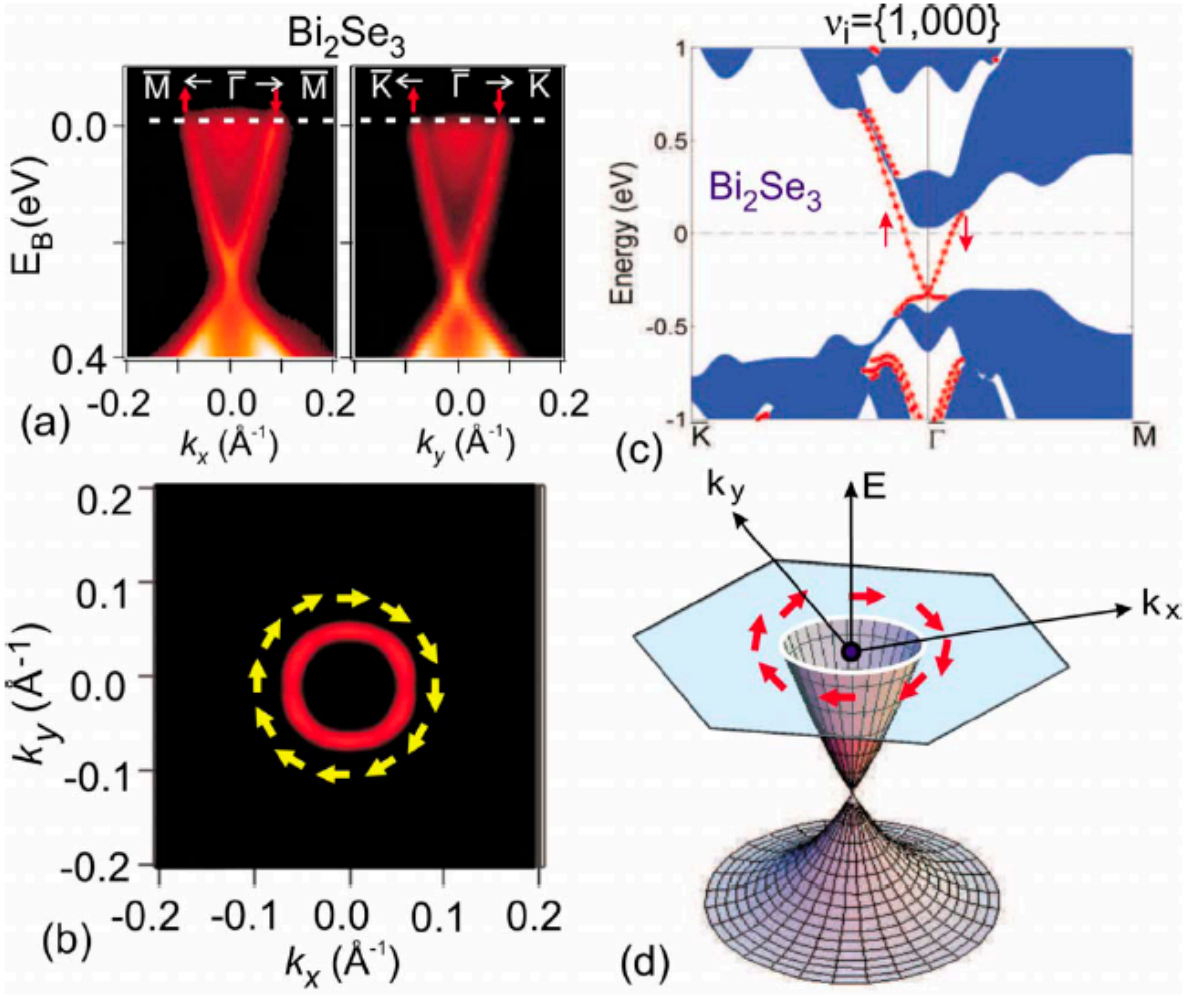
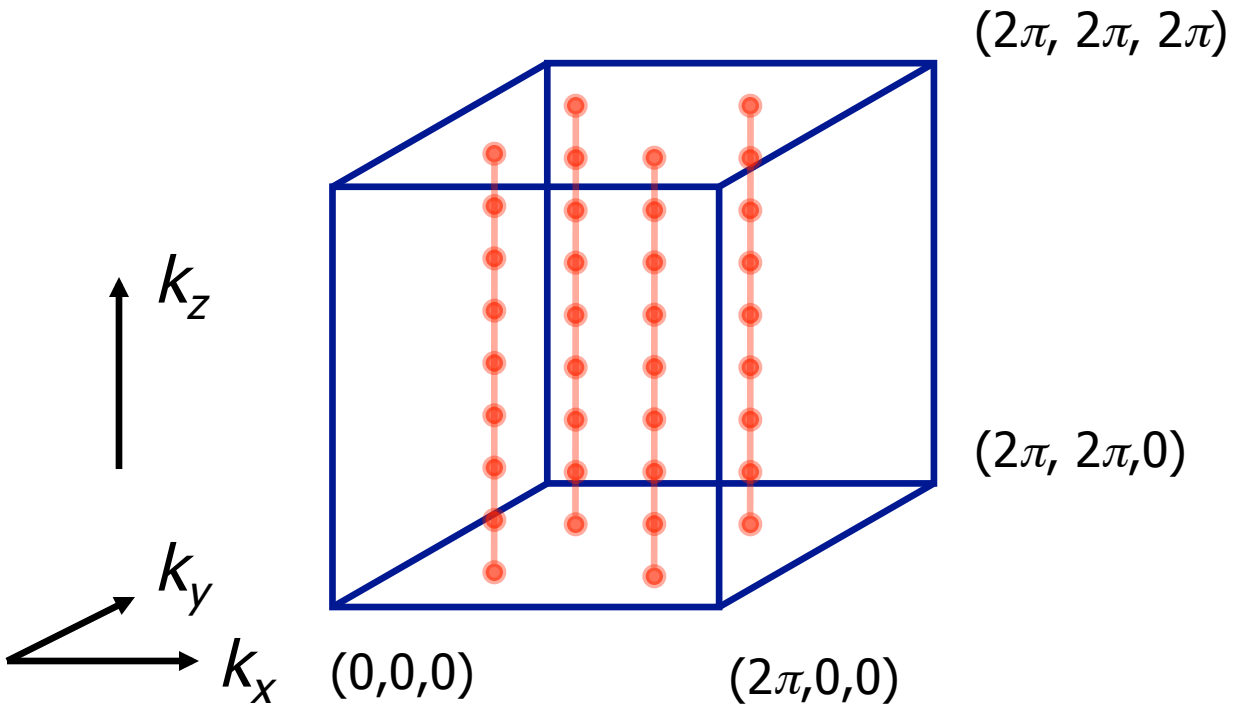
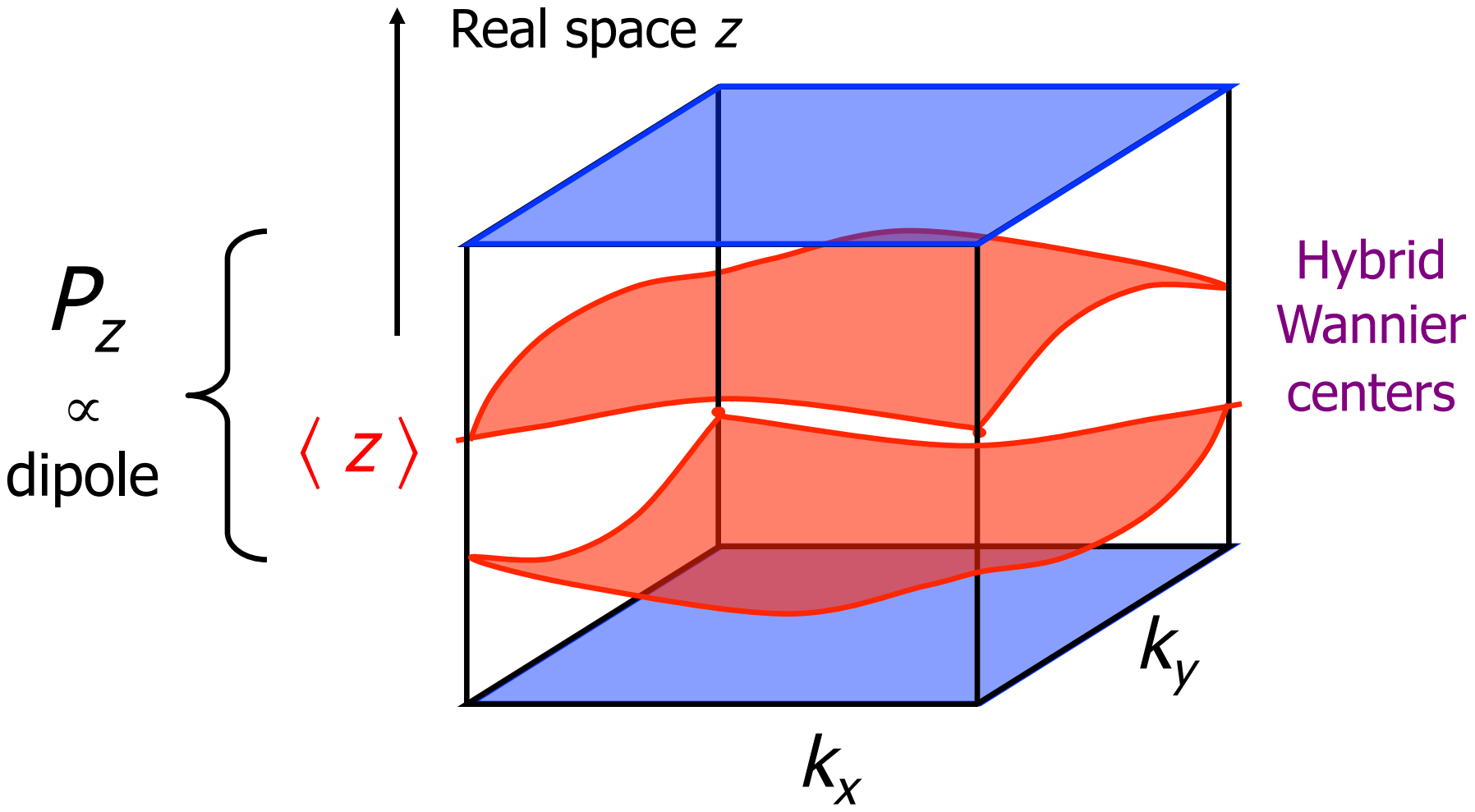


Figure from Hasan and Kane, RMP, 2010
(Adapted from Xia et al., 2008; Hsieh, Xia, Qian, Wray, et al., 2009a; and Xia, Qian, Hsieh, Wray, et al., 2009)

Reminder: Hybrid WF centers



2 occupied bands; no TR; trivial

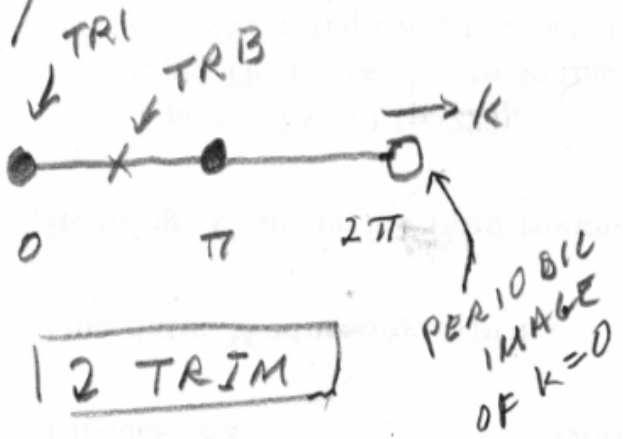


H_k IN TIME-REVERSAL-INVARIANT SYSTEMS

(TRI = TR INVARIANT TRB = TR-BROKEN)

