

3D Z_2 topological insulators

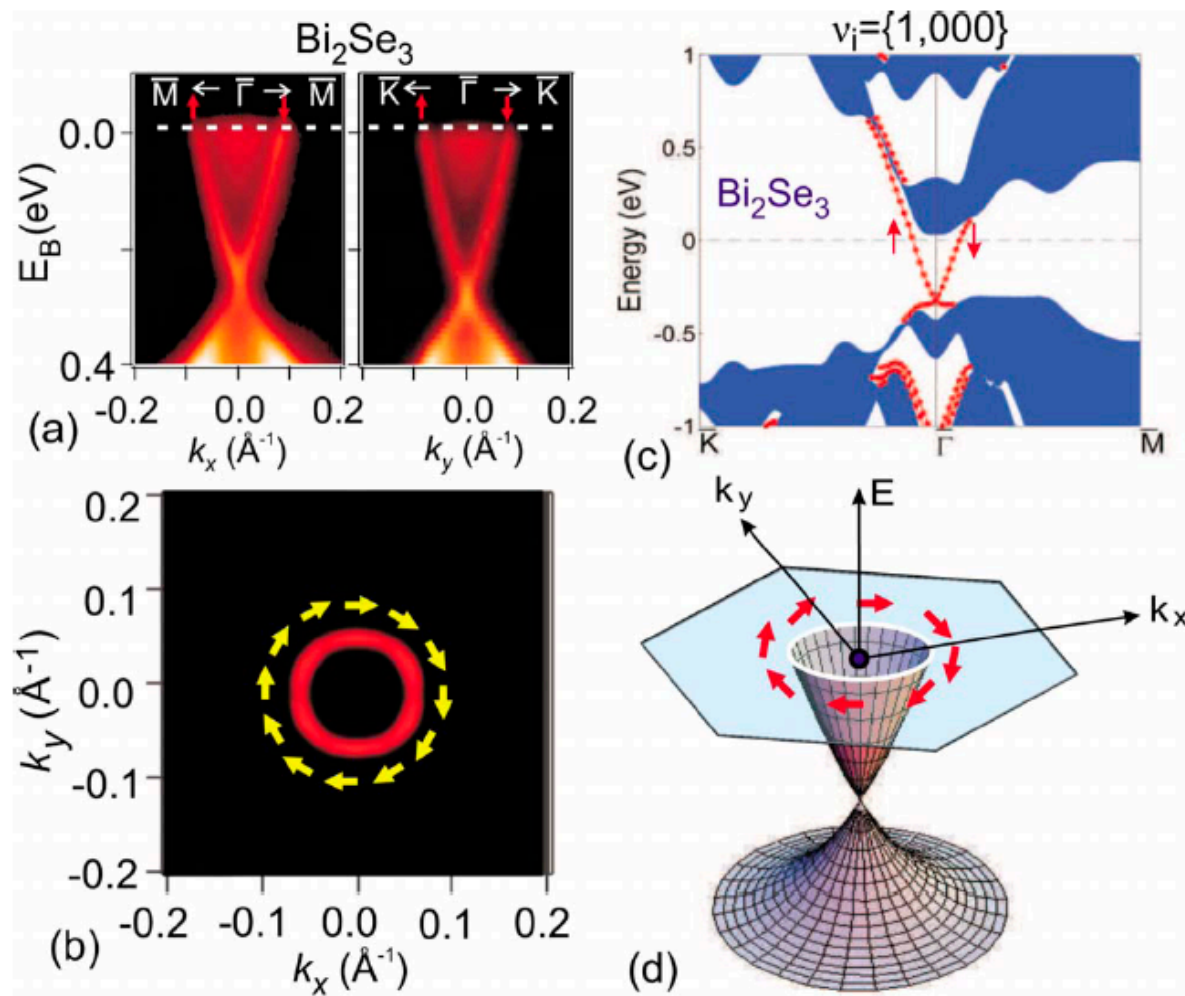
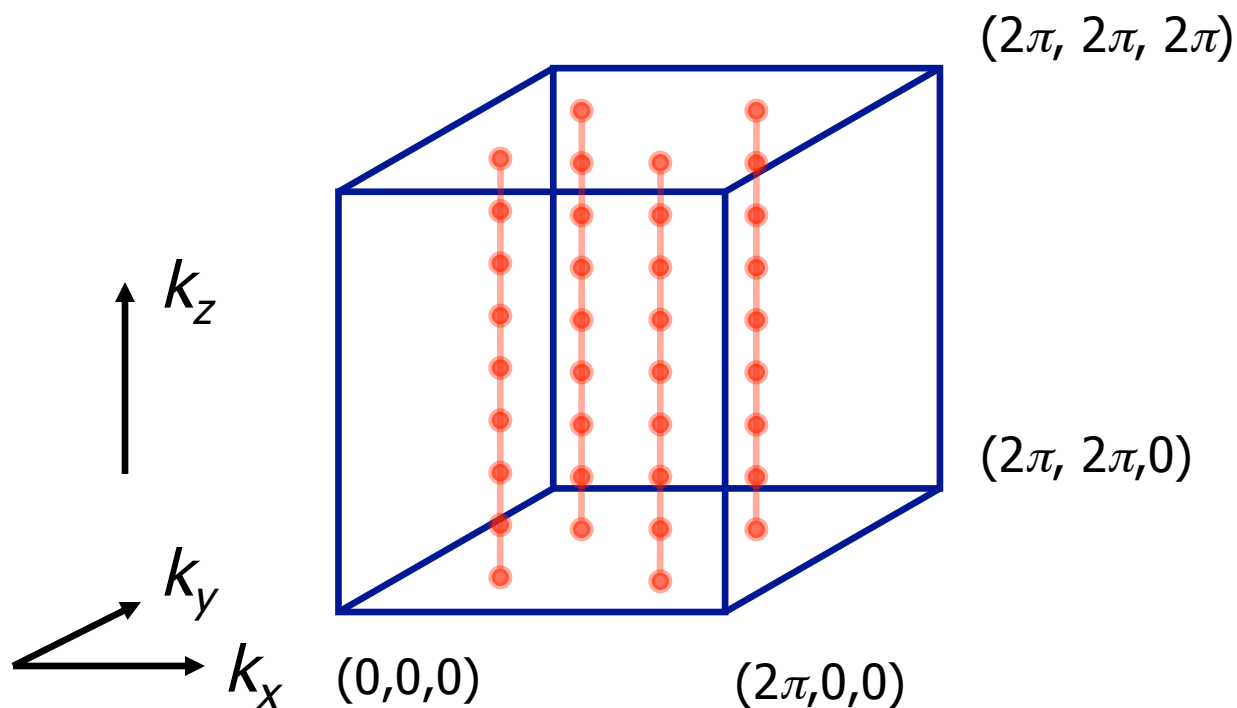


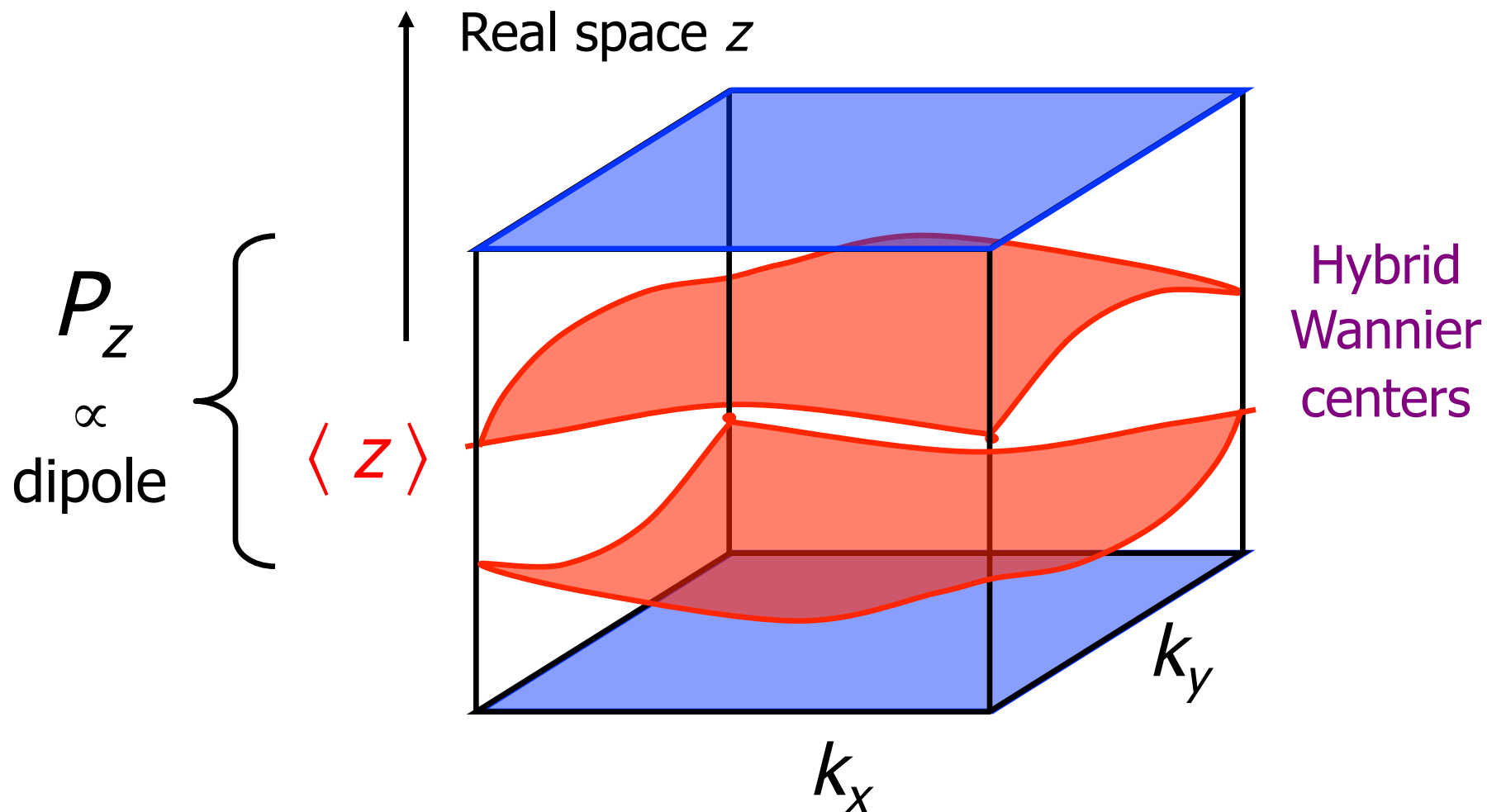
Figure from Hasan and Kane, RMP, 2010

(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



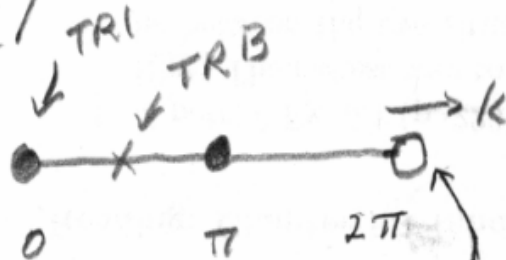
H_k IN TIME-REVERSAL-INVARIANT SYSTEMS

(TRI = TR INVARIANT TRB = TR - BROKEN)

0D

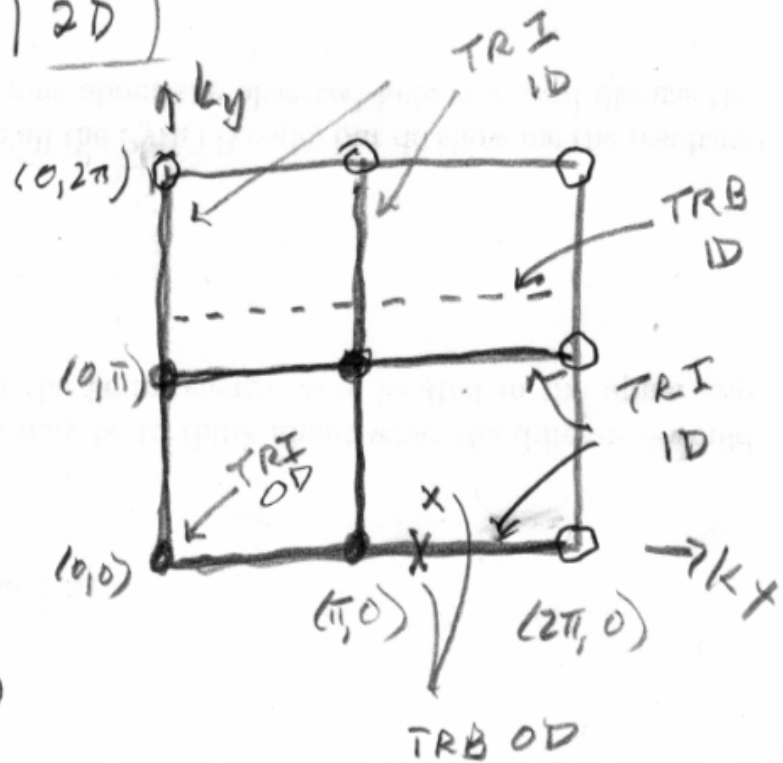
•
TRI

1D



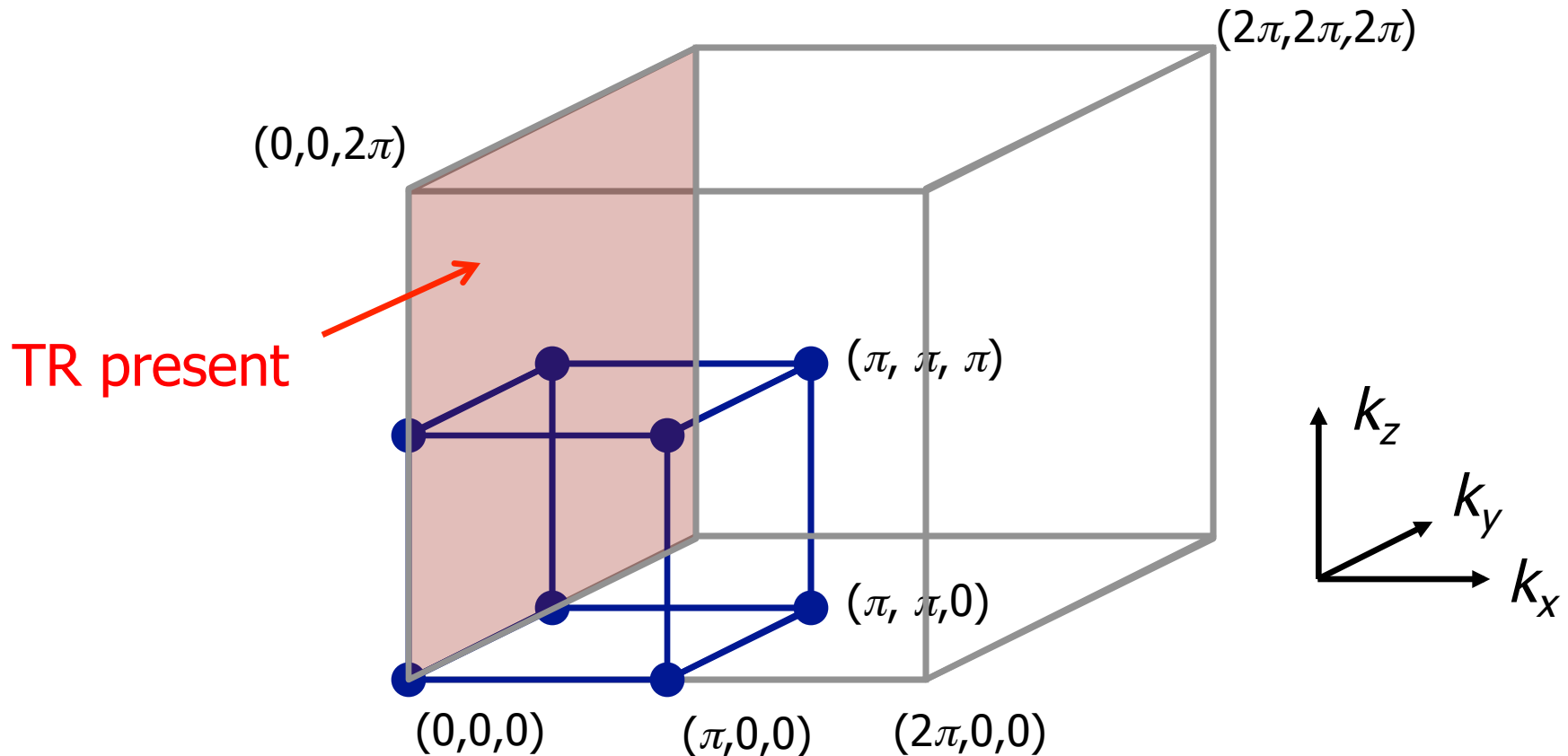
2 TRIM

2D



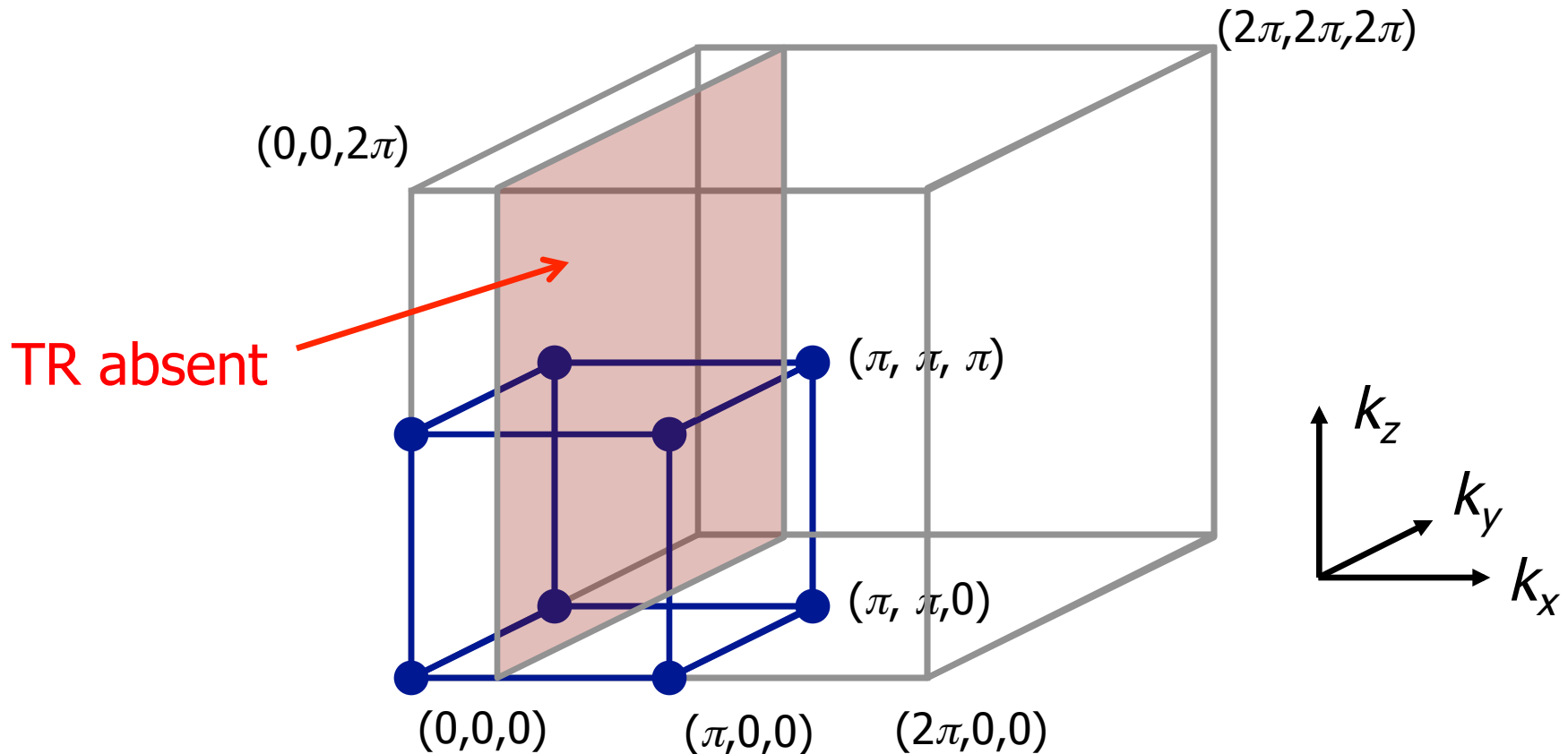
2 TRIM, 4 TRI LINES

3D Brillouin zone of TR-invariant ins.