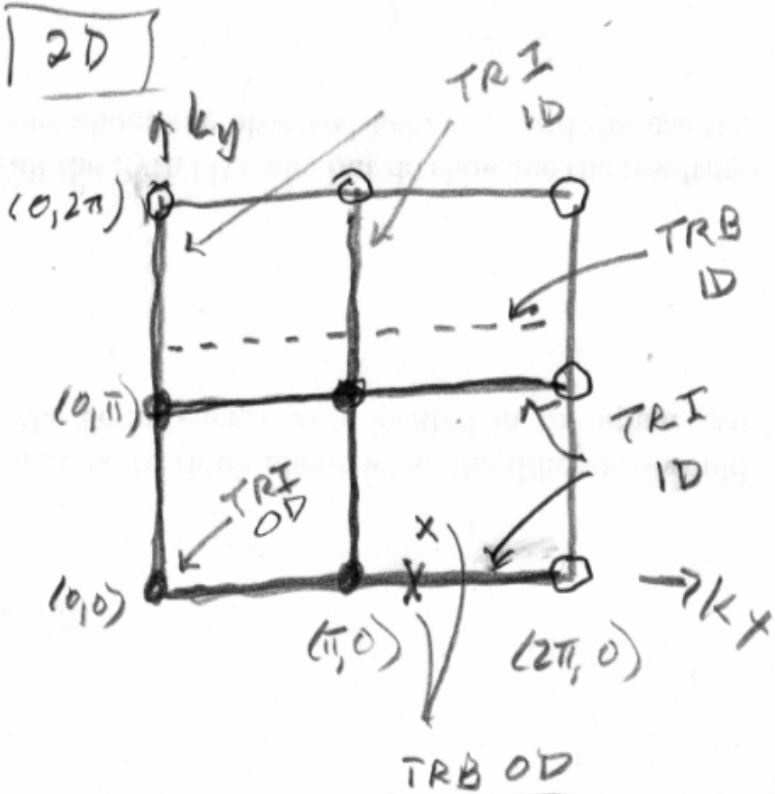
0D

1D



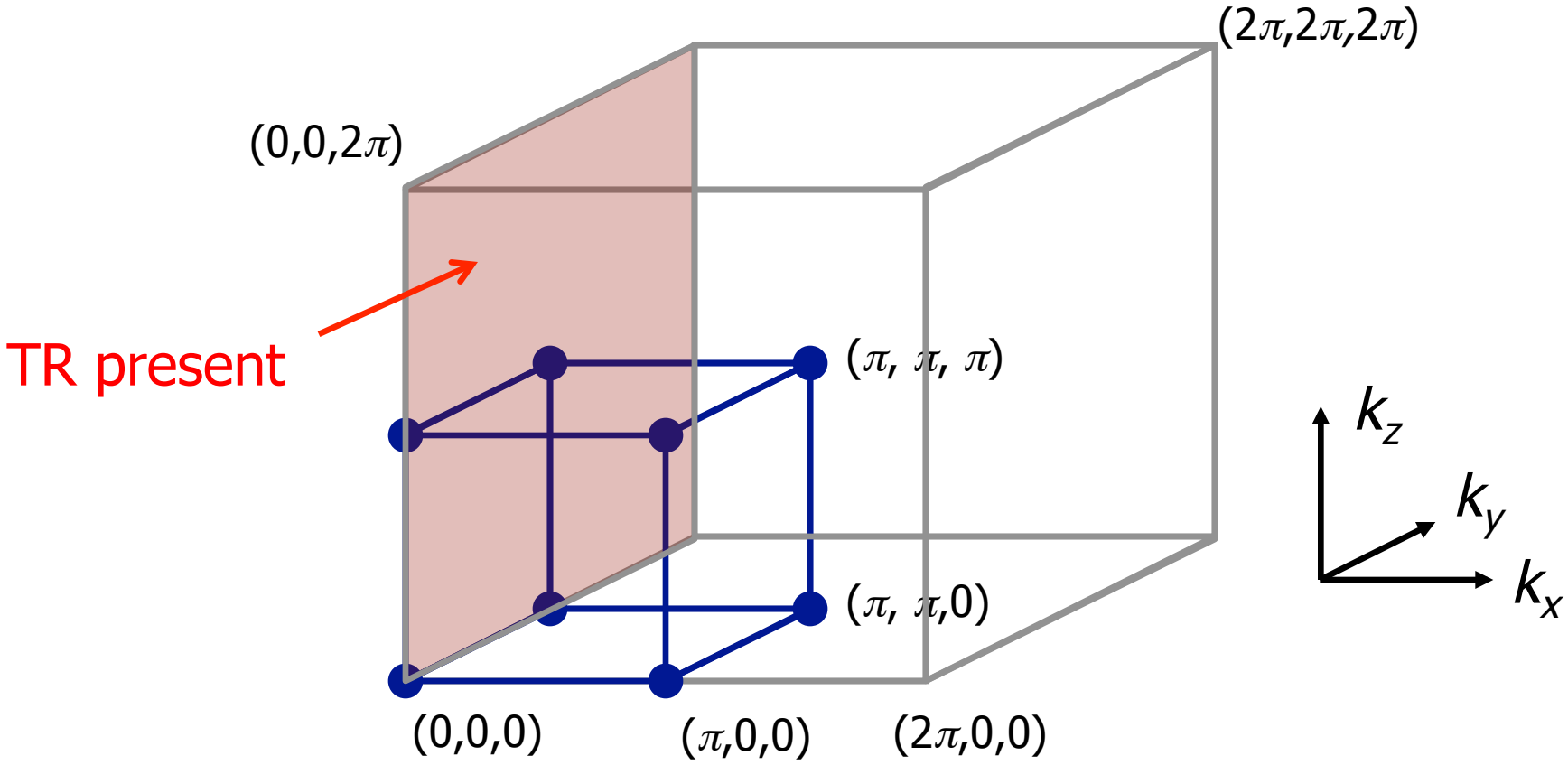
2 TRIM

2D



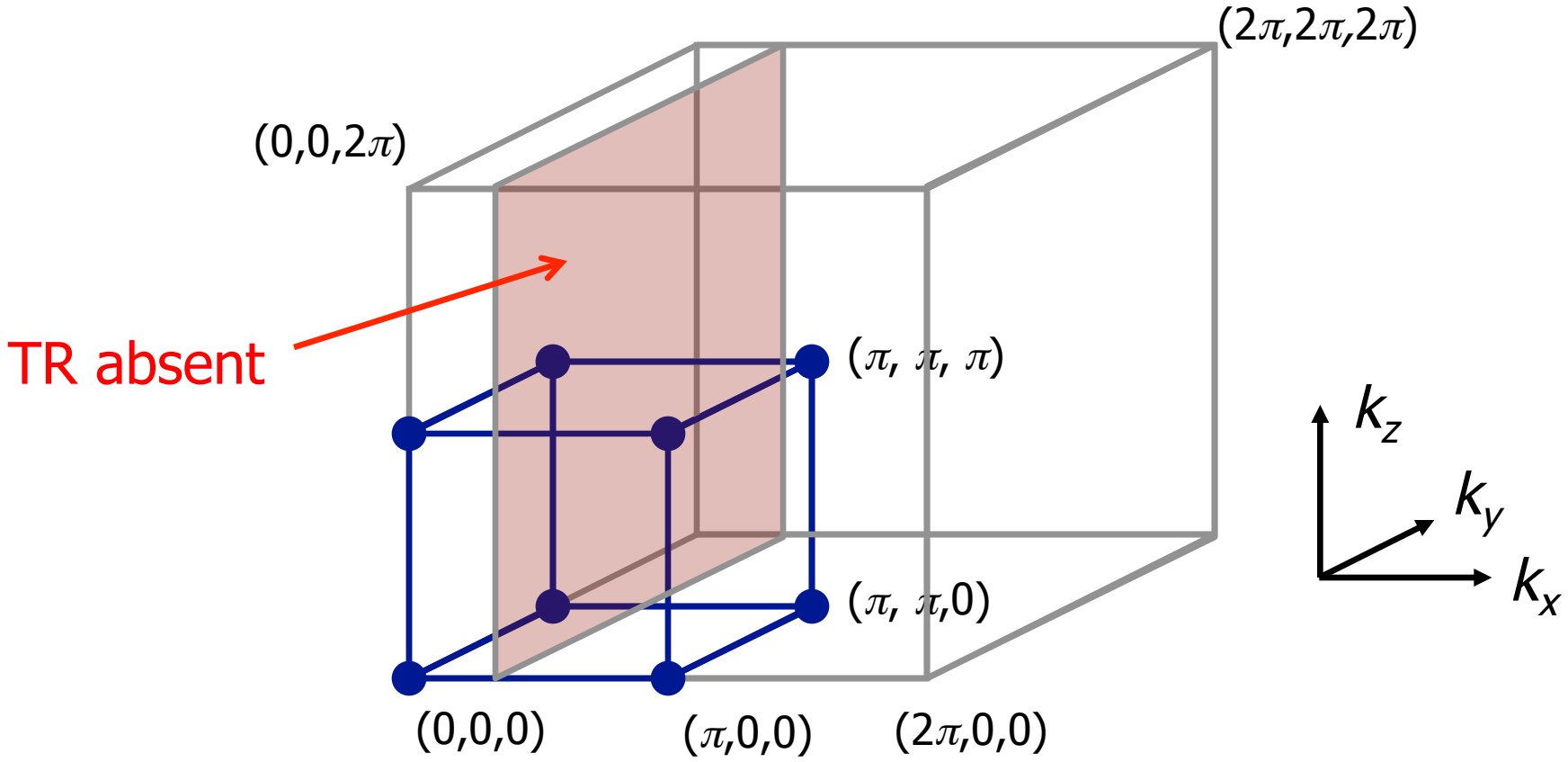
2 TRIM, 4 TRI LINES

3D Brillouin zone of TR-invariant ins.

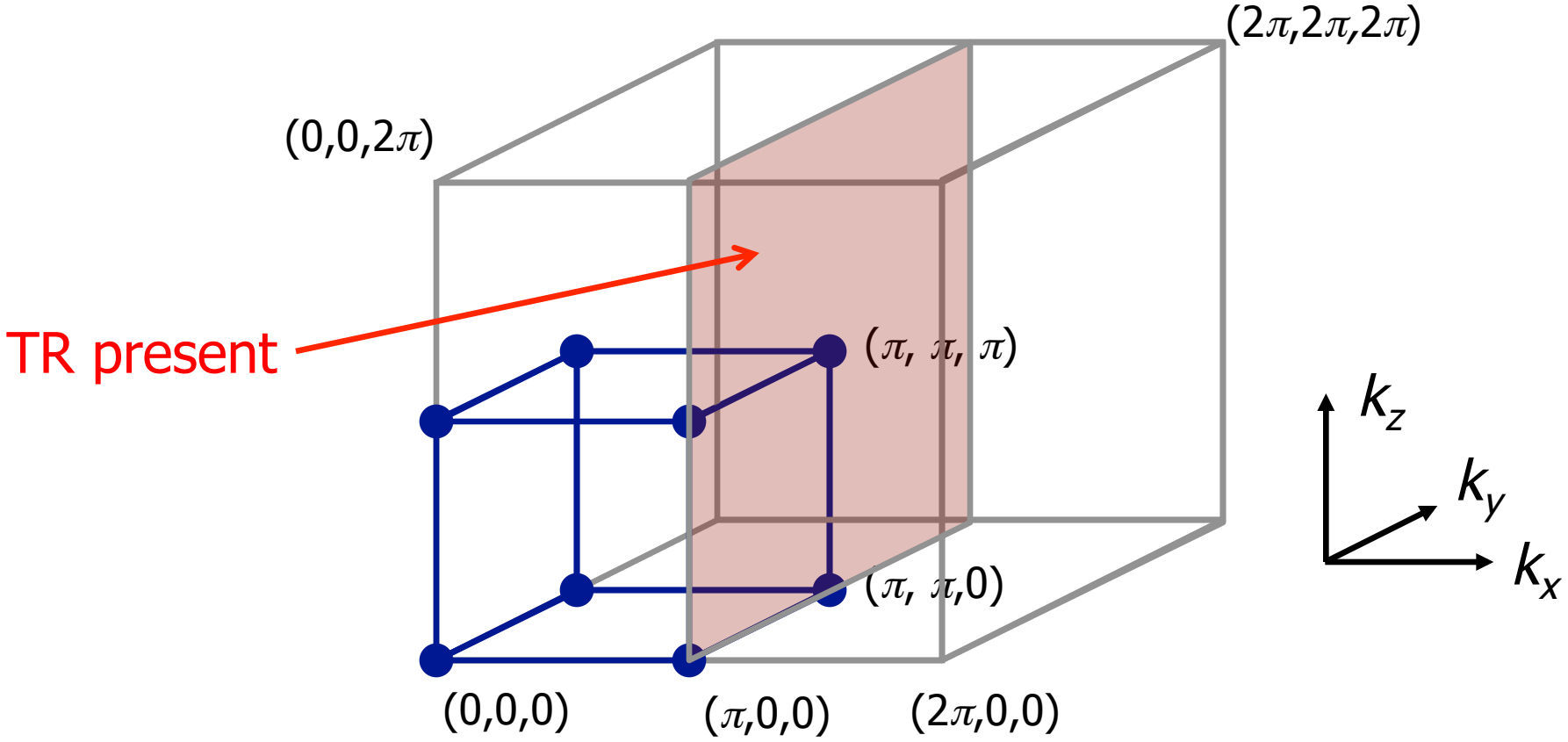


H_k is that of a 2D insulator with TR

3D Brillouin zone of TR-invariant ins.

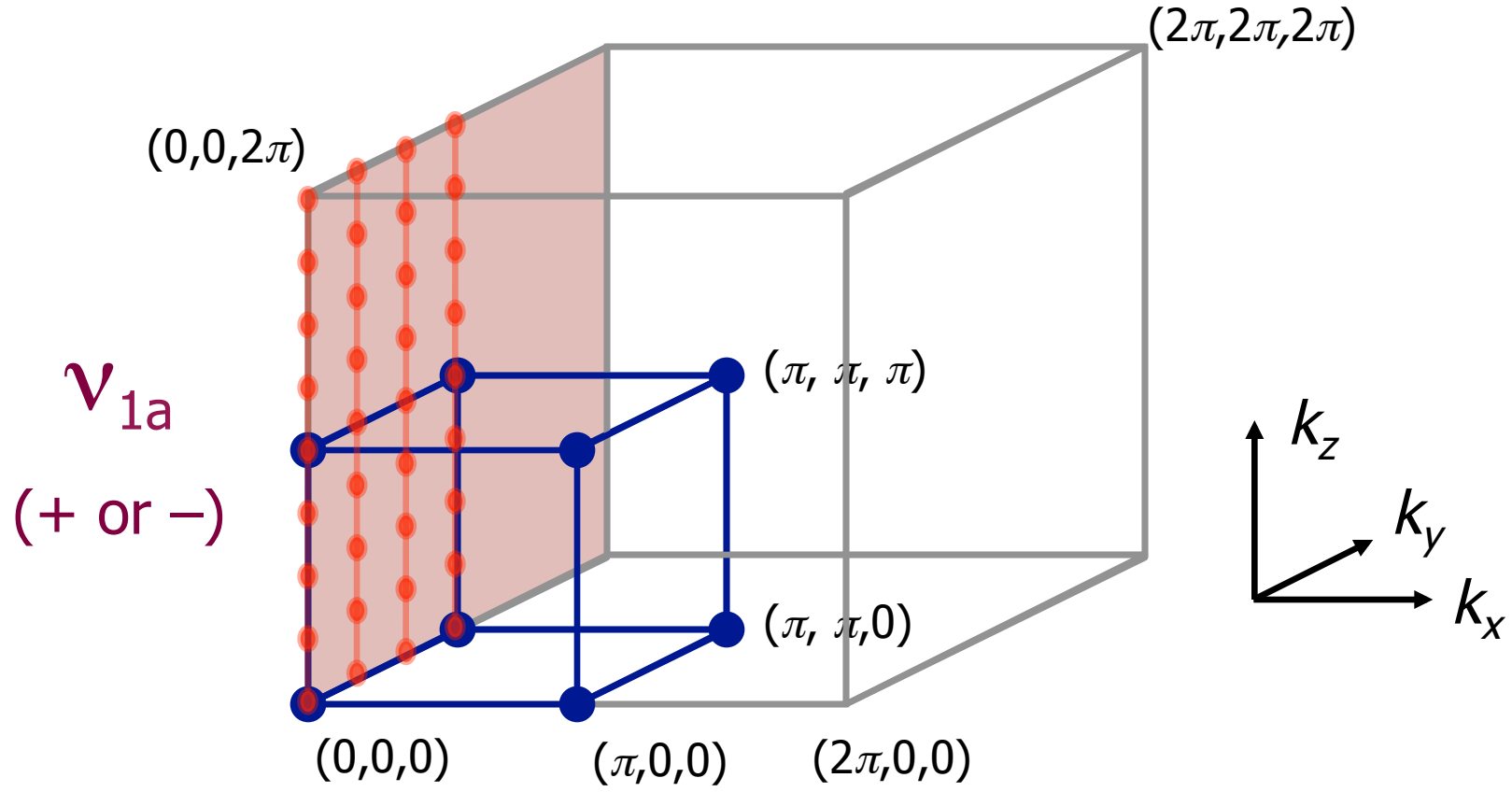


3D Brillouin zone of TR-invariant ins.