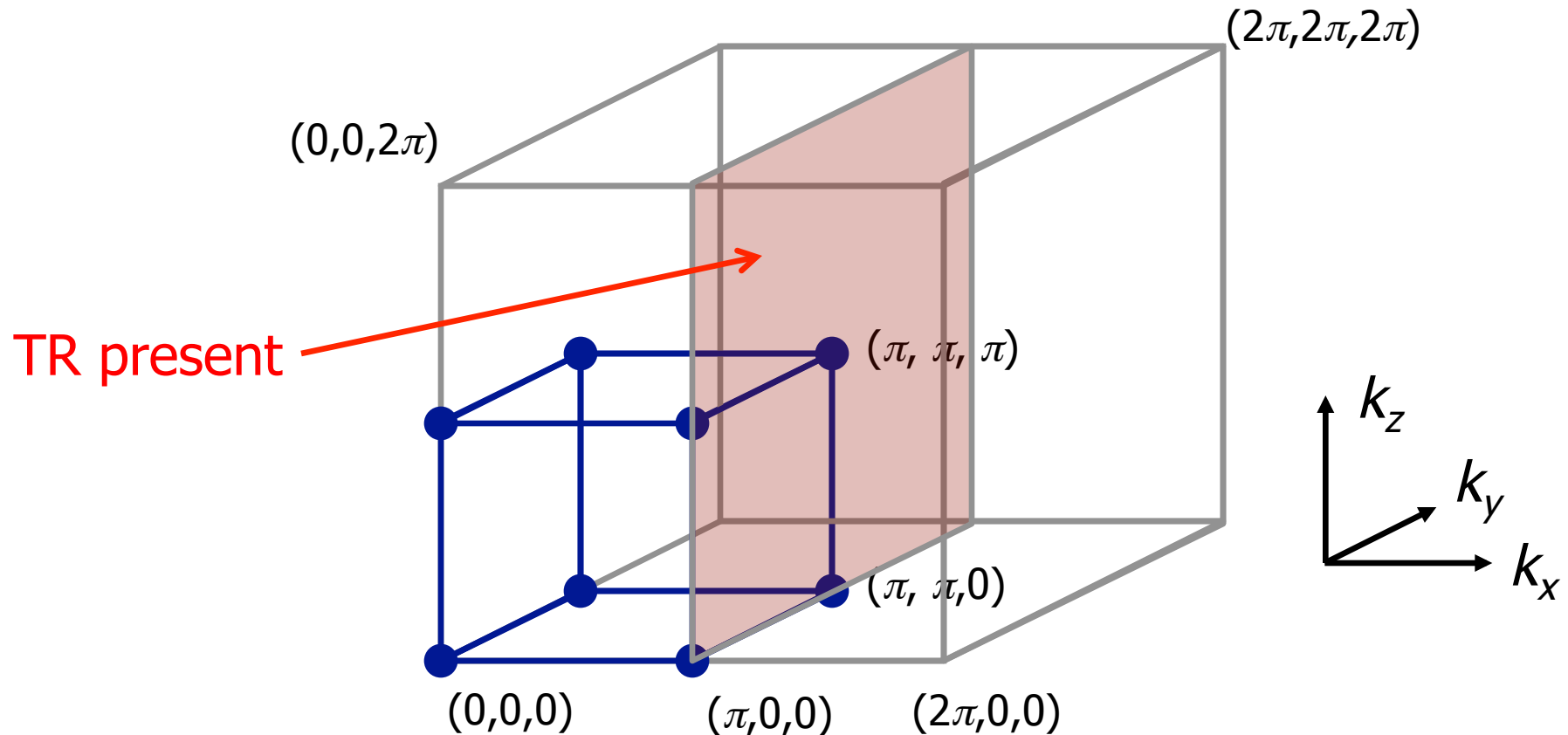


H_k is that of a 2D insulator with TR

3D Brillouin zone of TR-invariant ins.

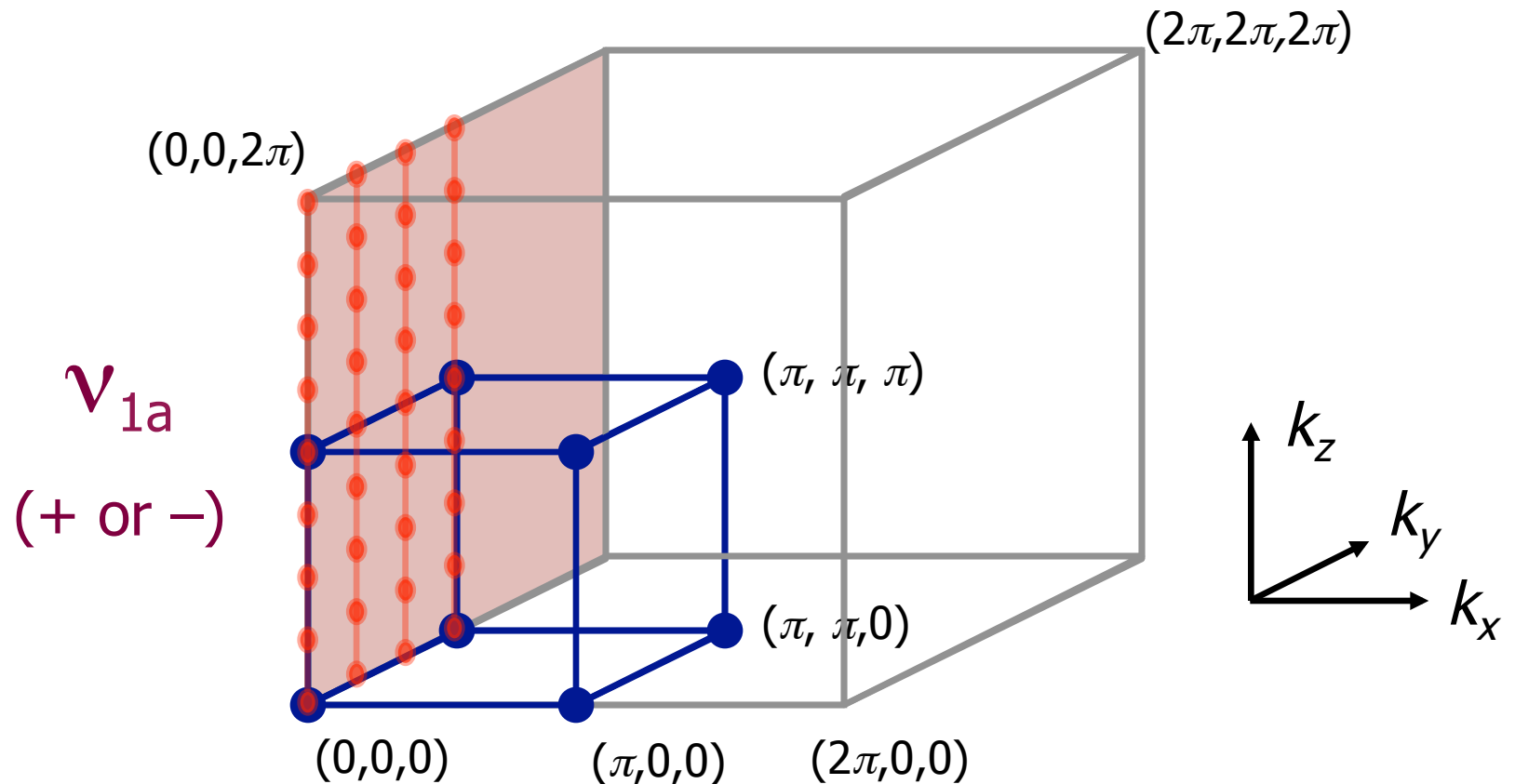


3D Brillouin zone of TR-invariant ins.

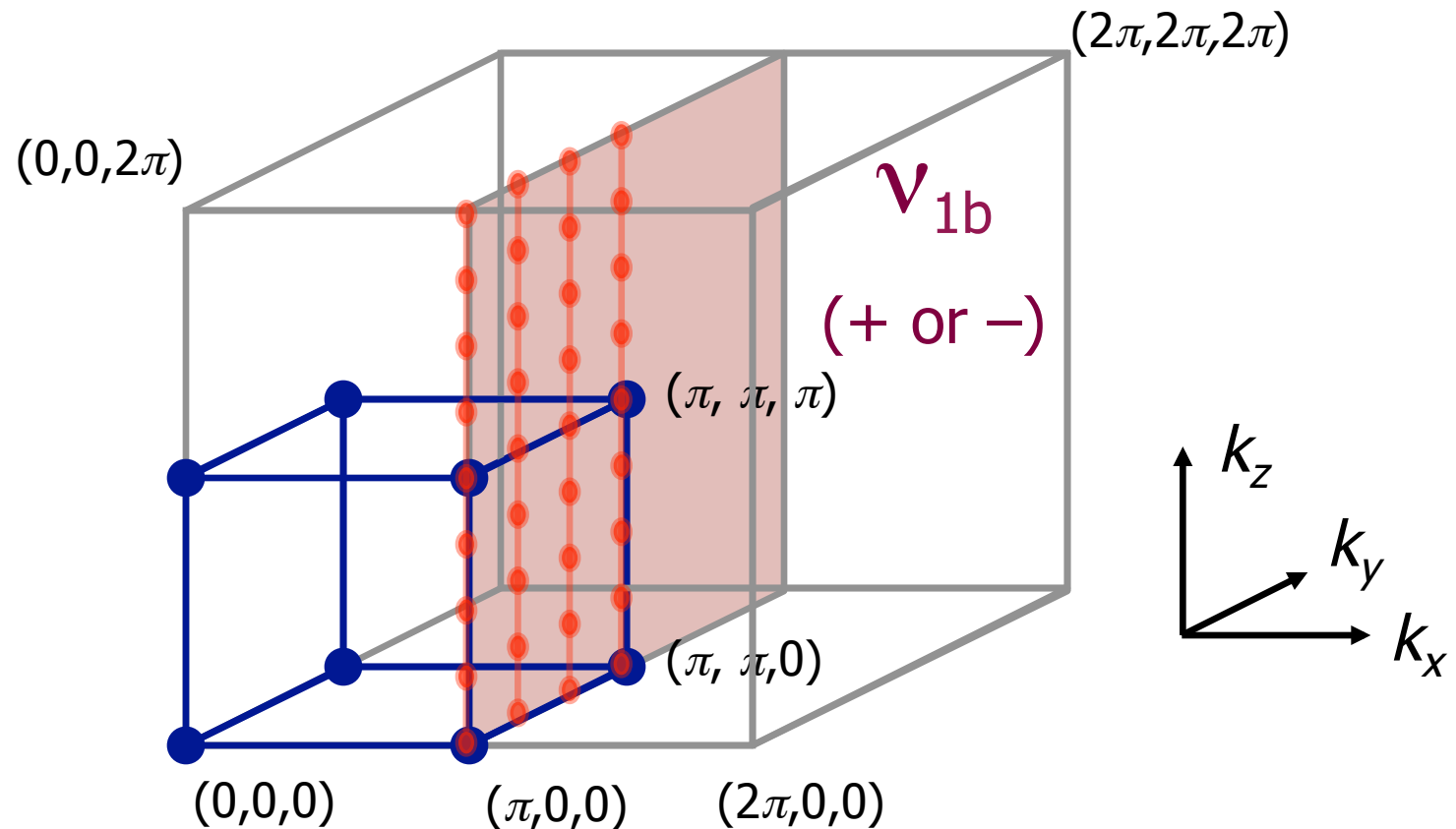


H_k is that of a 2D insulator with TR

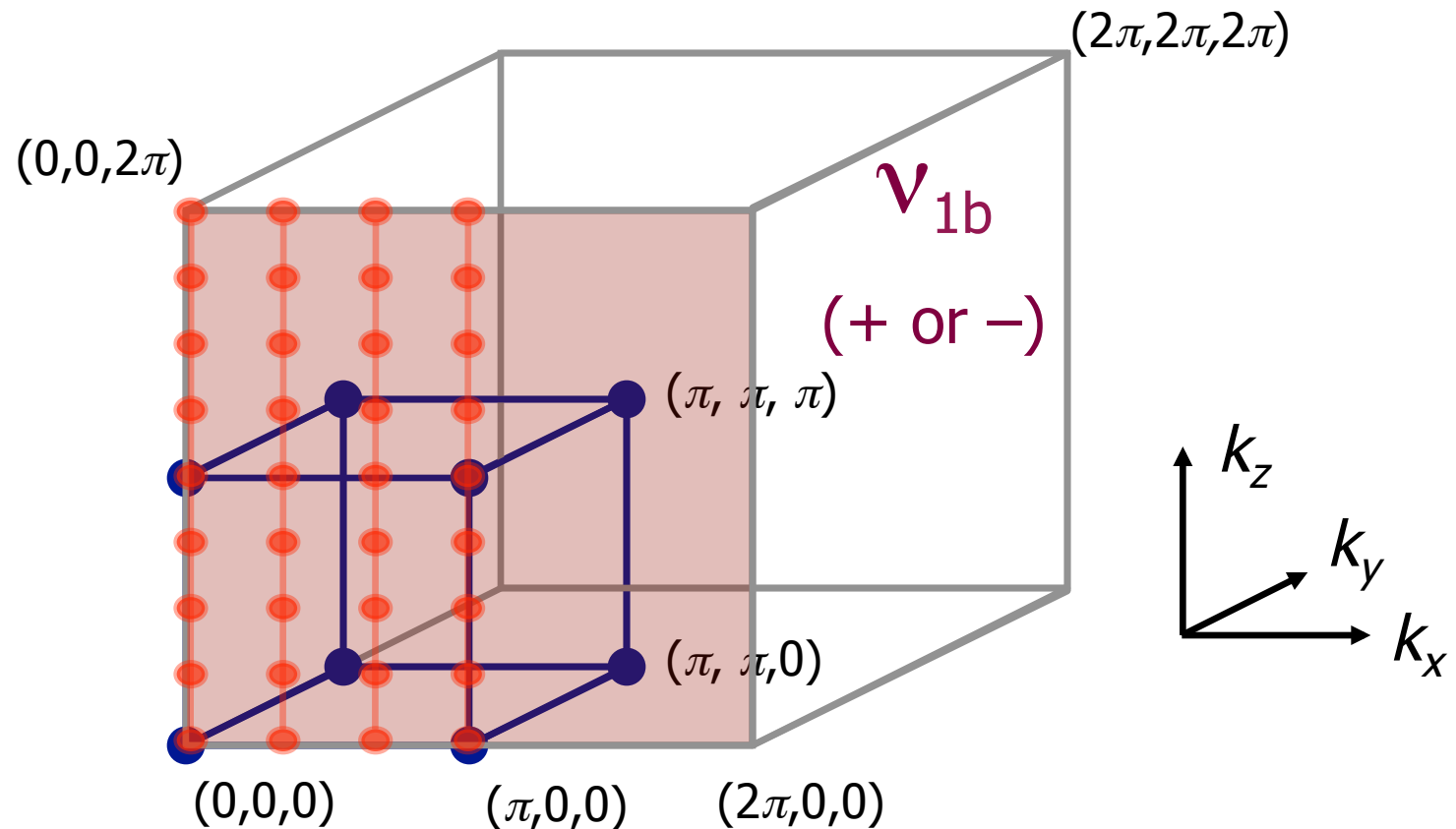
3D Brillouin zone of TR-invariant ins.



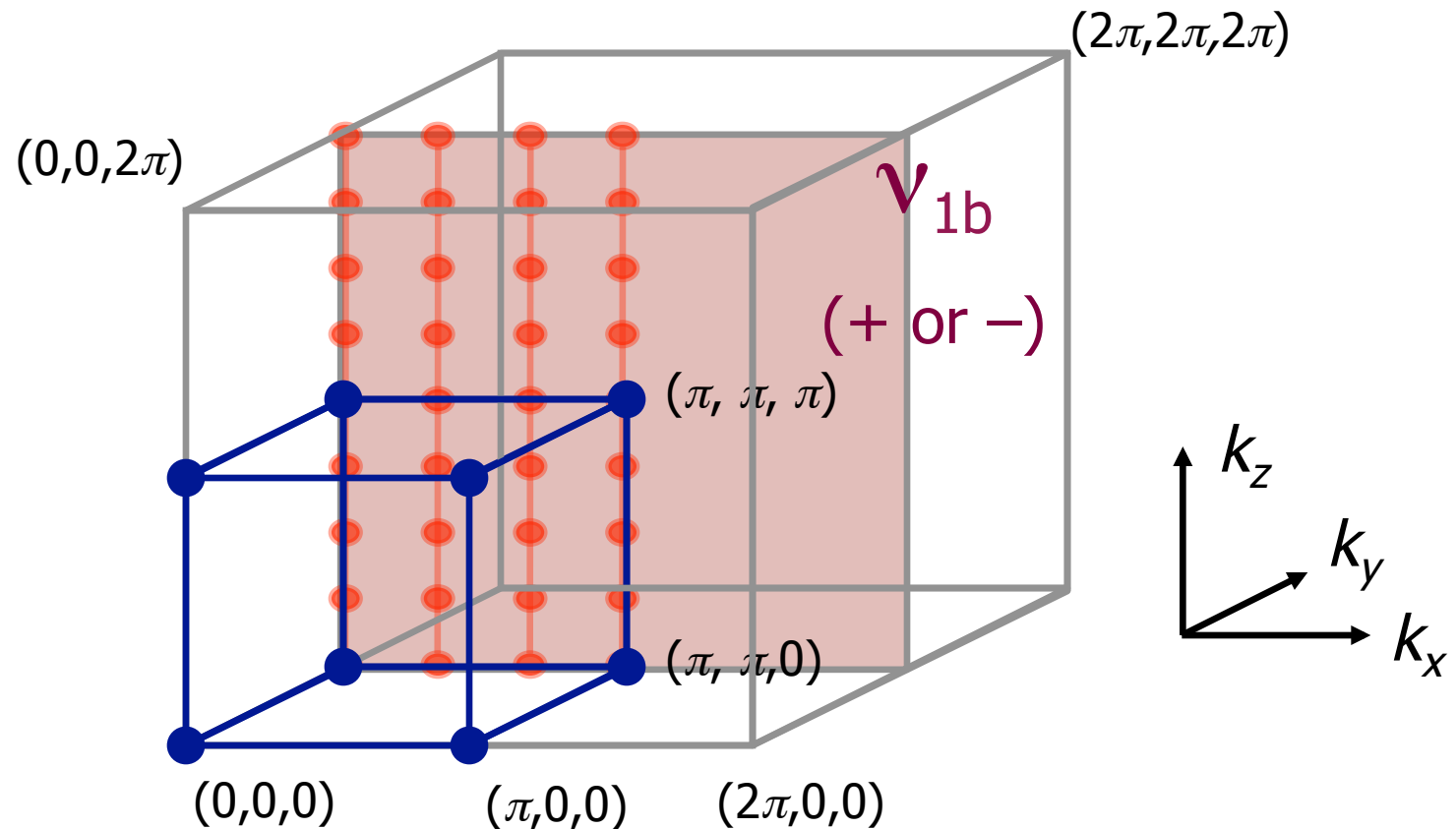
3D Brillouin zone of TR-invariant ins.



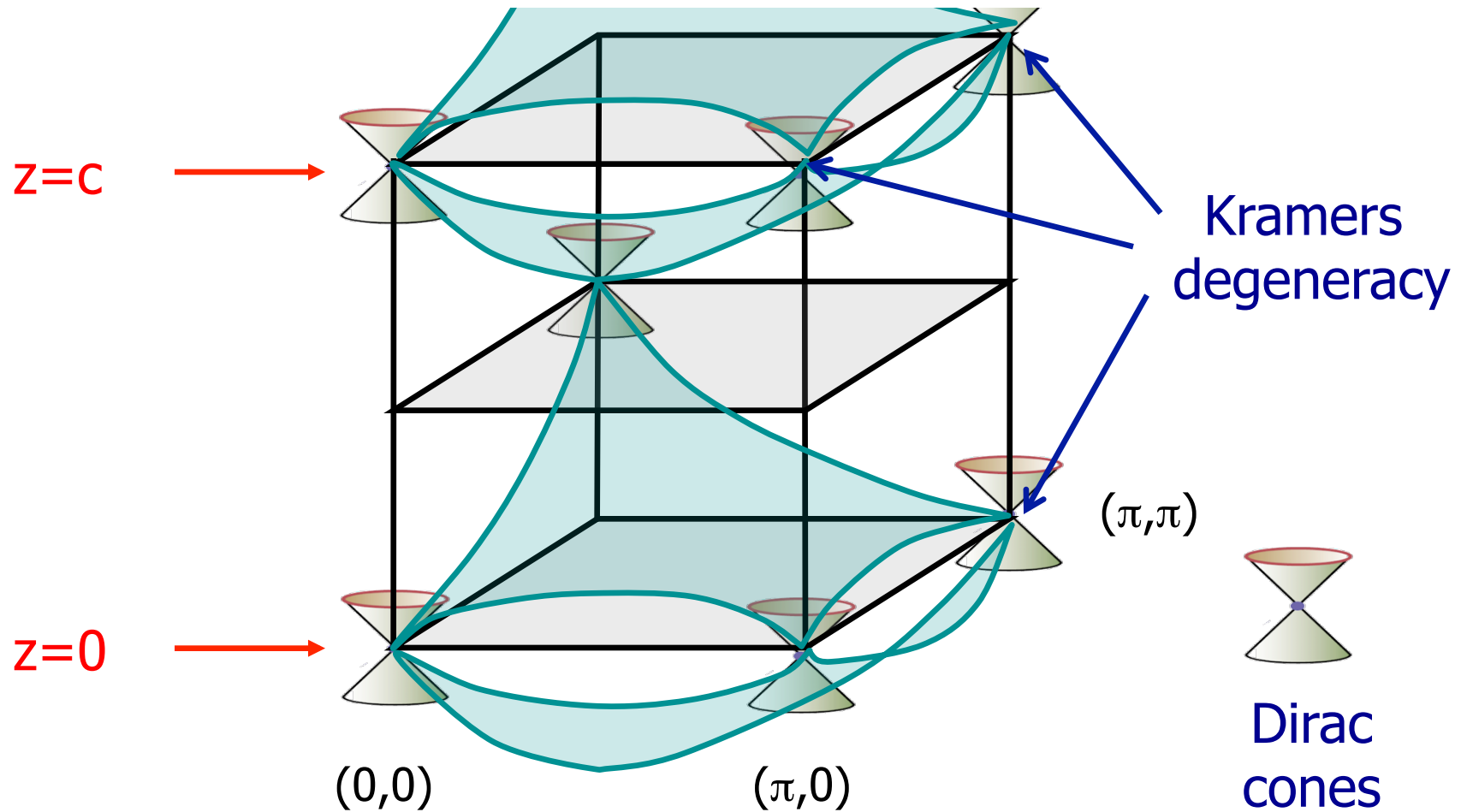
3D Brillouin zone of TR-invariant ins.