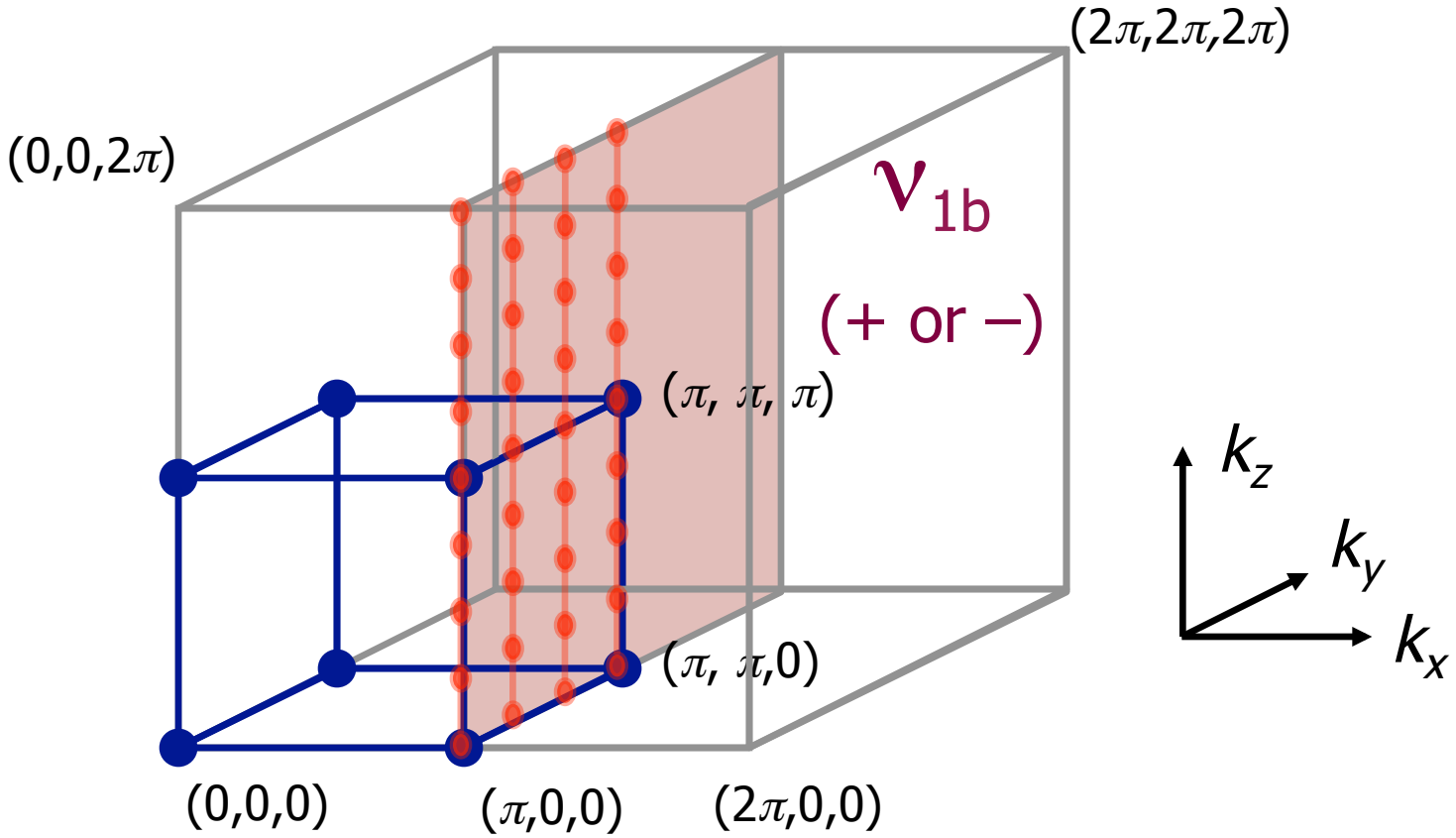


H_k is that of a 2D insulator with TR

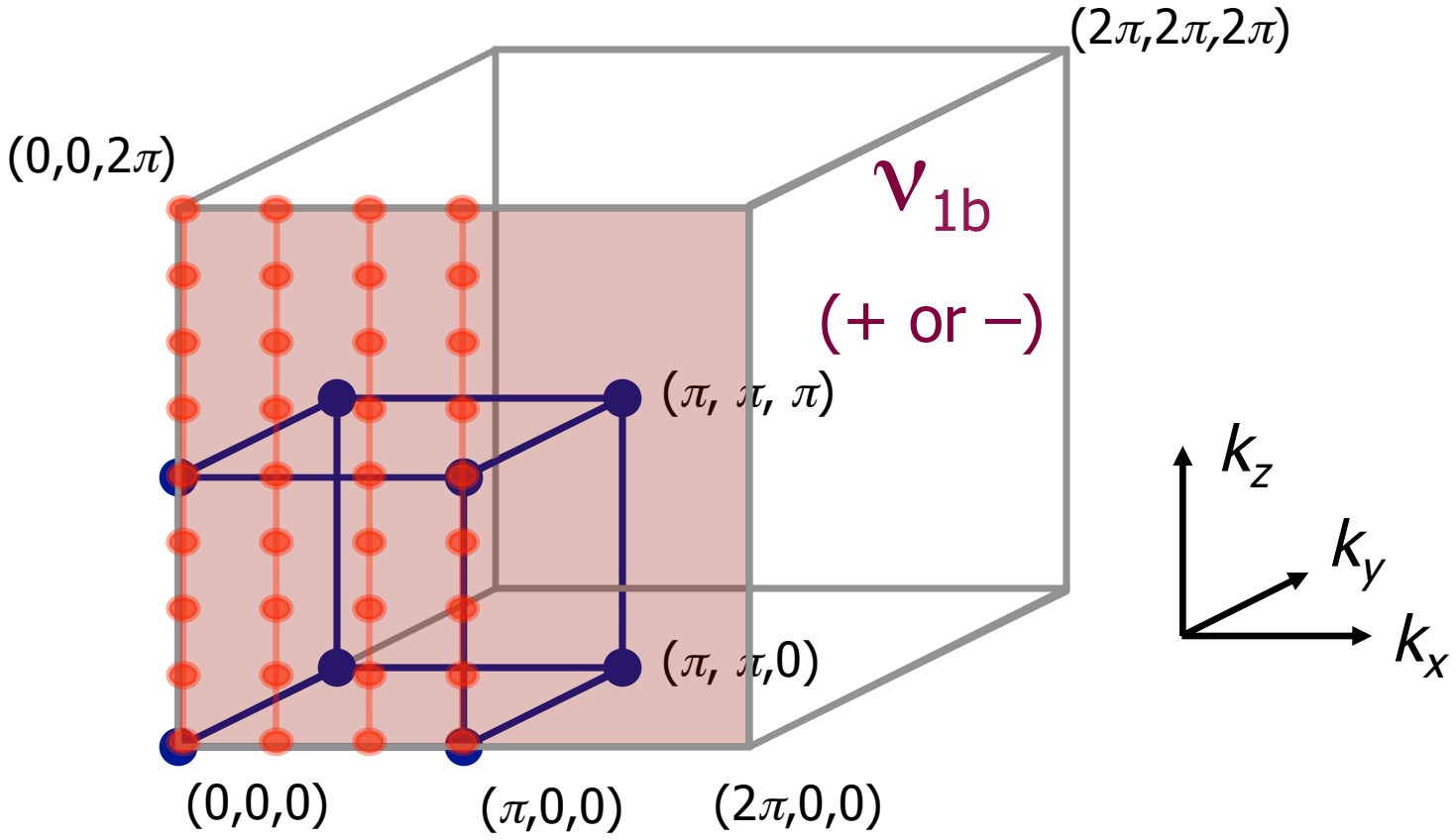
3D Brillouin zone of TR-invariant ins.



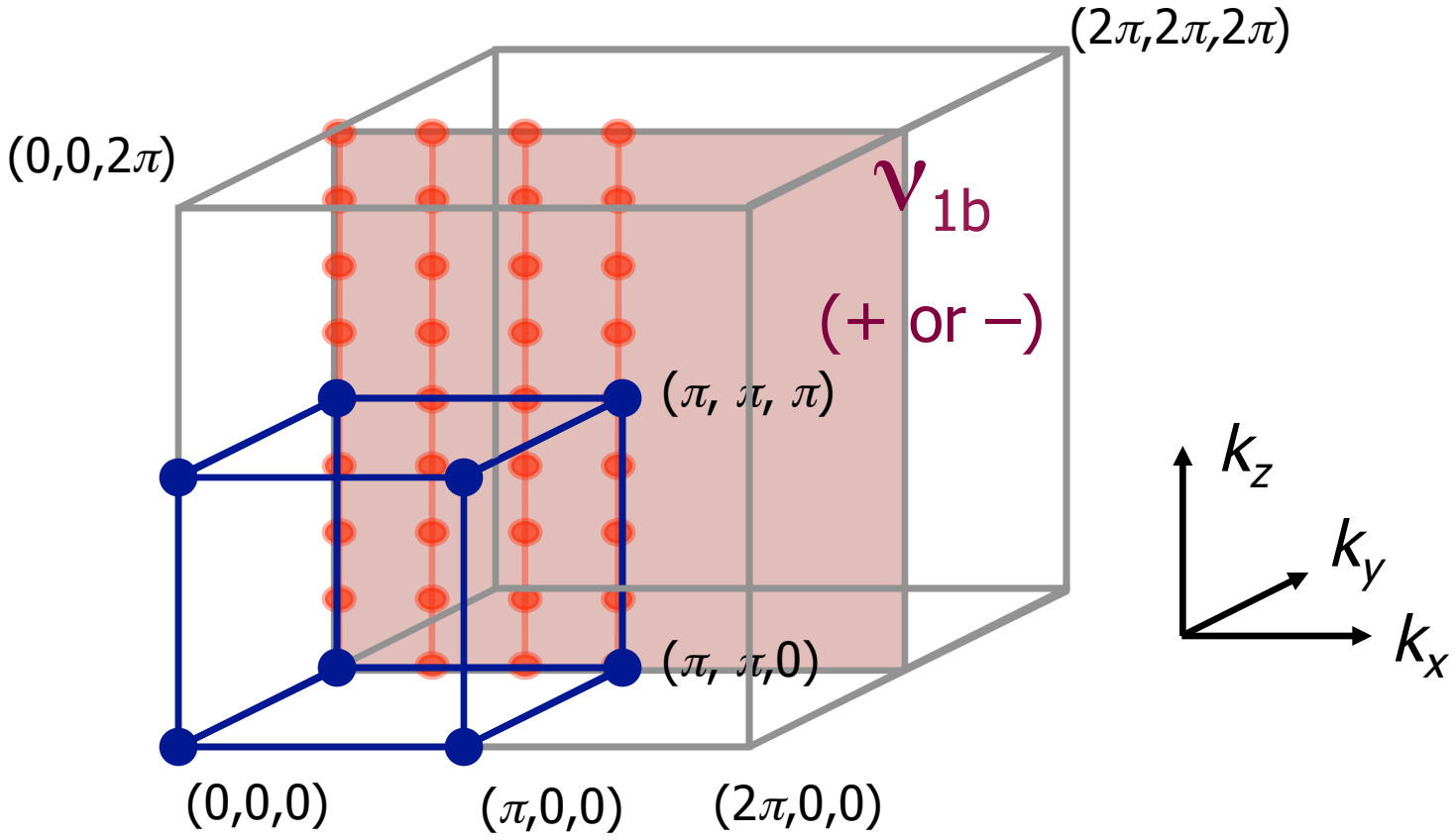
3D Brillouin zone of TR-invariant ins.



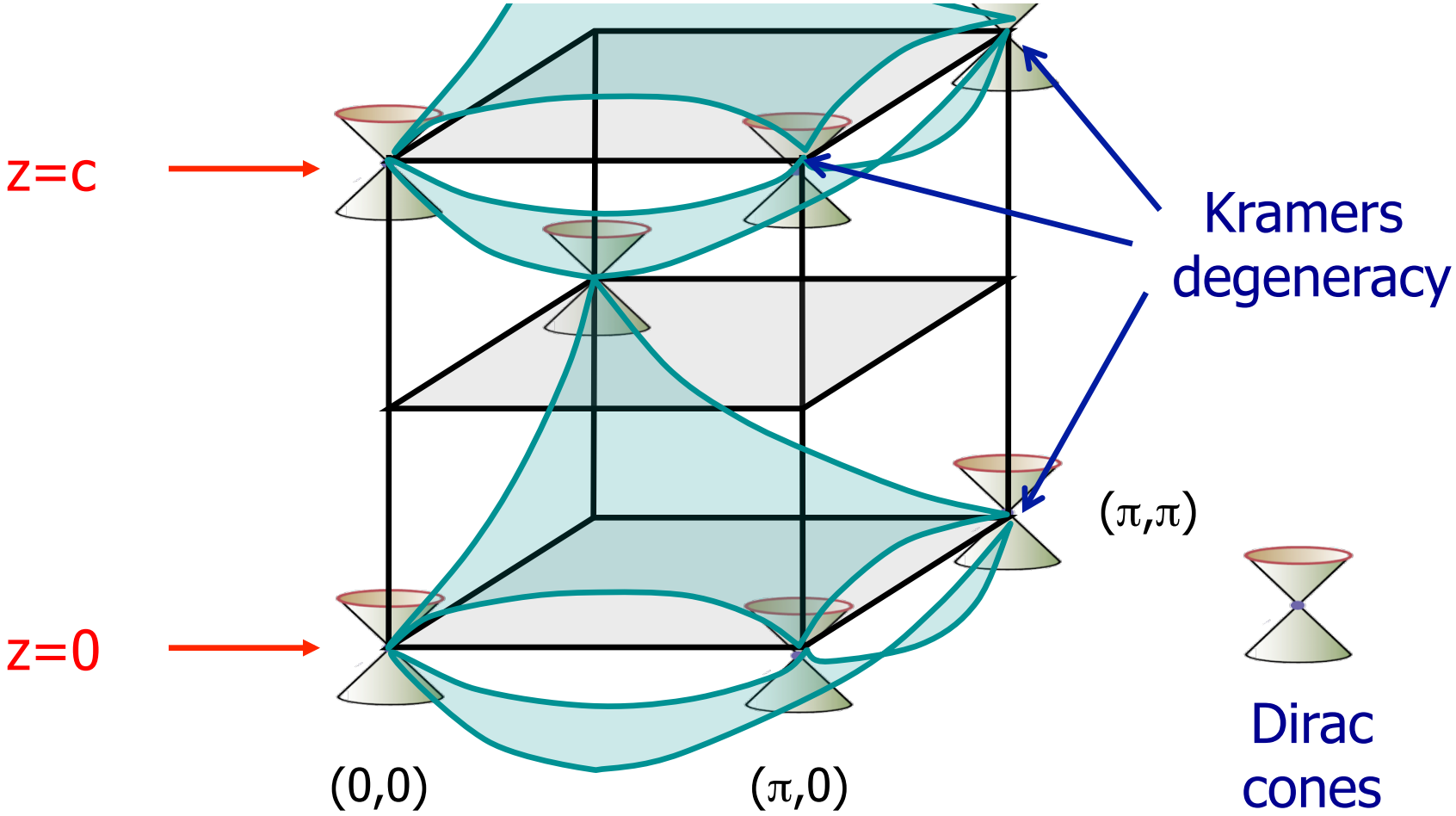
3D Brillouin zone of TR-invariant ins.



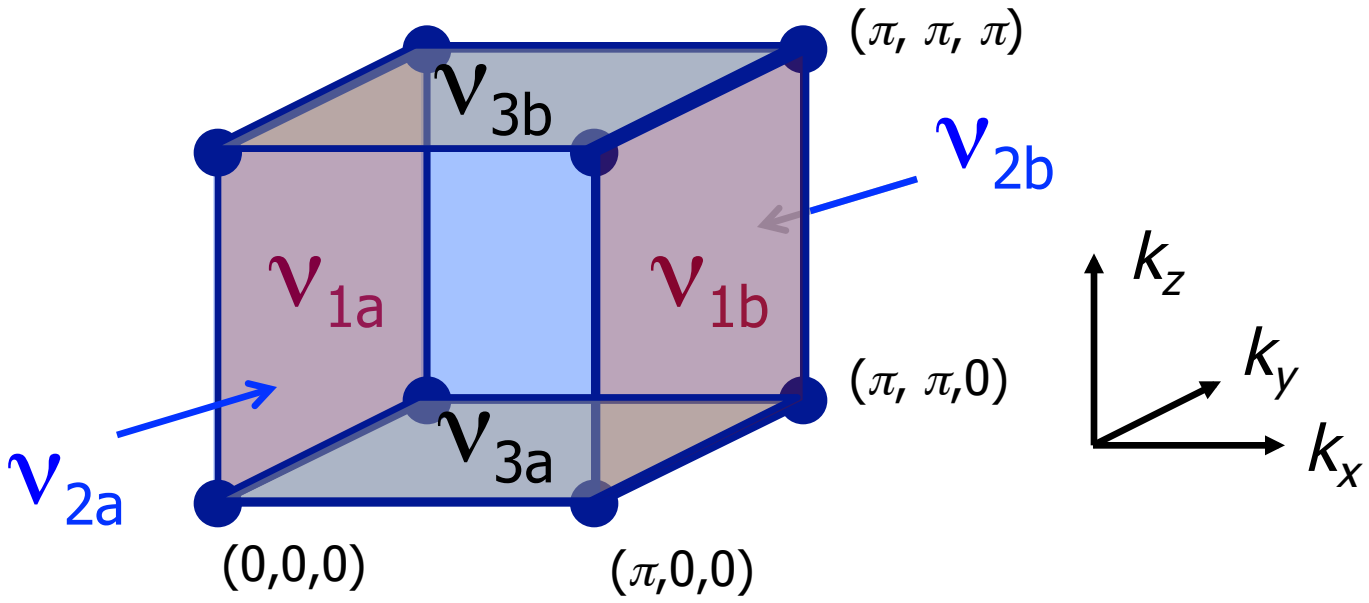
3D Brillouin zone of TR-invariant ins.



Hybrid WF sheets



3D Brillouin zone of TR-invariant ins.