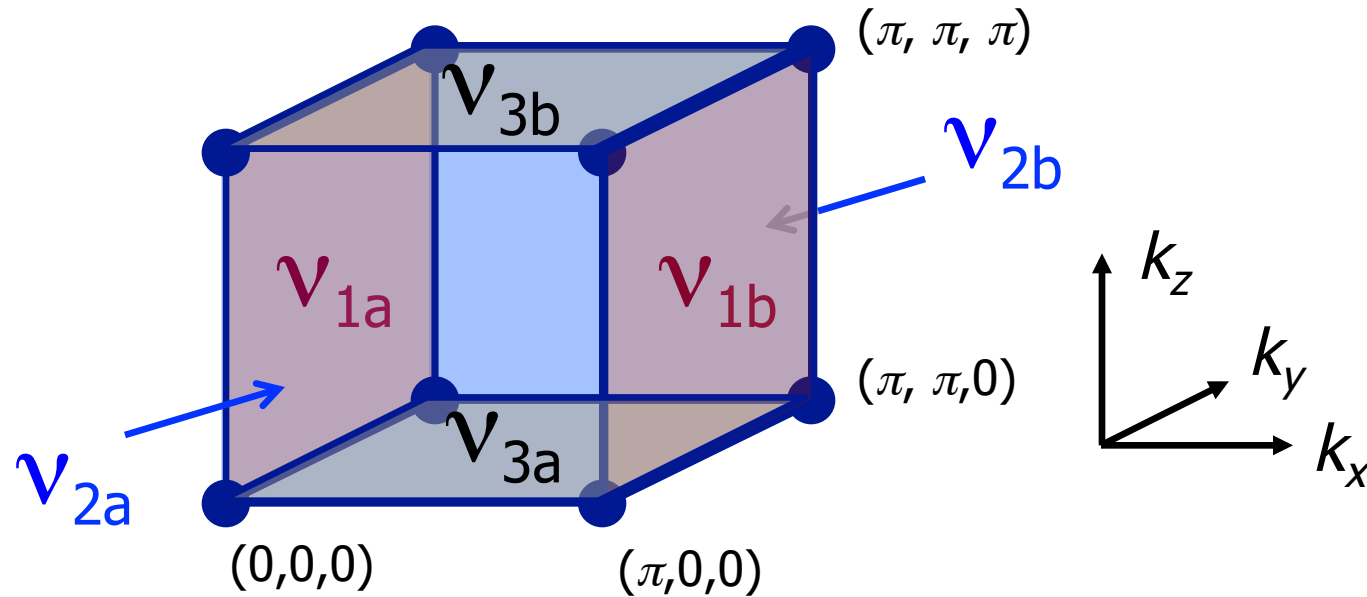
3D Brillouin zone of TR-invariant ins.



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

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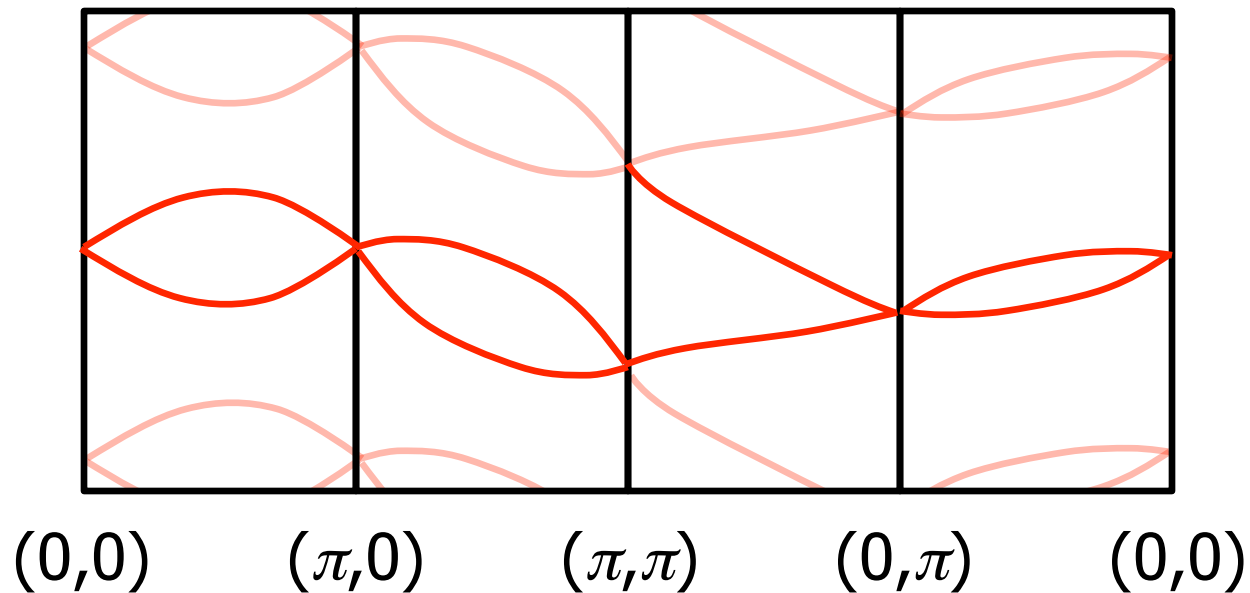
$$\nu_0 = \nu_{1a}\nu_{1b} = \nu_{2a}\nu_{2b} = \nu_{3a}\nu_{3b}$$

$\nu_0 = (+)$: Opposite faces have same indices

$\nu_0 = (-)$: Opposite faces have opposite indices
“Strong Topological Insulator” (STI)

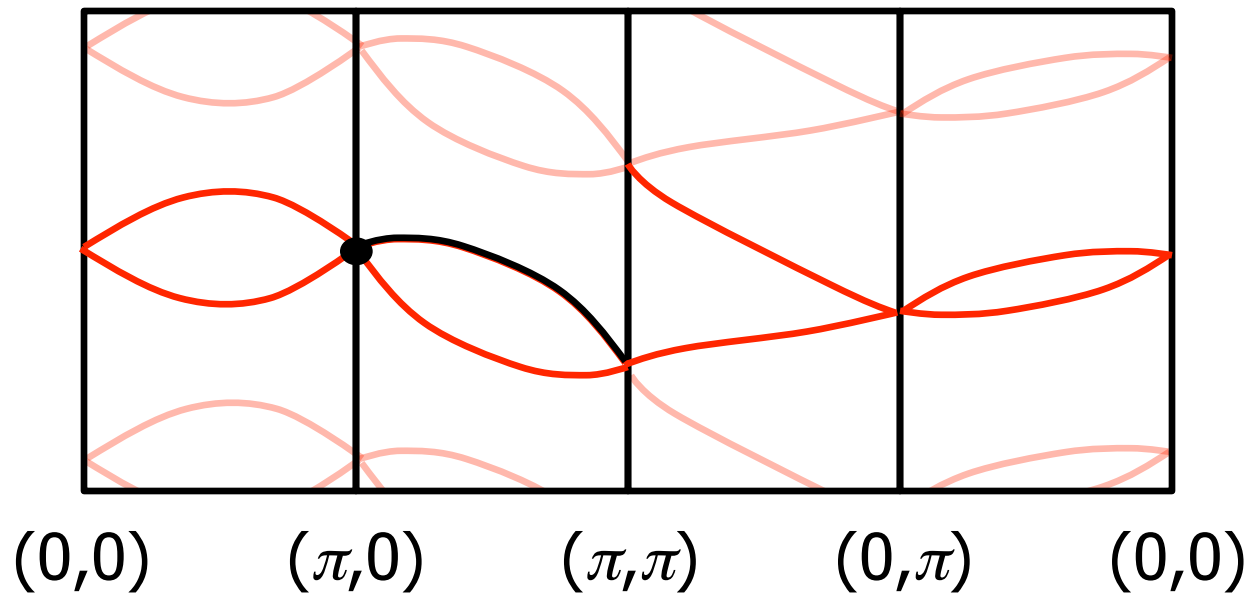
Full index set: $(\nu_0; \nu_{1b} \nu_{2b} \nu_{3b})$