6 independent Z_2 indices? No, only 4…

(Moore and Balents , 2007)

Moore-Balents rule

6 independent Z_2 indices? No, only 4…

(Moore and Balents , 2007)

$$\nu_0 = \nu_{1a}\nu_{1b} = \nu_{2a}\nu_{2b} = \nu_{3a}\nu_{3b}$$

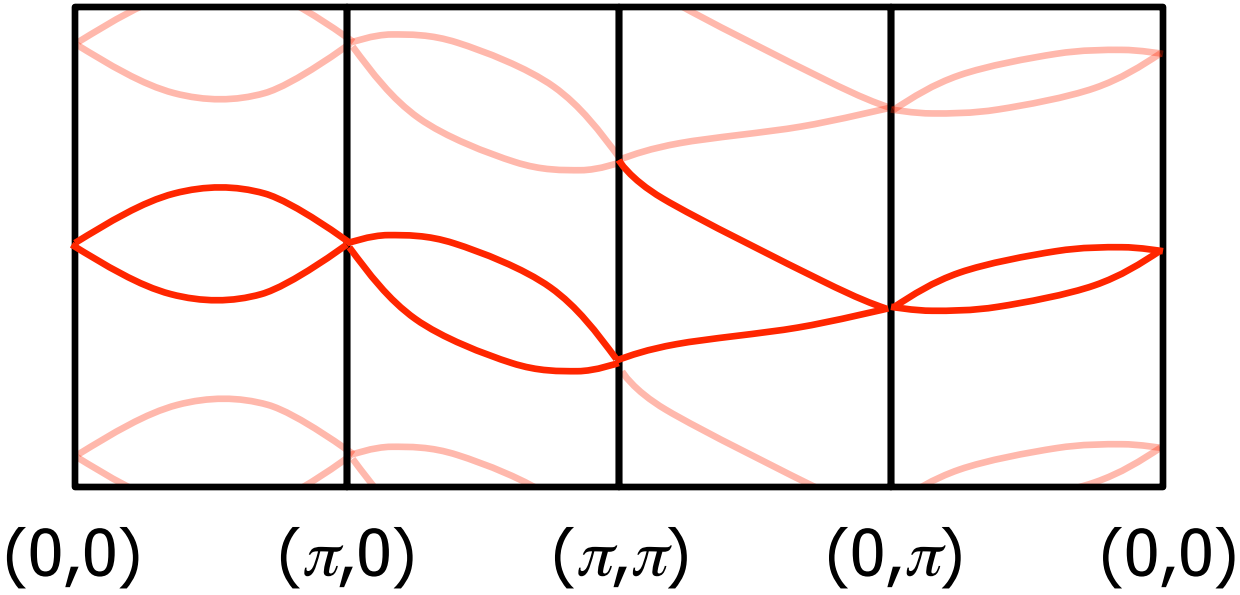
ν_0 = (+) : Opposite faces have same indices

ν_0 = (–) : Opposite faces have opposite indices

"Strong Topological Insulator" (STI)

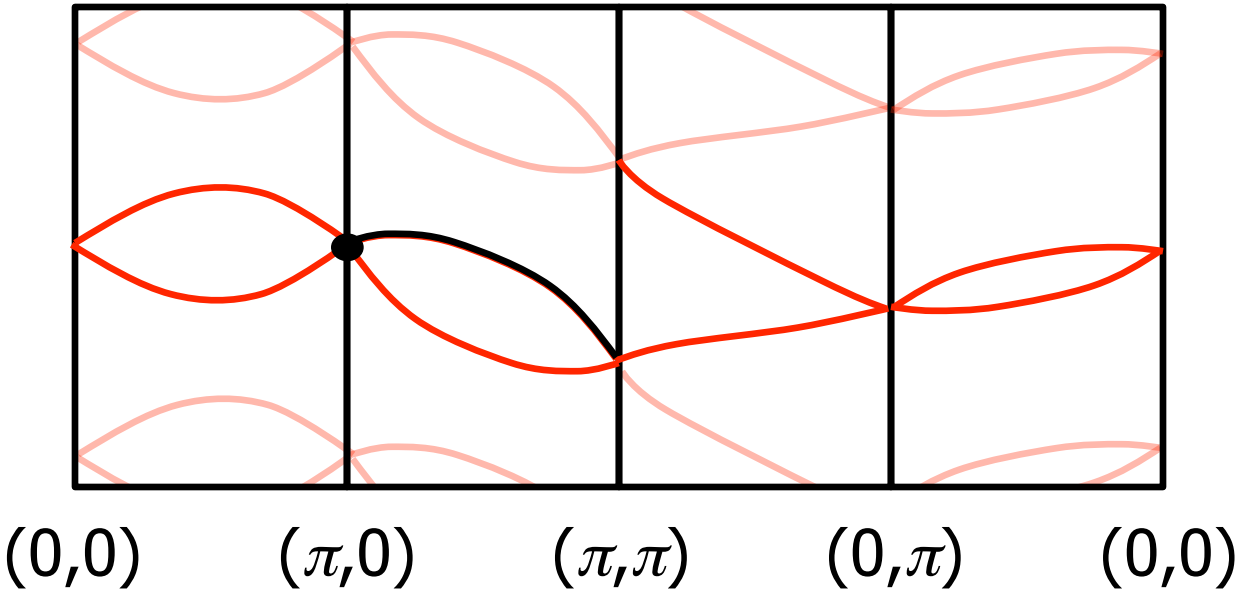
Full index set: $(\nu_0; \nu_{1b}\, \nu_{2b}\, \nu_{3b})$

Moore-Balents rule



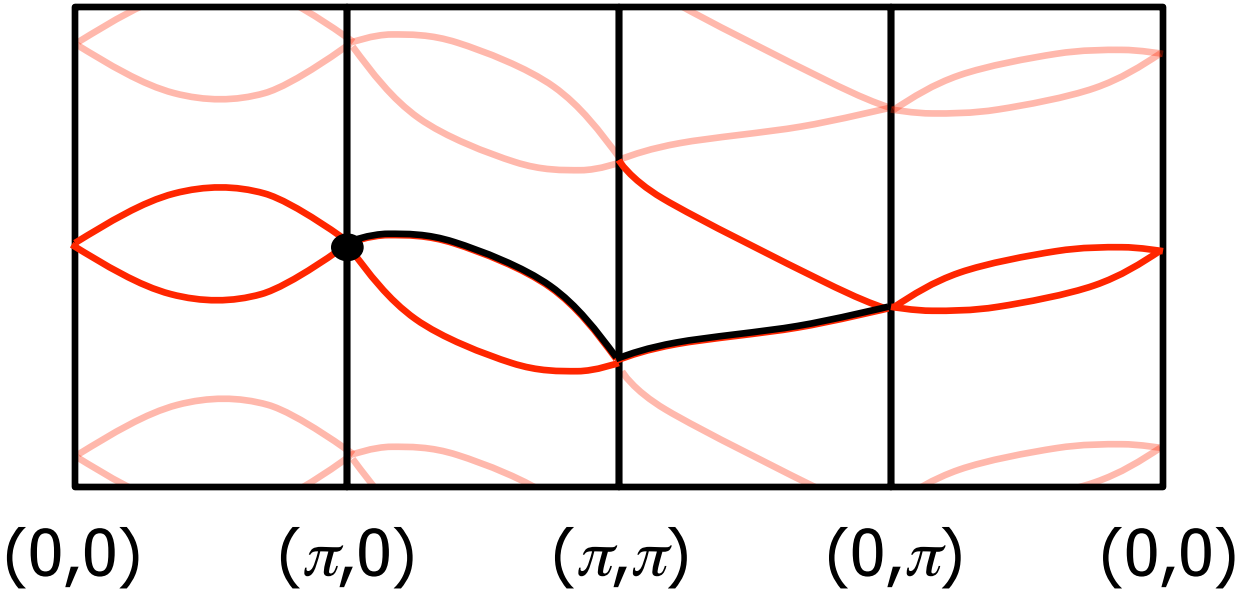
This would violate the Moore-Balents rule
Is it possible?

Moore-Balents rule



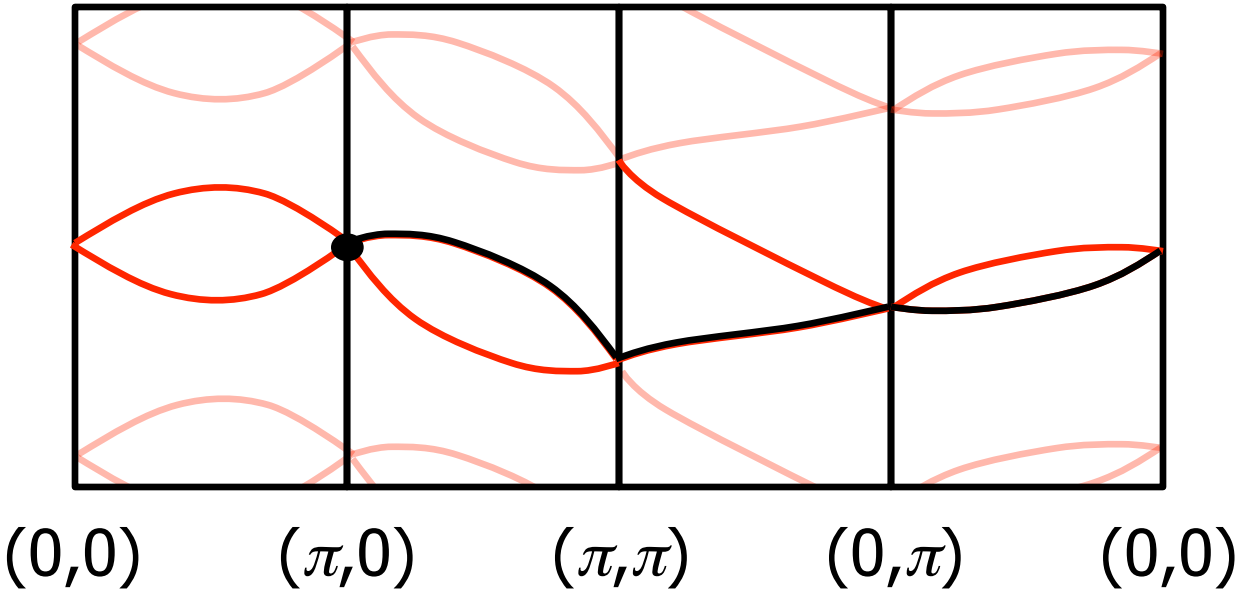
This would violate the Moore-Balents rule
Is it possible?

Moore-Balents rule



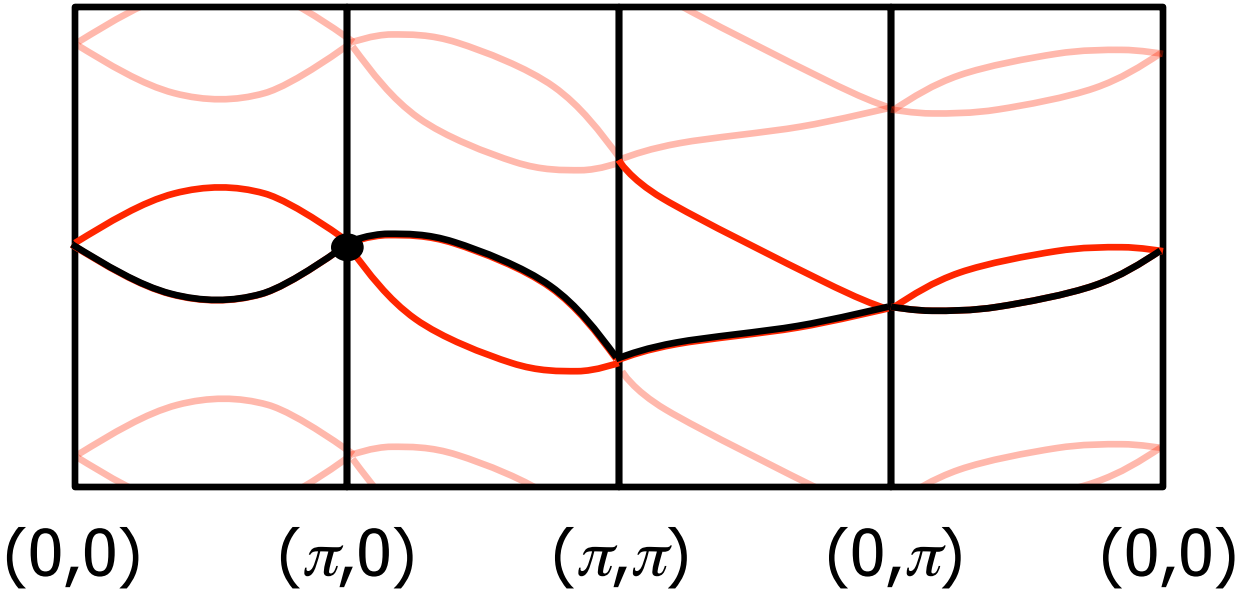
This would violate the Moore-Balents rule
Is it possible?

Moore-Balents rule



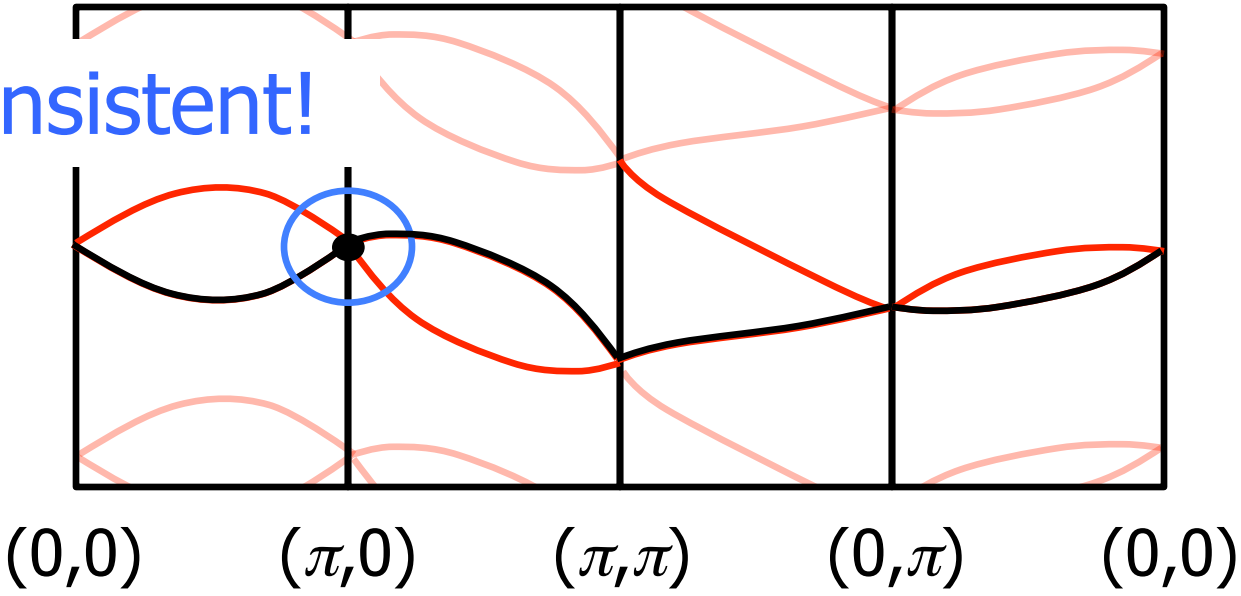
This would violate the Moore-Balents rule
Is it possible?

Moore-Balents rule



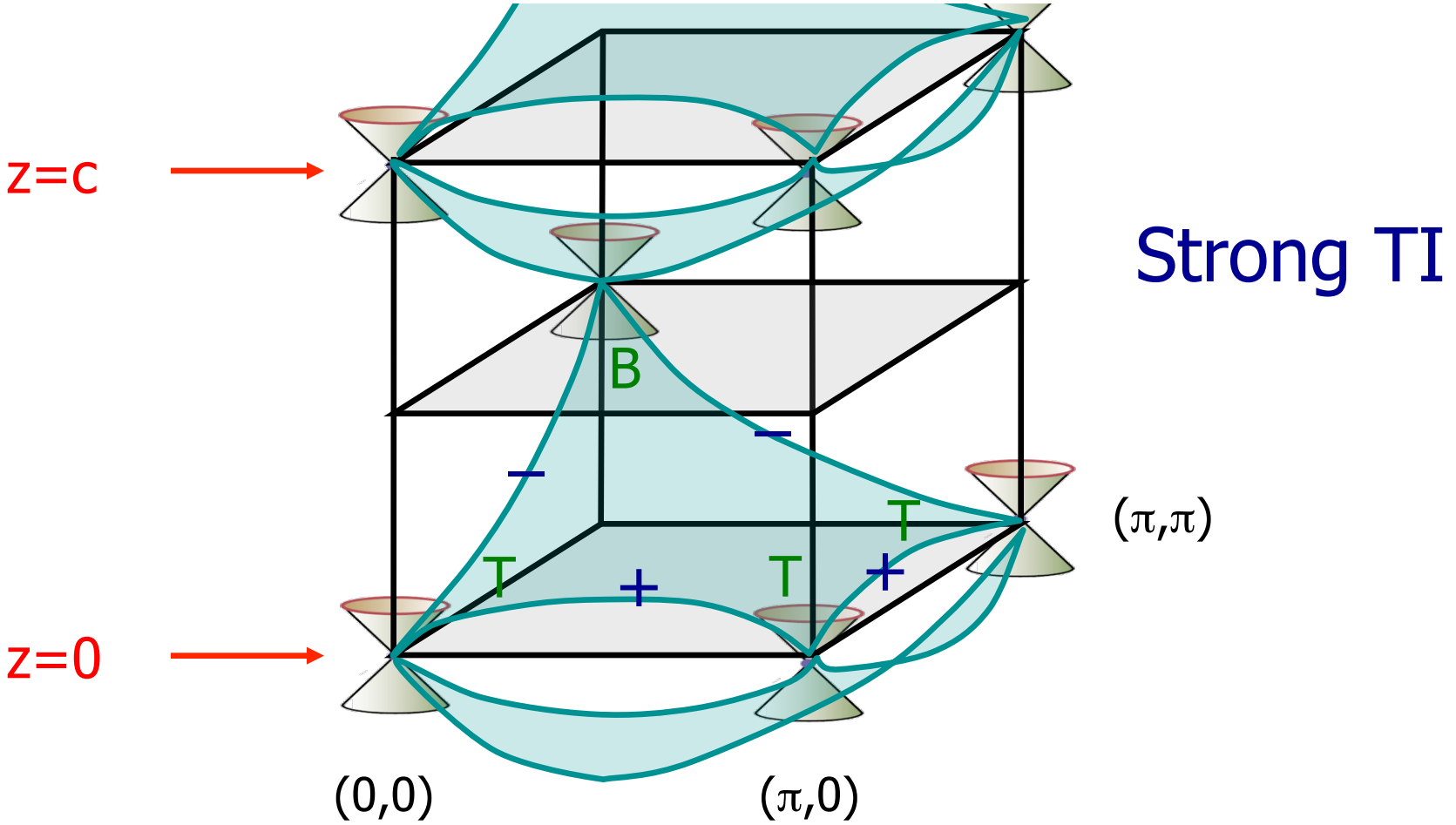
This would violate the Moore-Balents rule
Is it possible?