Moore-Balents rule



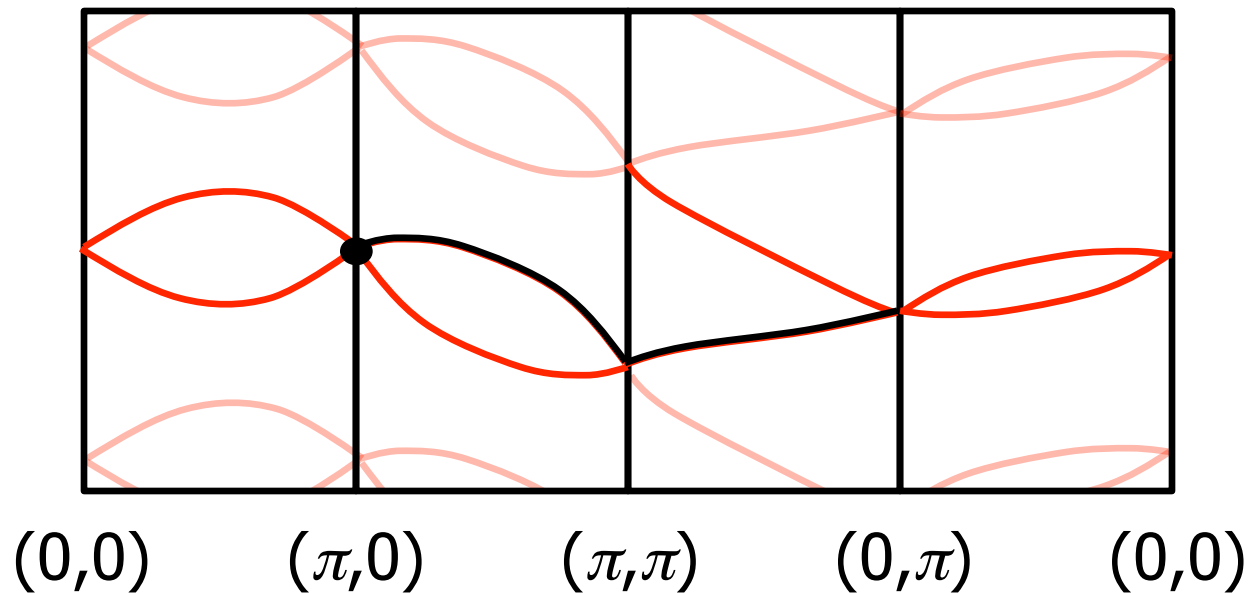
This would violate the Moore-Balents rule
Is it possible?

Moore-Balents rule



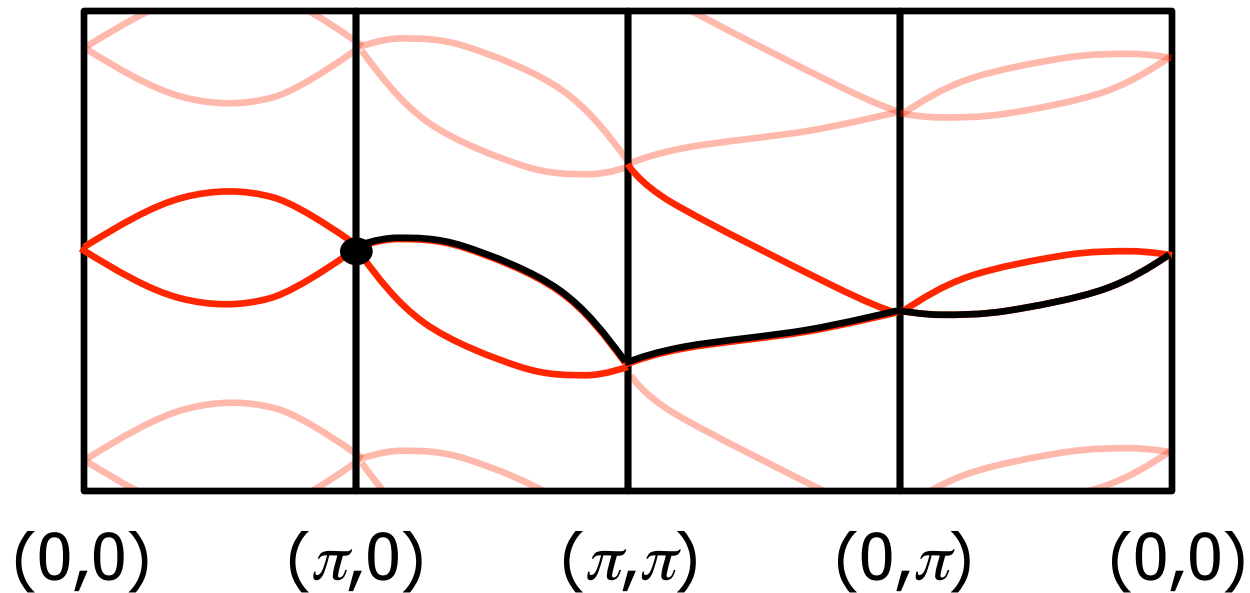
This would violate the Moore-Balents rule
Is it possible?

Moore-Balents rule



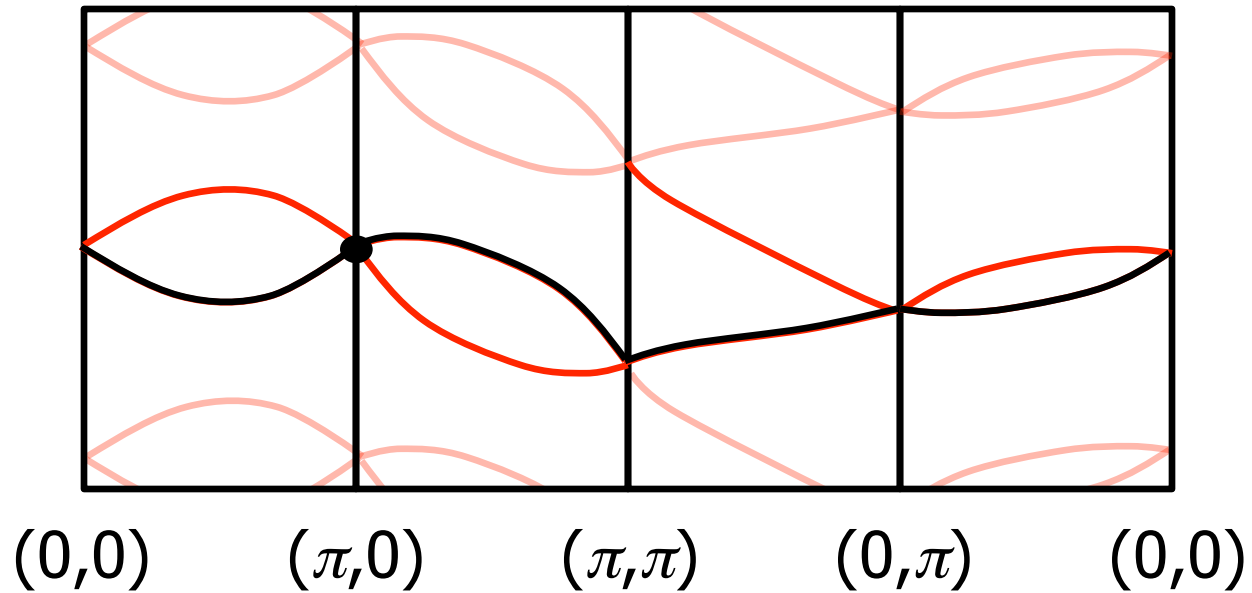
This would violate the Moore-Balents rule
Is it possible?

Moore-Balents rule



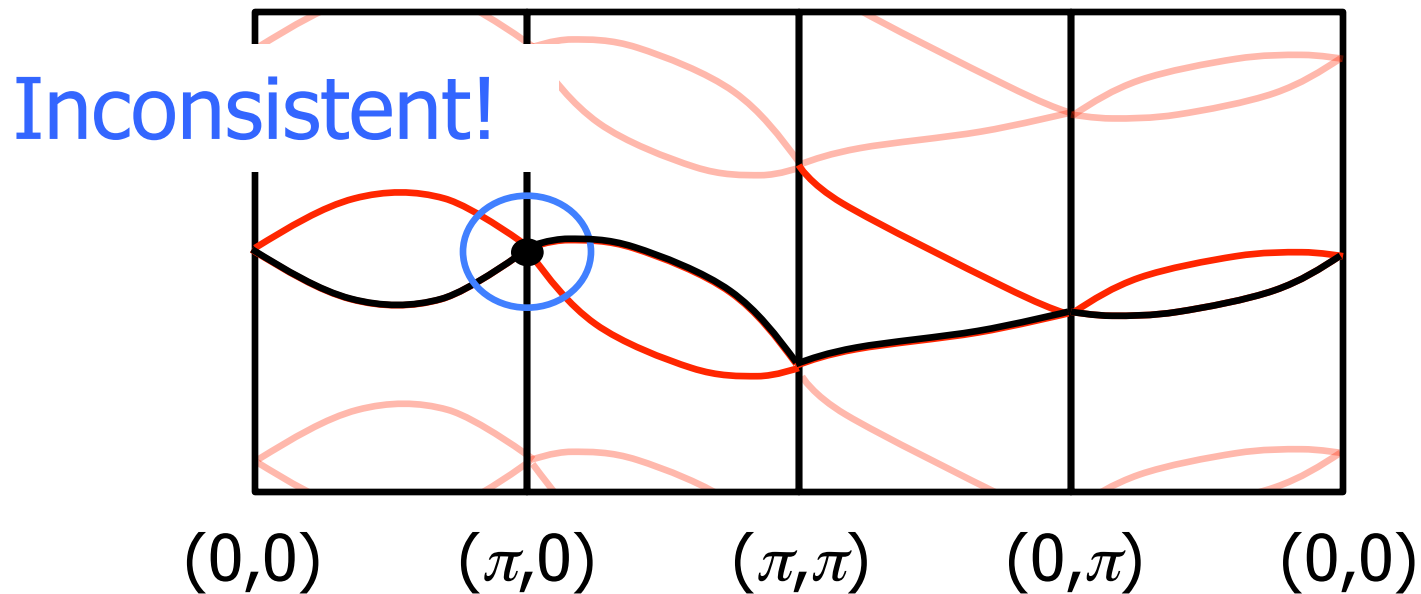
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Moore-Balents rule