Moore-Balents rule

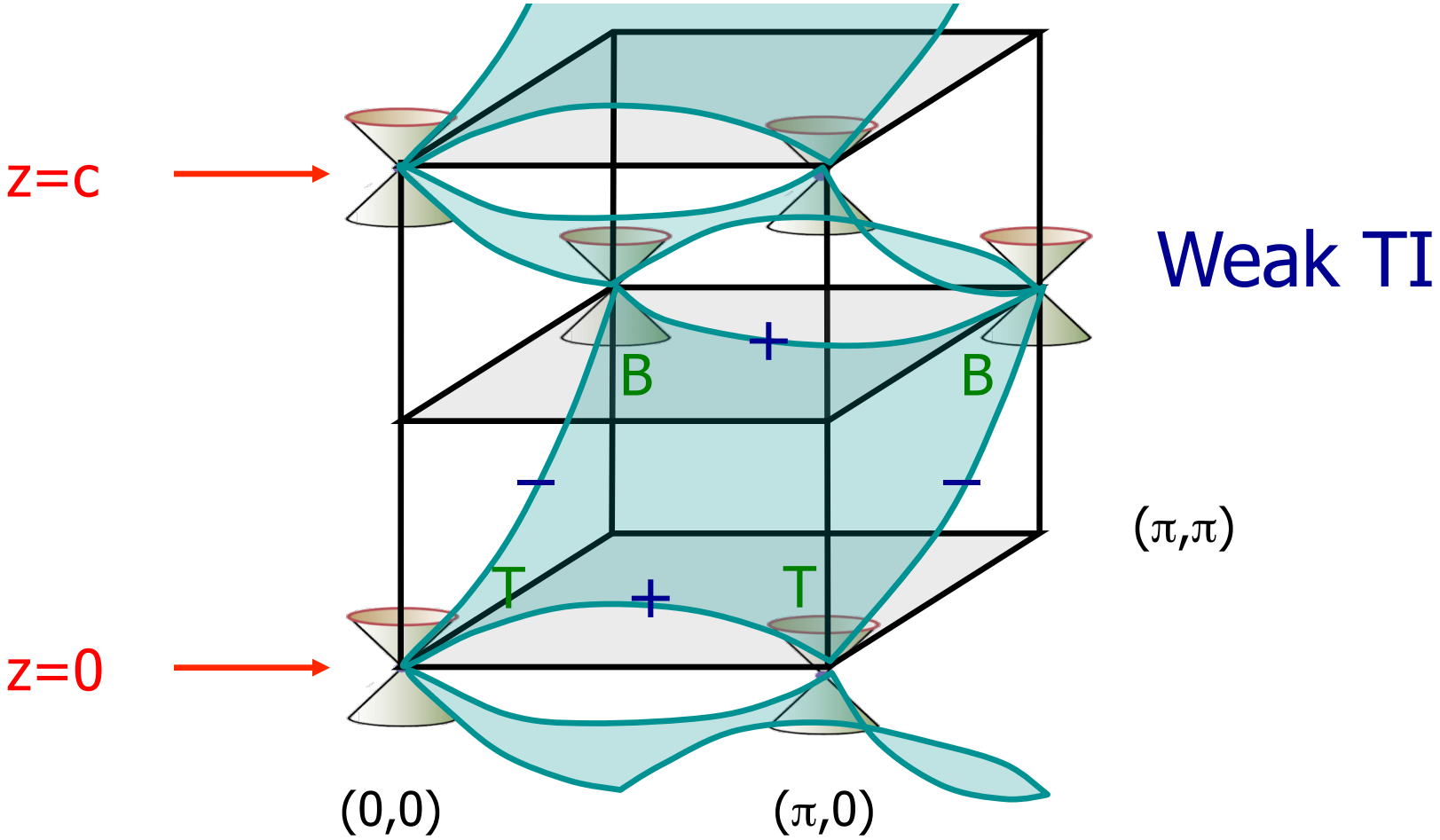


This would violate the Moore-Balents rule
Is it possible?

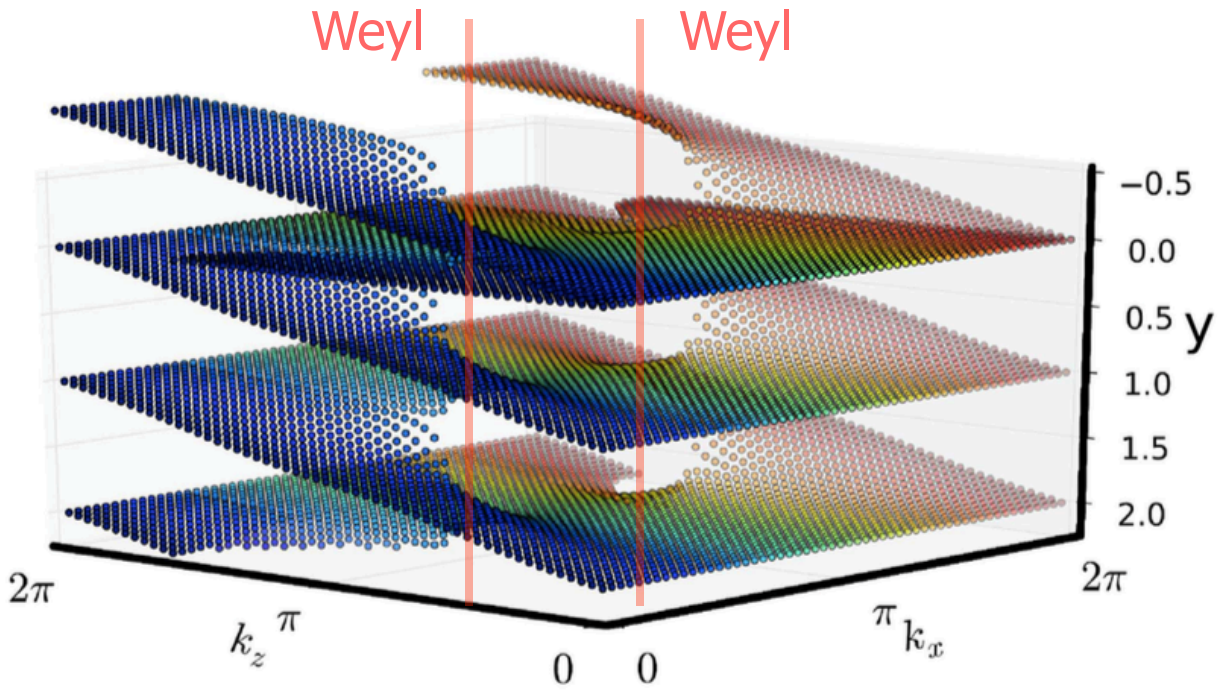
Hybrid WF sheets



Hybrid WF sheets



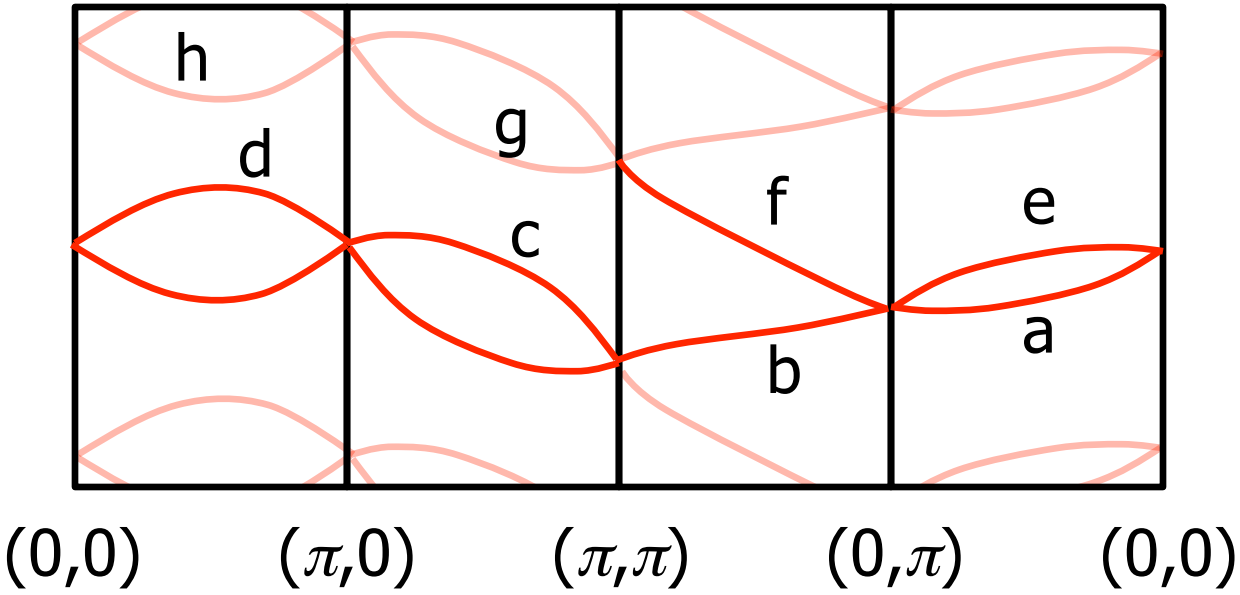
Weyl semimetal



WCCs along $\hat{y}$ vs. (k_x, k_z) for Weyl semimetal.

One Weyl point in the ¼ 2D BZ allows violation of the Moore-Balents rule

Moore-Balents rule



One Weyl point in the ¼ 2D BZ allows violation of the Moore-Balents rule

Bulk-boundary correspondence: 2D

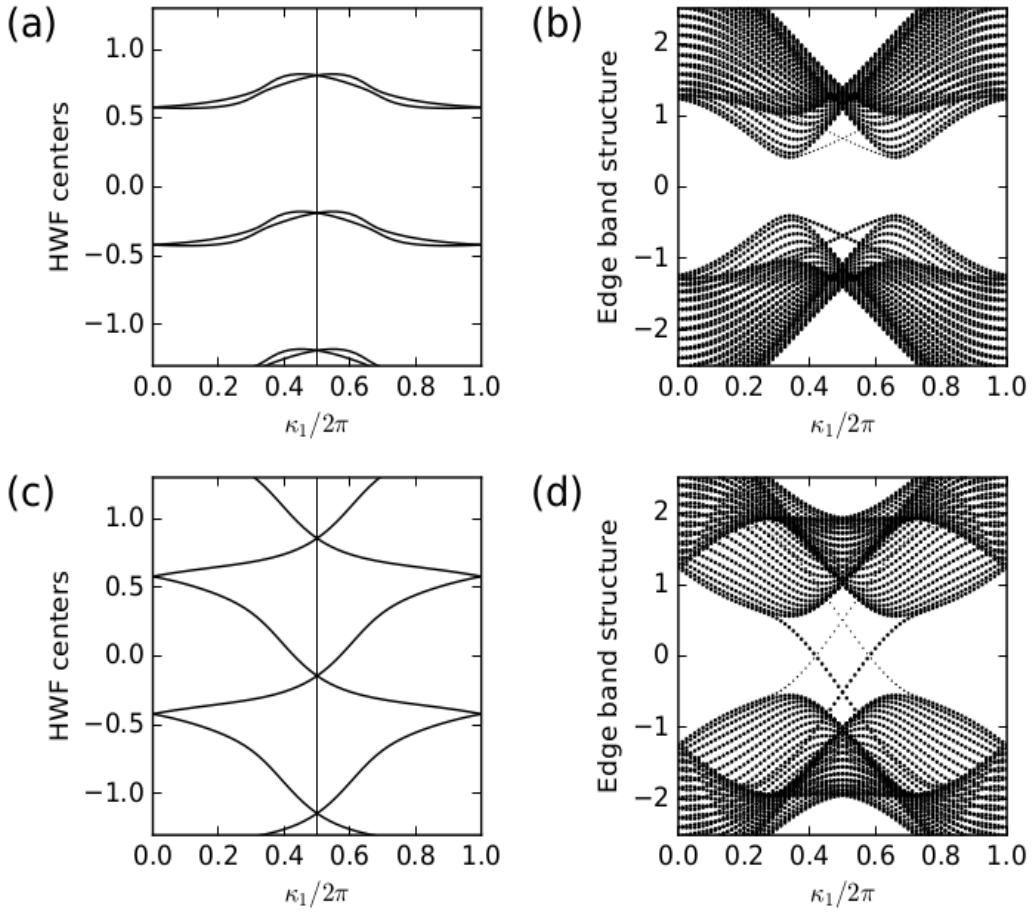
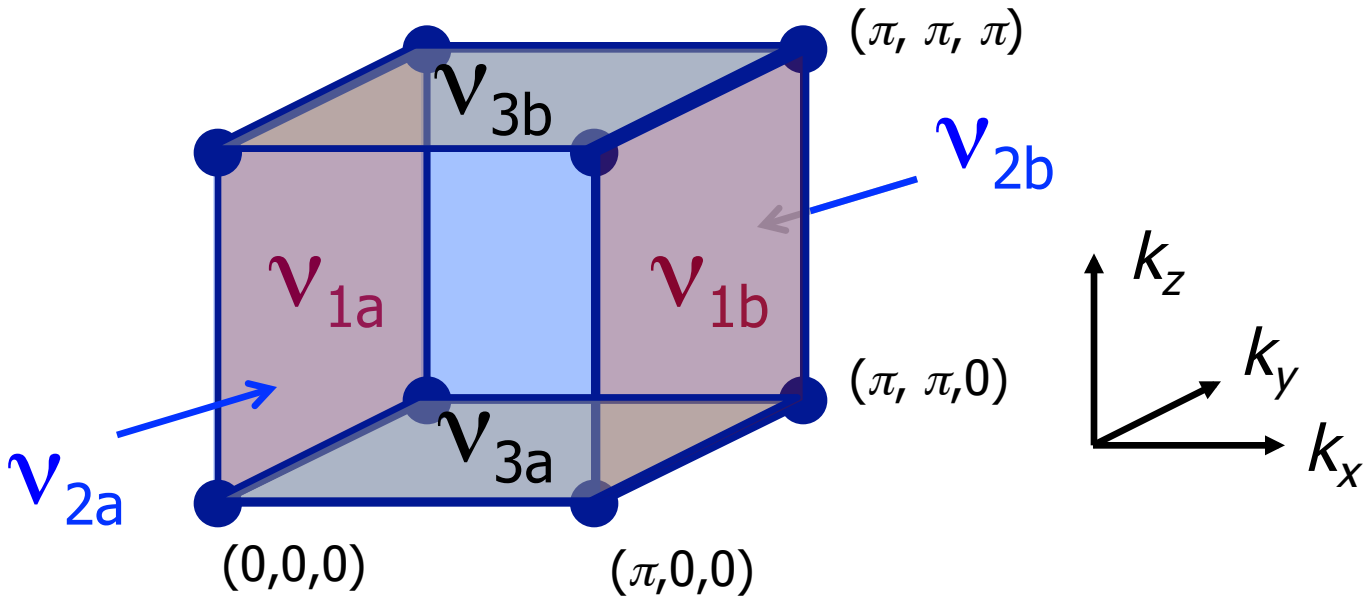


Figure 5.13 (a) Flow of hybrid Wannier centers for a Kane-Mele model in the trivial phase with $\Delta = 0.7$, $t_1 = -1.0$, $\lambda_R = 0.05$, and $\lambda_{SO} = -0.06$. (b) Edge states on a ribbon cut from the same model; those on the top and bottom edges of the ribbon are indicated by full and reduced intensity respectively. (c-d) Same as (a-b), but in the topological phase, $\lambda_{SO} = -0.24$.