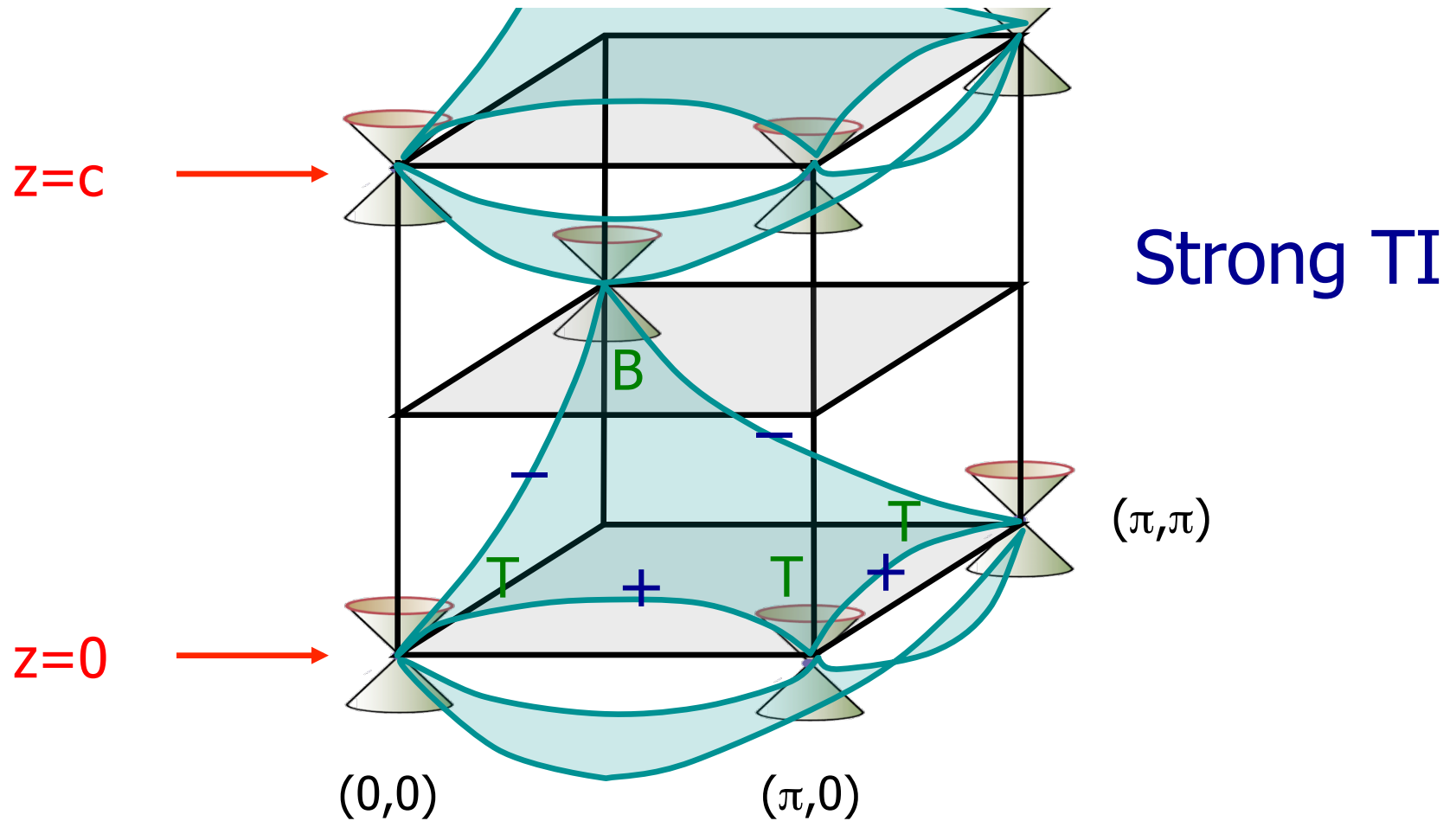
This would violate the Moore-Balents rule
Is it possible?

Moore-Balents rule

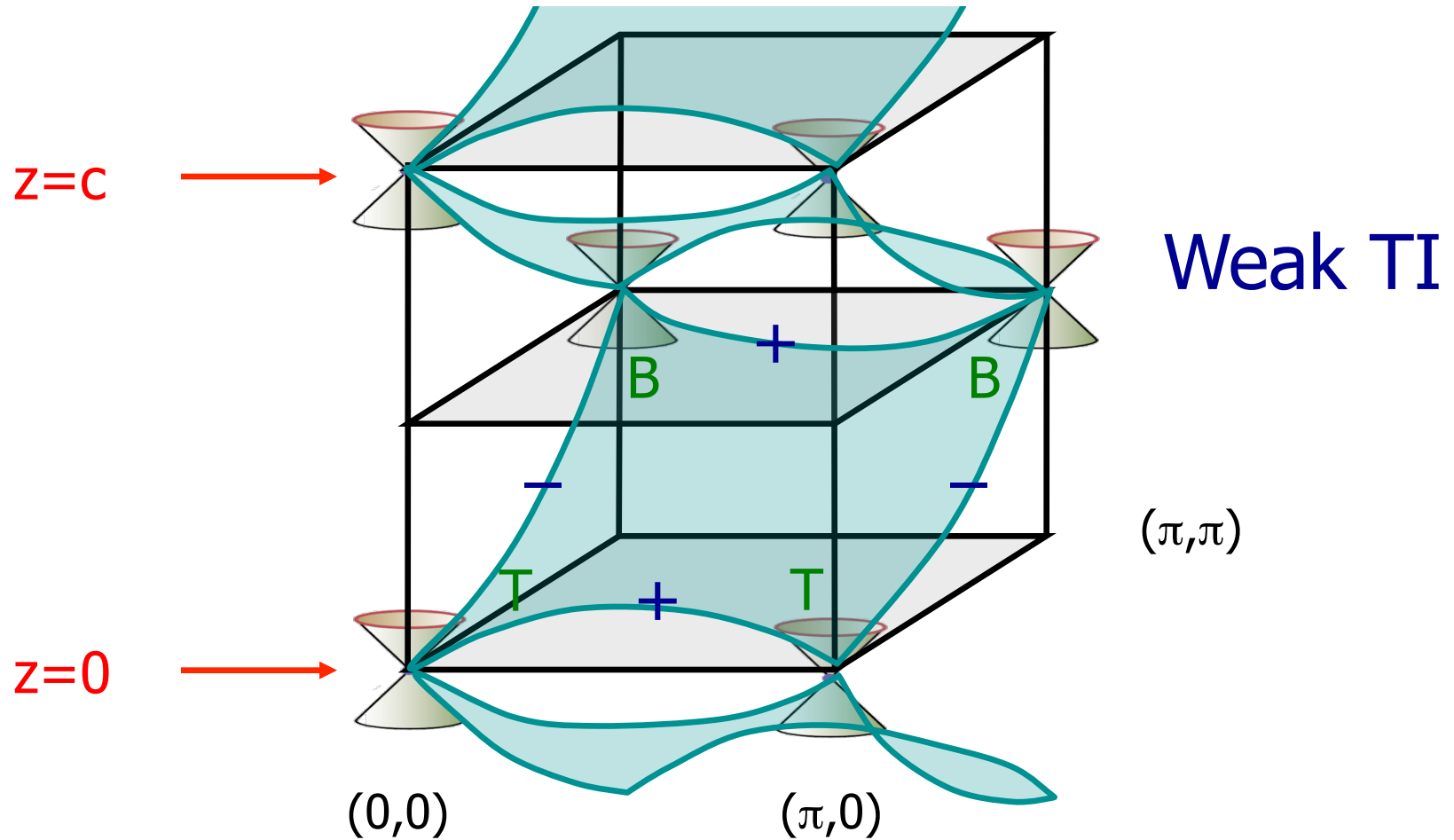


This would violate the Moore-Balents rule
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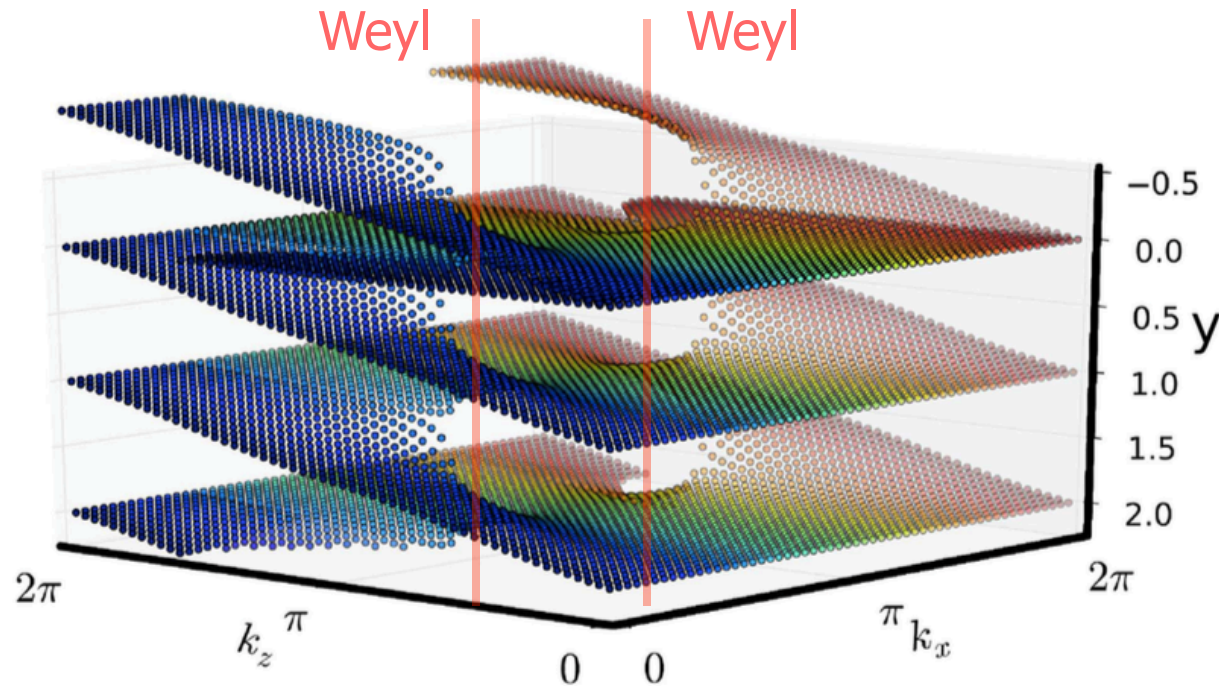
Hybrid WF sheets