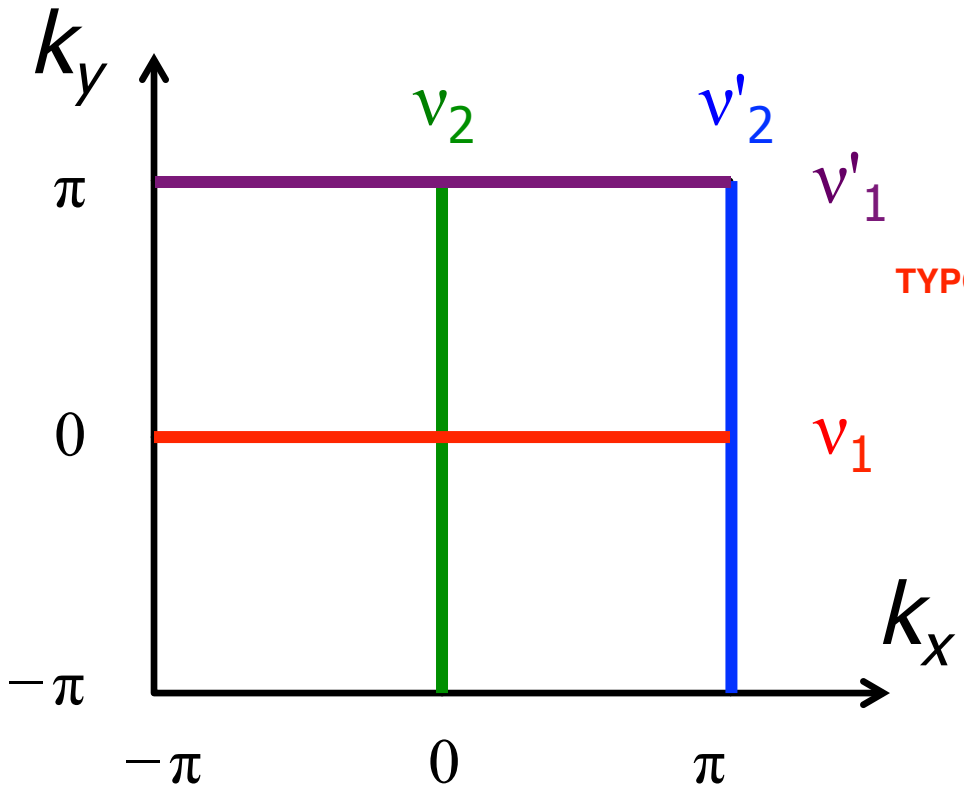
3D Brillouin zone of TR-invariant ins.



6 independent Z_2 indices? No, only 4…

(Moore and Balents , 2007)

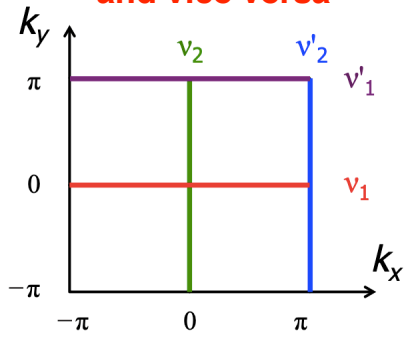
(001) surface Fermi structure



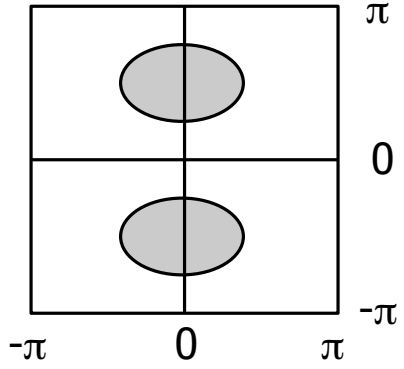
TYPO: change the indices 1 and 2 so nu_1 should be nu_2

Fig. 5.17: $(\nu_1\ \nu'_1\,;\nu_2\ \nu'_2) = ?$

TYPO: change the indices 1 and 2 so nu_1 should be nu_2 and vice versa

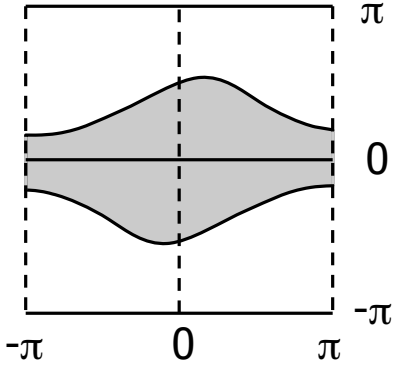


(a)



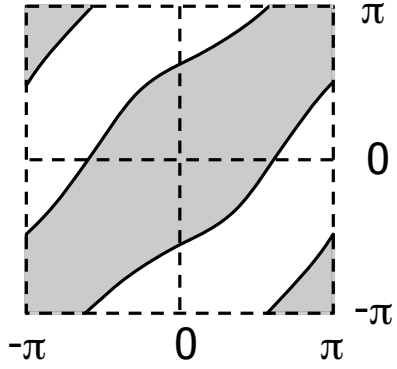
(00;00)

(b)



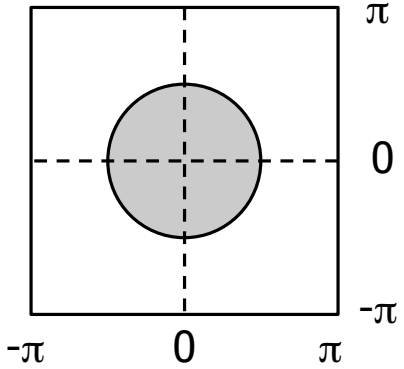
(11;00)

(c)



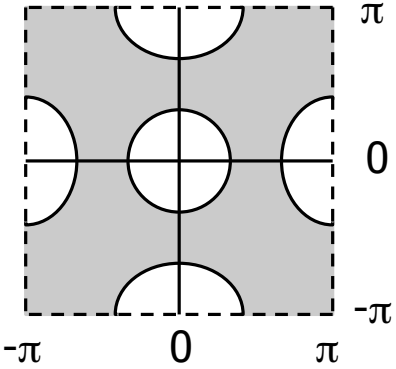
(11;11)

(d)



(10;10)

(e)



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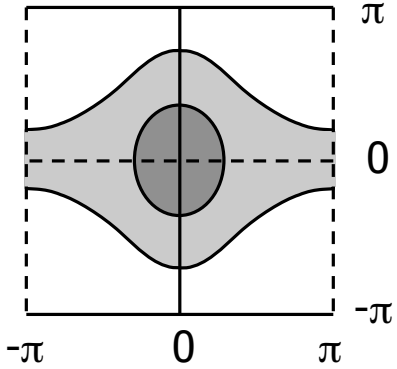
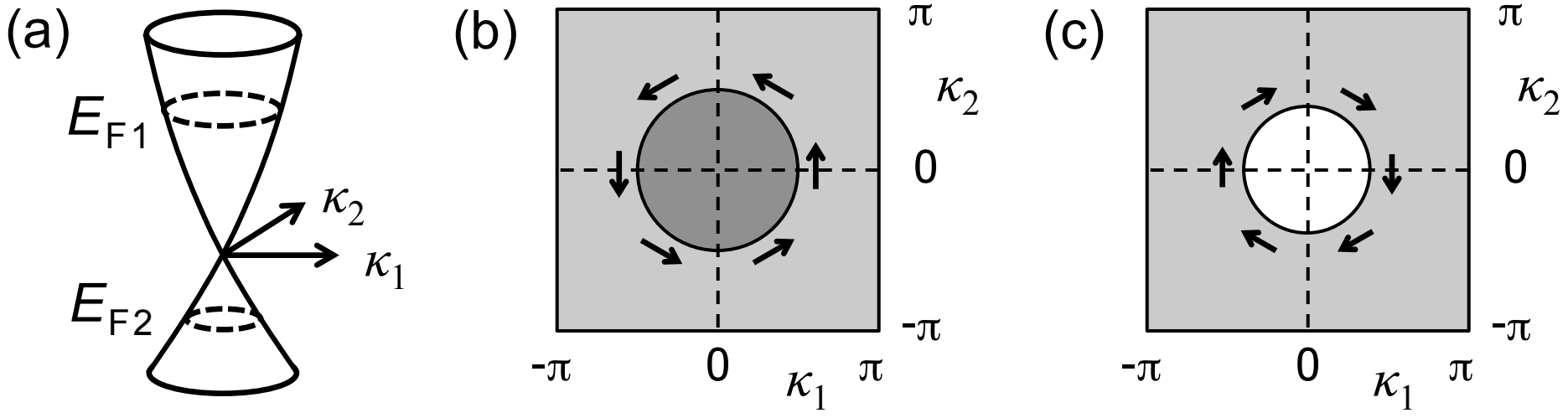
(f)

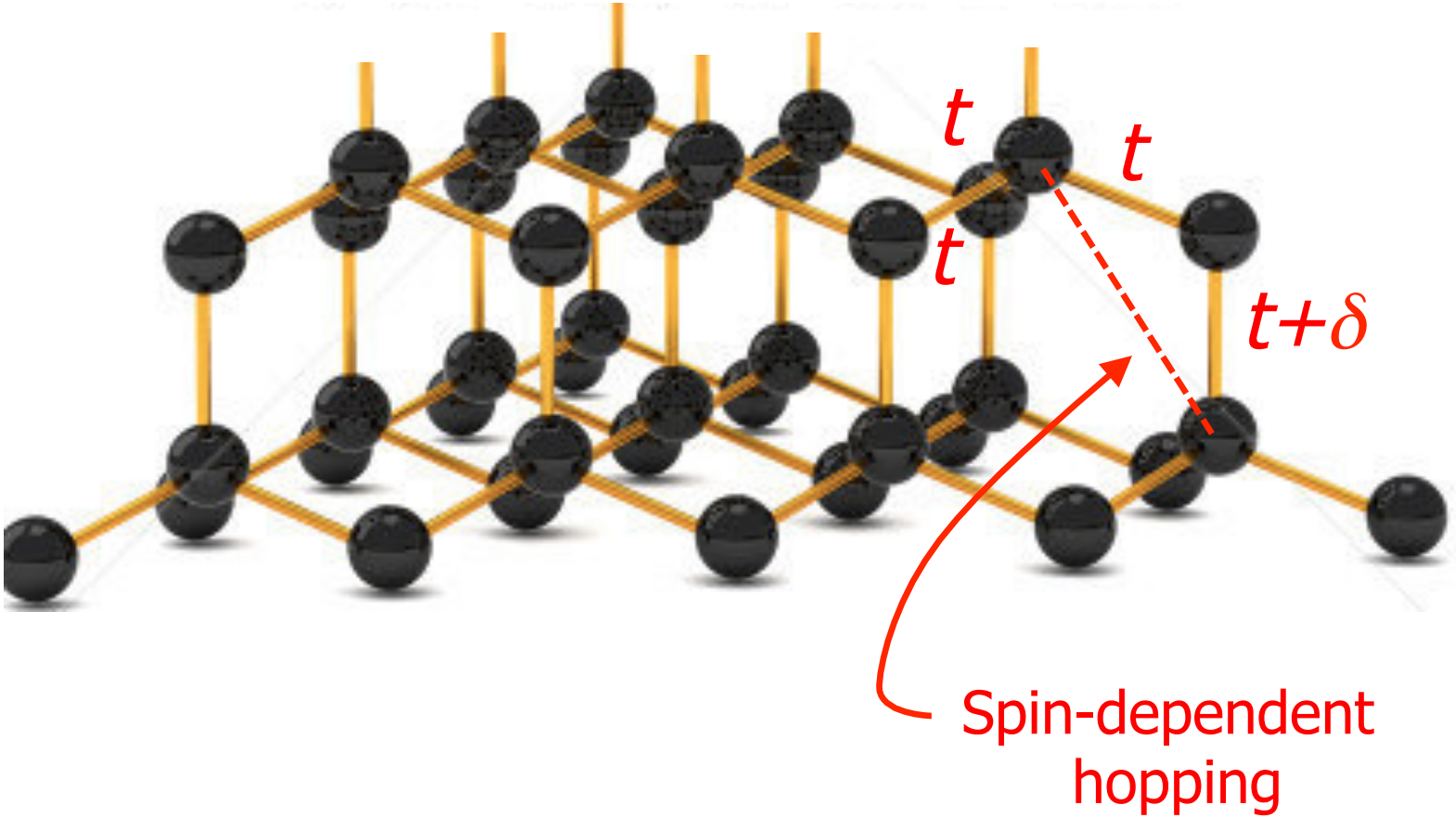


(01;10)

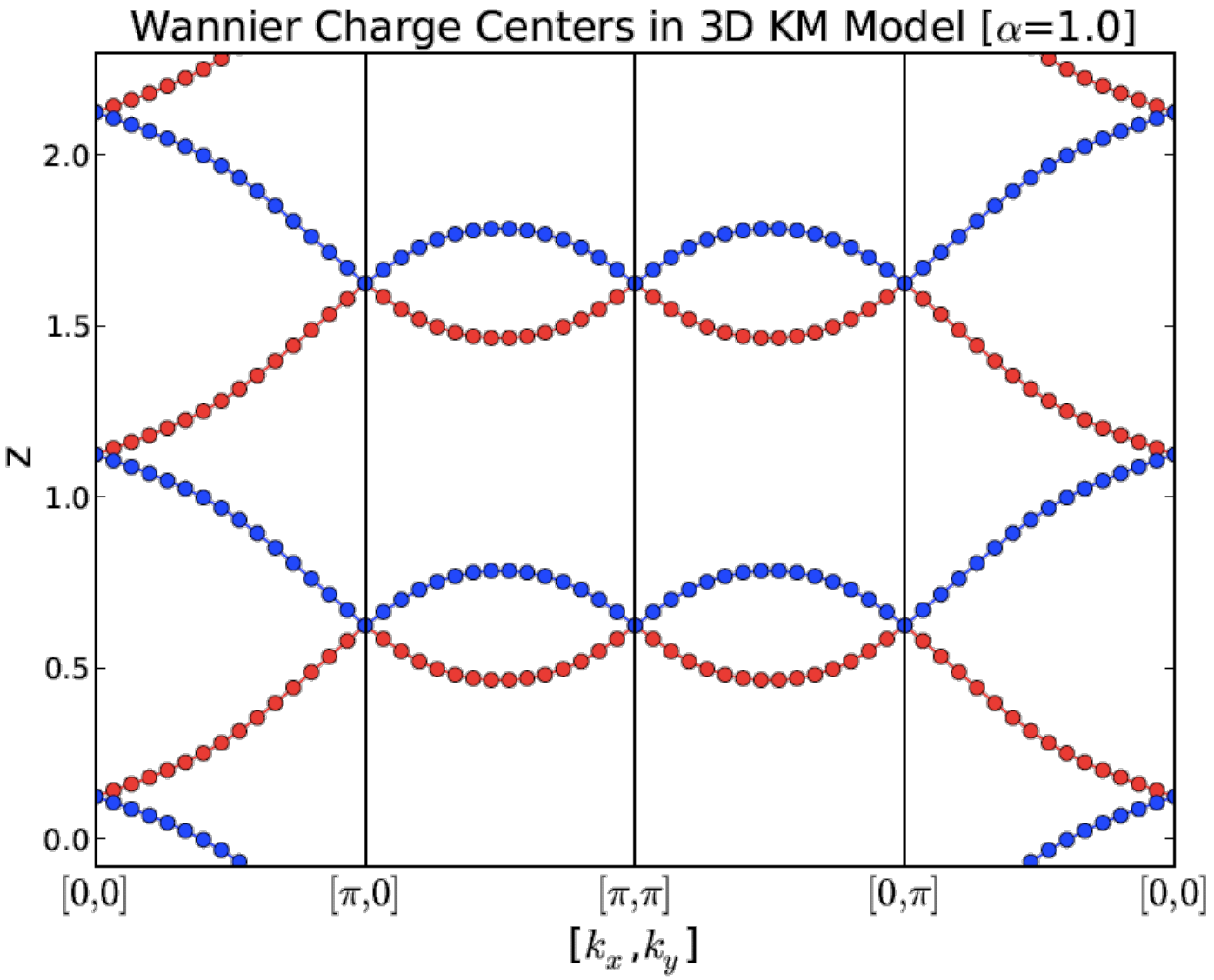
Fig. 5.18


(a)
E_{F1}
E_{F2}
κ_2
κ_1
(b)
π
κ_2
0
-π
-π
0
κ_1
π
(c)
π
κ_2
0
-π
-π
0
κ_1
π

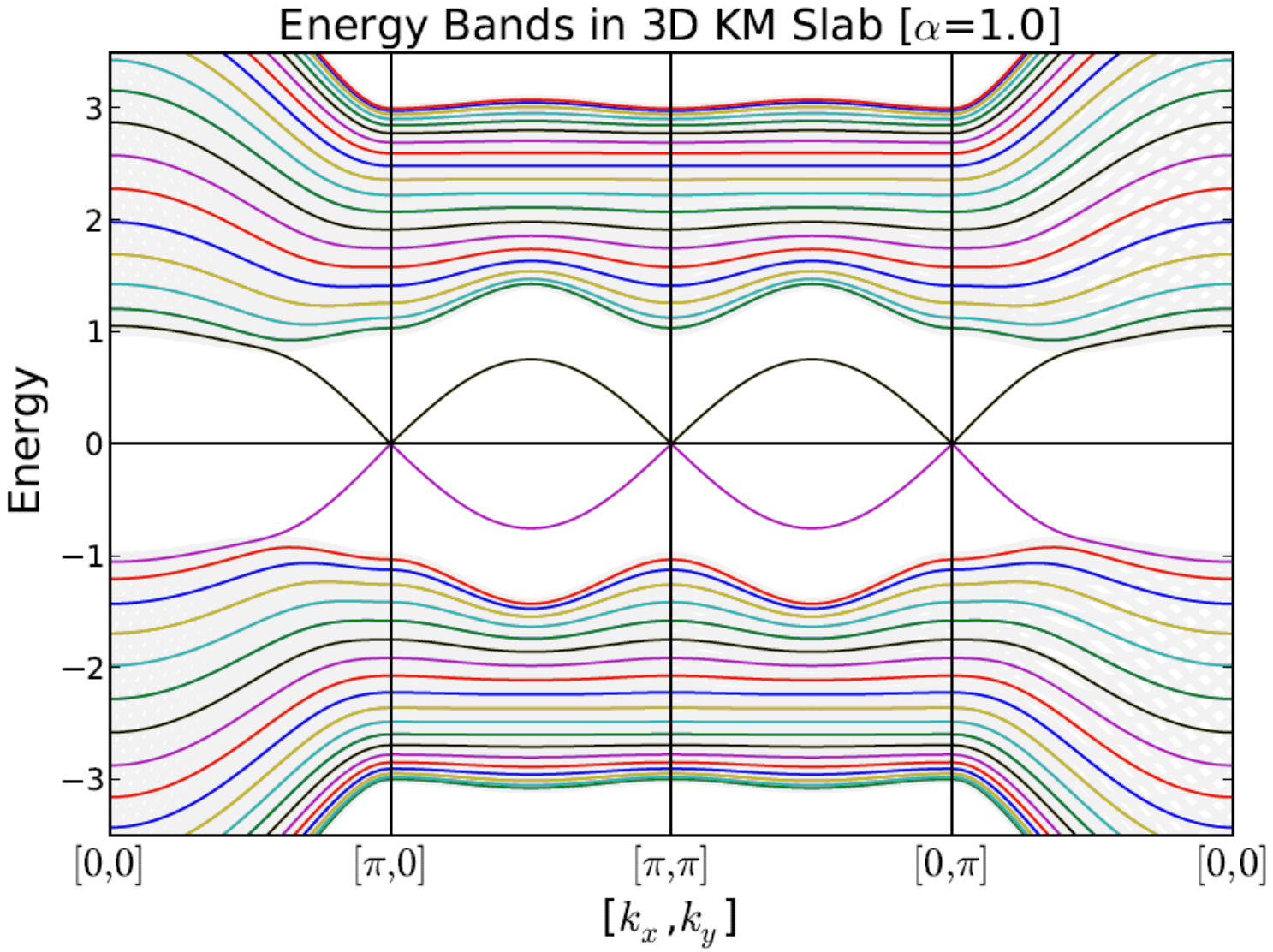
3D Kane-Mele model



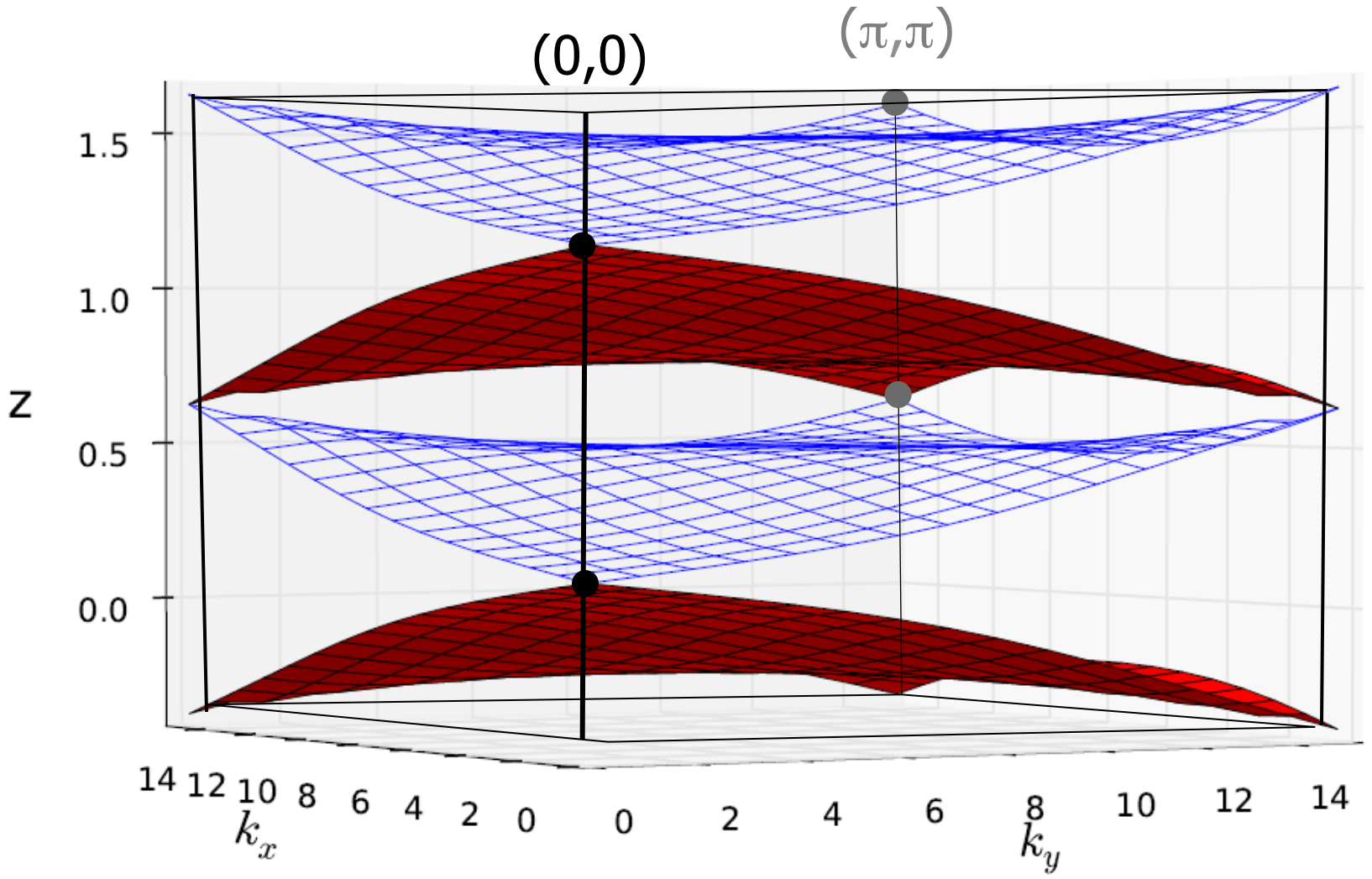
Hybrid WF sheets



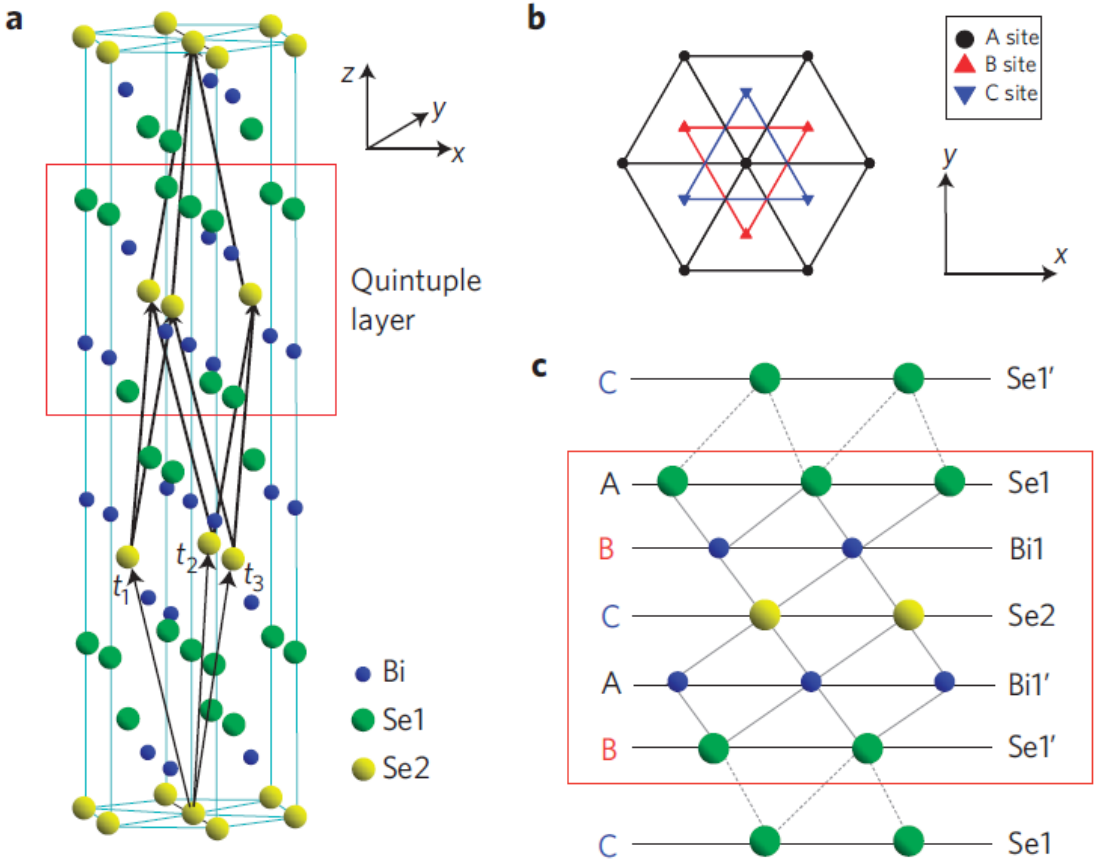
Surface energy bands



Hybrid WF sheets

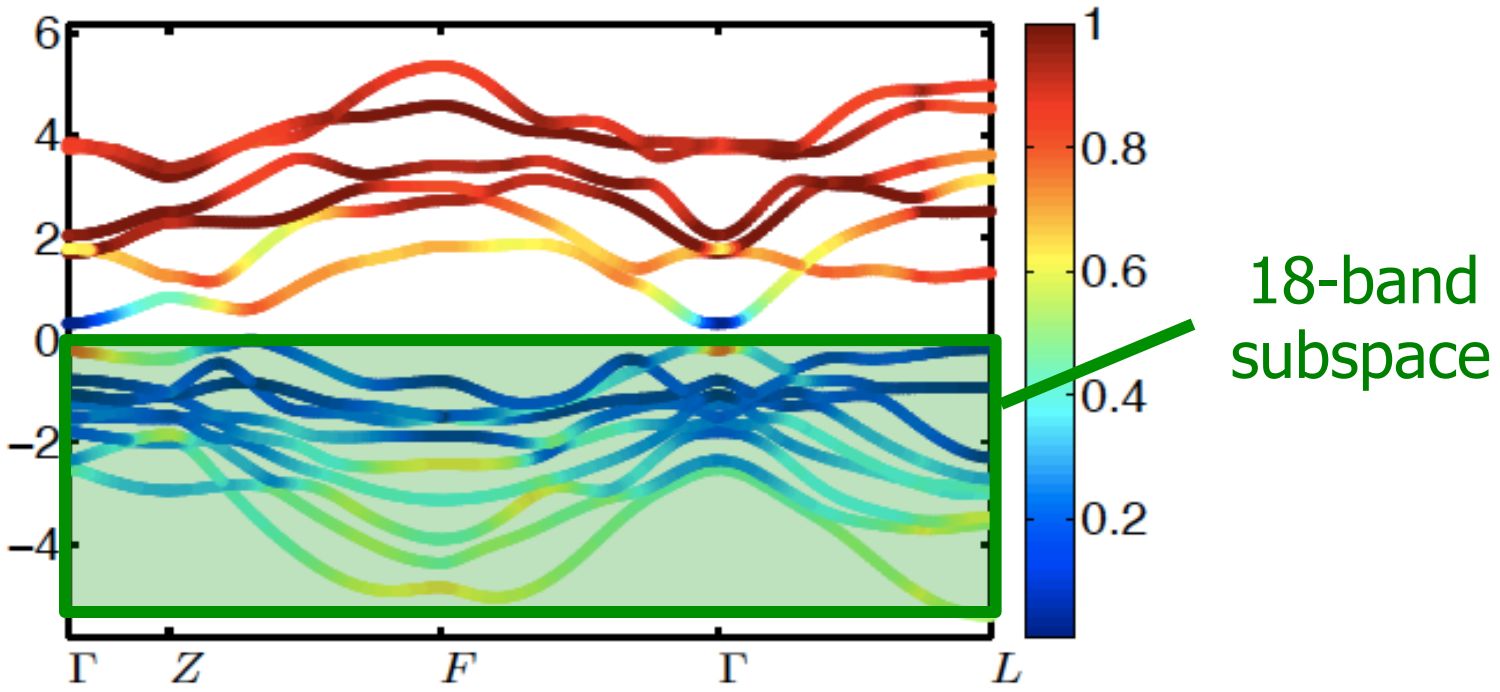


First-principles calculation: Bi_2Se_3



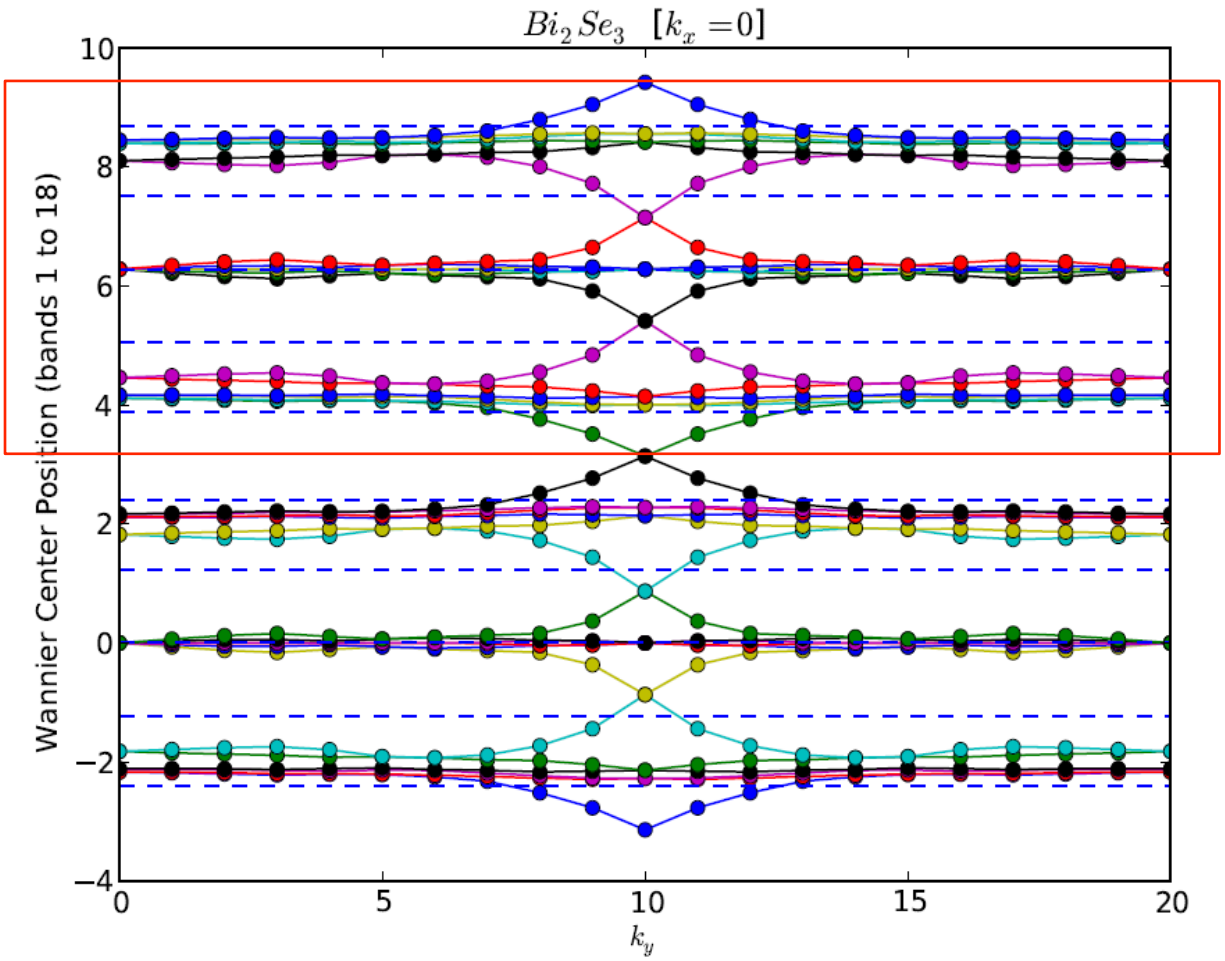
H. Zhang et al., Nature Physcis **5**, 2009

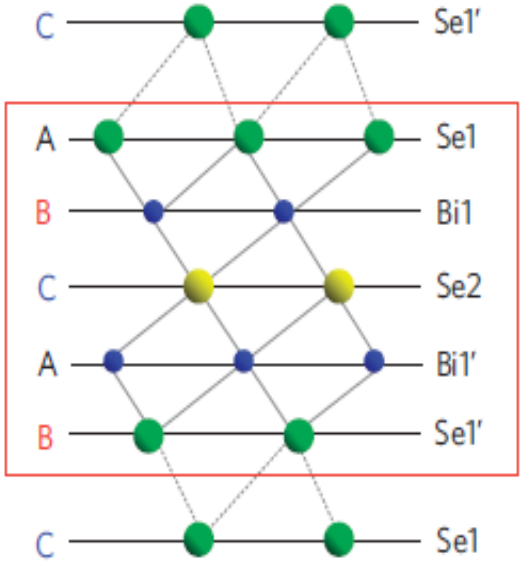
First-principles calculation: Bi_2Se_3



bulk bandstructure of Bi_2Se_3 projected onto Bi 6p orbitals

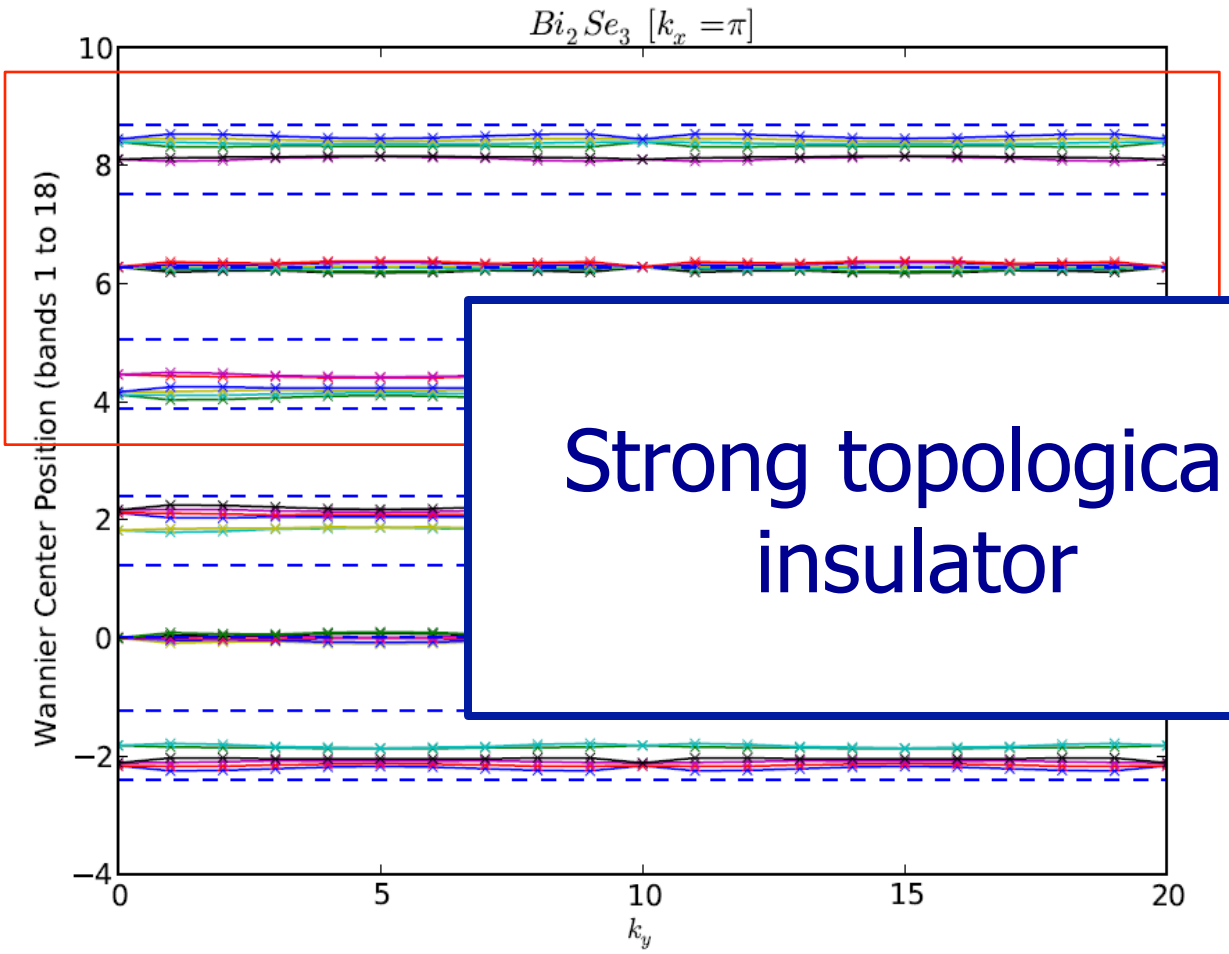
First-principles Bi_2Se_3 Wannier centers

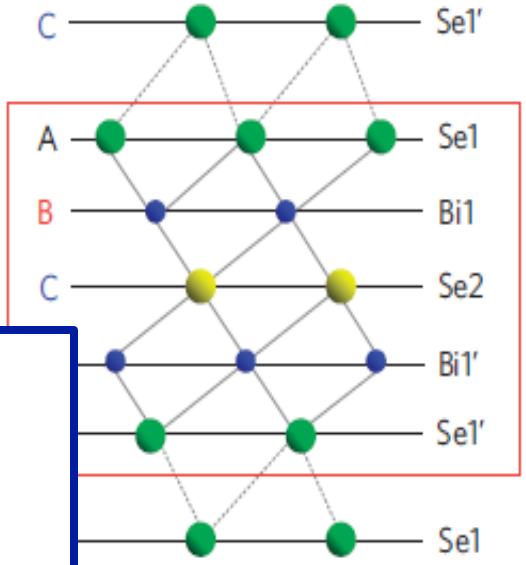




$\nu_{1a} = \nu(k_x=0) = (-)$

First-principles Bi_2Se_3 Wannier centers

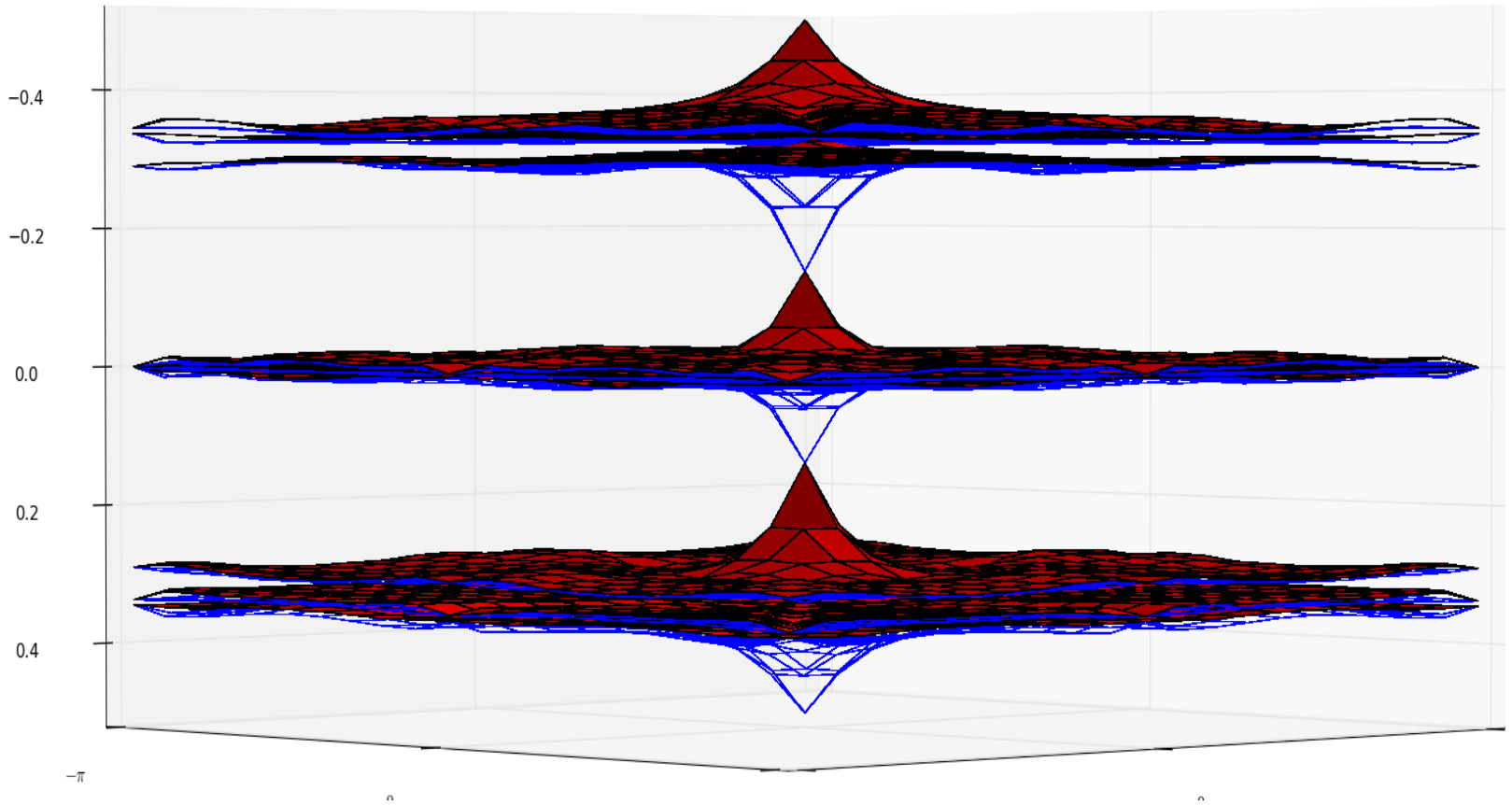




Strong topological insulator

$\nu_{1b} = \nu(k_x=\pi) = (+)$

First-principles Bi_2Se_3 Wannier centers



3D Z_2 topological insulators

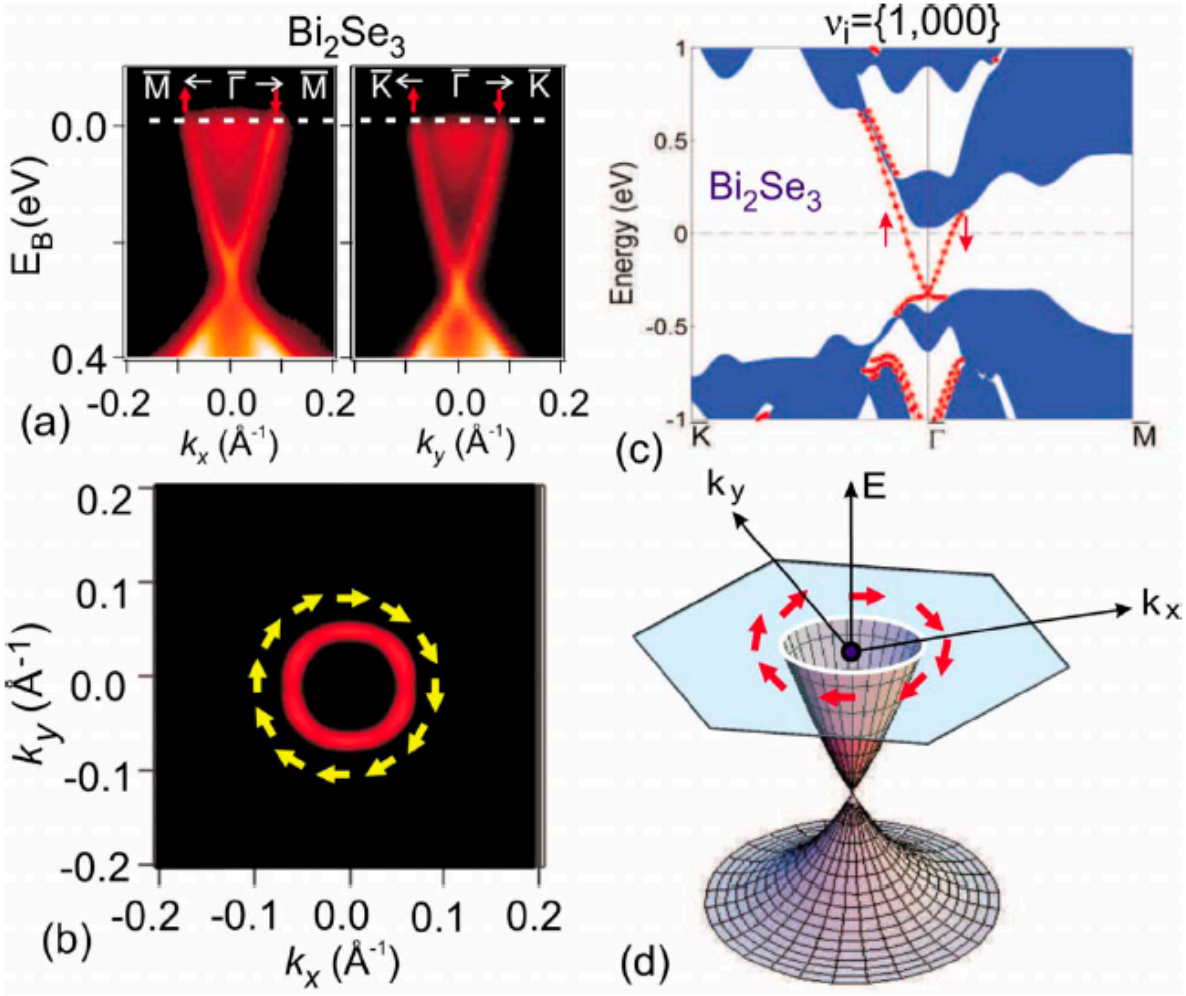


Figure from Hasan and Kane, RMP, 2010
(Adapted from Xia et al., 2008; Hsieh, Xia, Qian, Wray, et al., 2009a; and Xia, Qian, Hsieh, Wray, et al., 2009)