Hybrid WF sheets



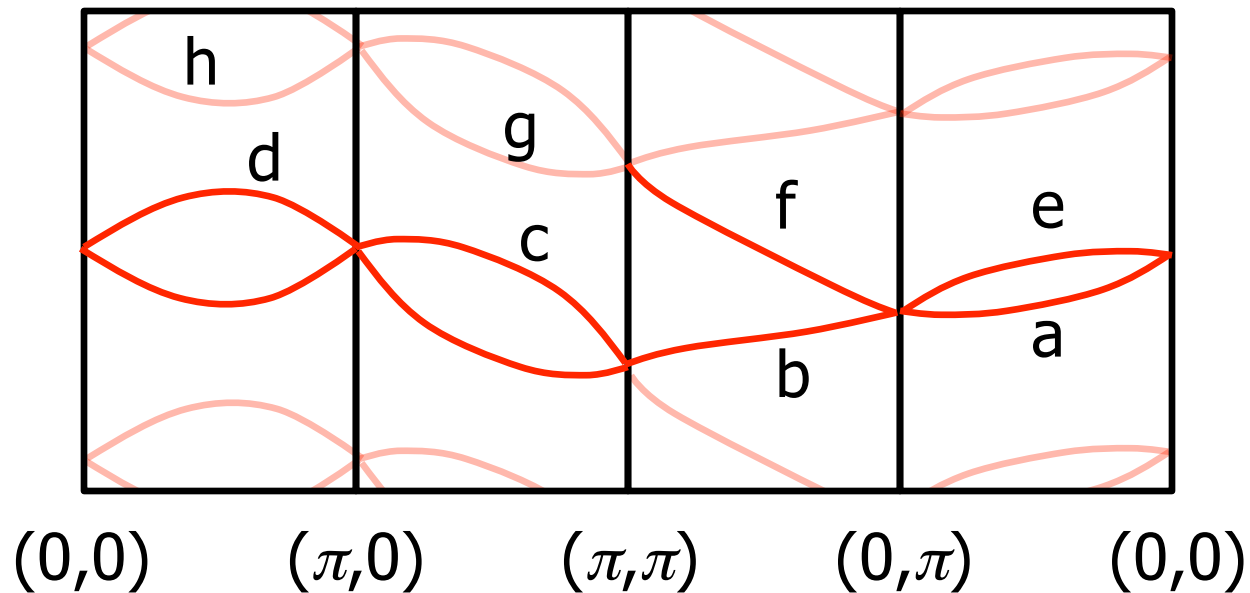
Weyl semimetal



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

One Weyl point in the $\frac{1}{4}$ 2D BZ allows violation of the Moore-Balents rule

Moore-Balents rule



One Weyl point in the $\frac{1}{4}$ 2D BZ allows violation of the Moore-Balents rule

Bulk-boundary correspondence: 2D

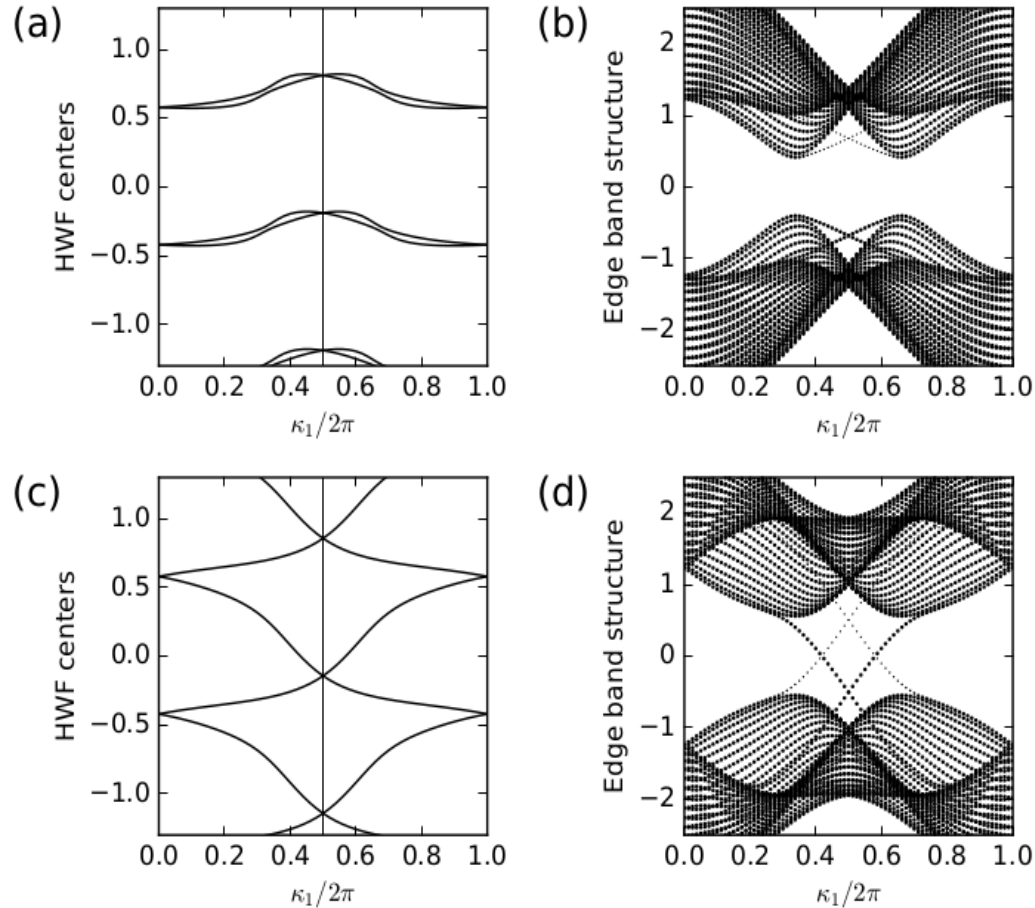
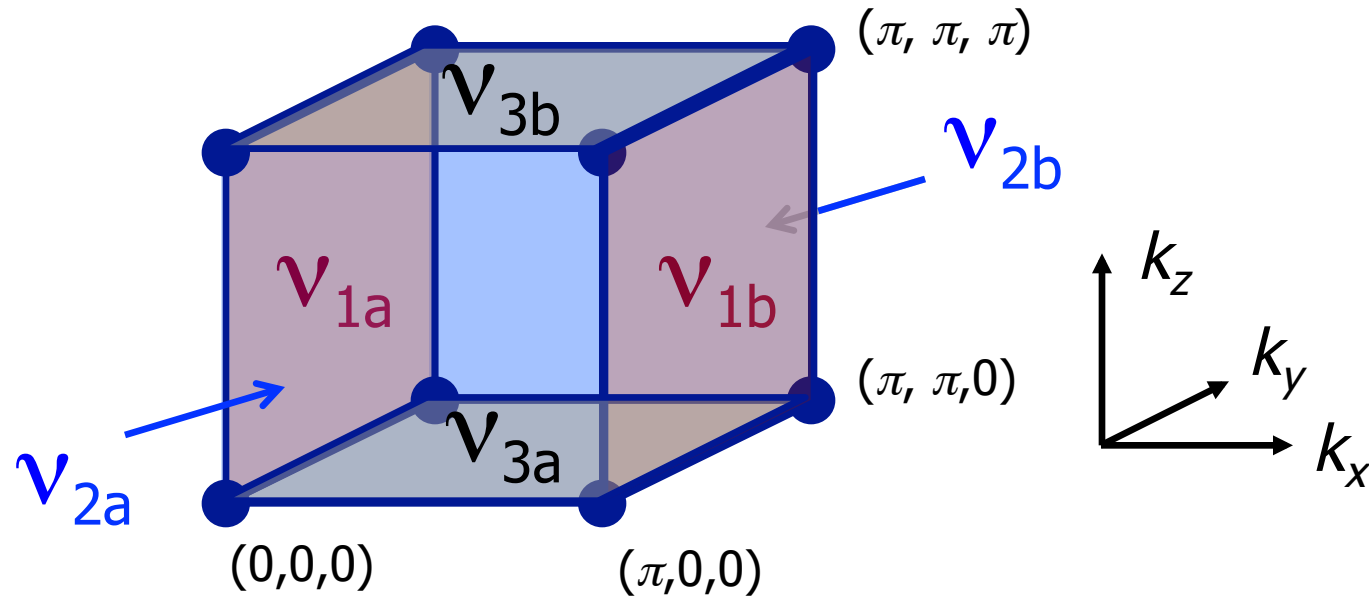


Figure 5.13 (a) Flow of hybrid Wannier centers for a Kane-Mele model in the trivial phase with $\Delta = 0.7$, $t_1 = -1.0$, $\lambda_R = 0.05$, and $\lambda_{SO} = -0.06$. (b) Edge states on a ribbon cut from the same model; those on the top and bottom edges of the ribbon are indicated by full and reduced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

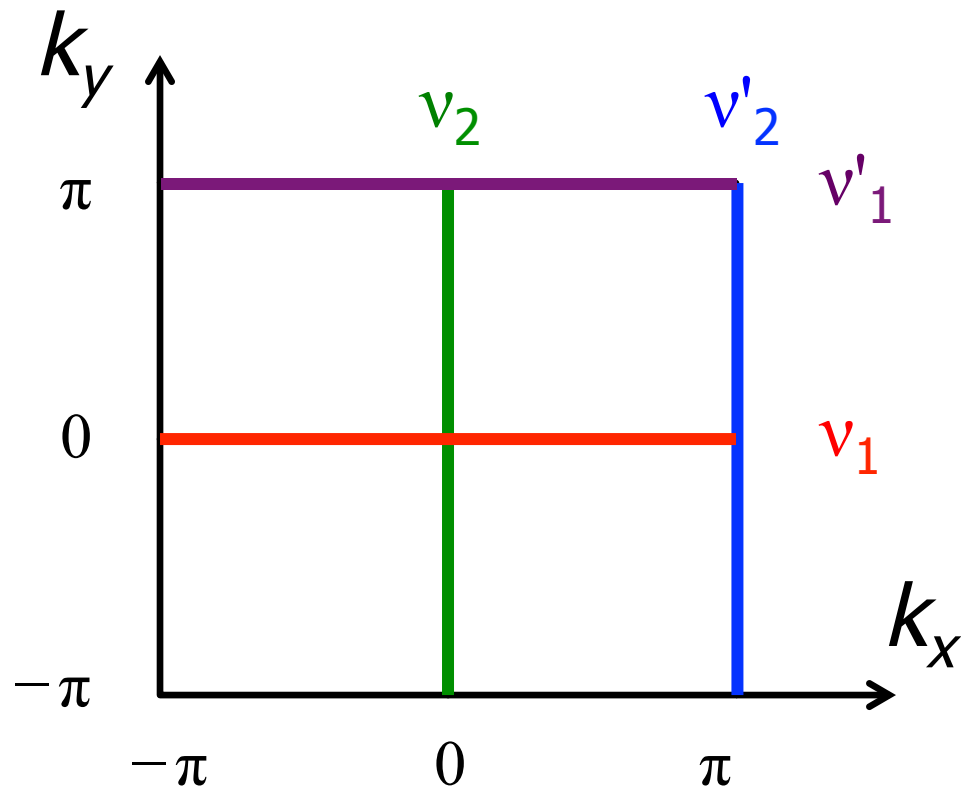


Fig. 5.17: $(v_1 \ v'_1; v_2 \ v'_2) = ?$

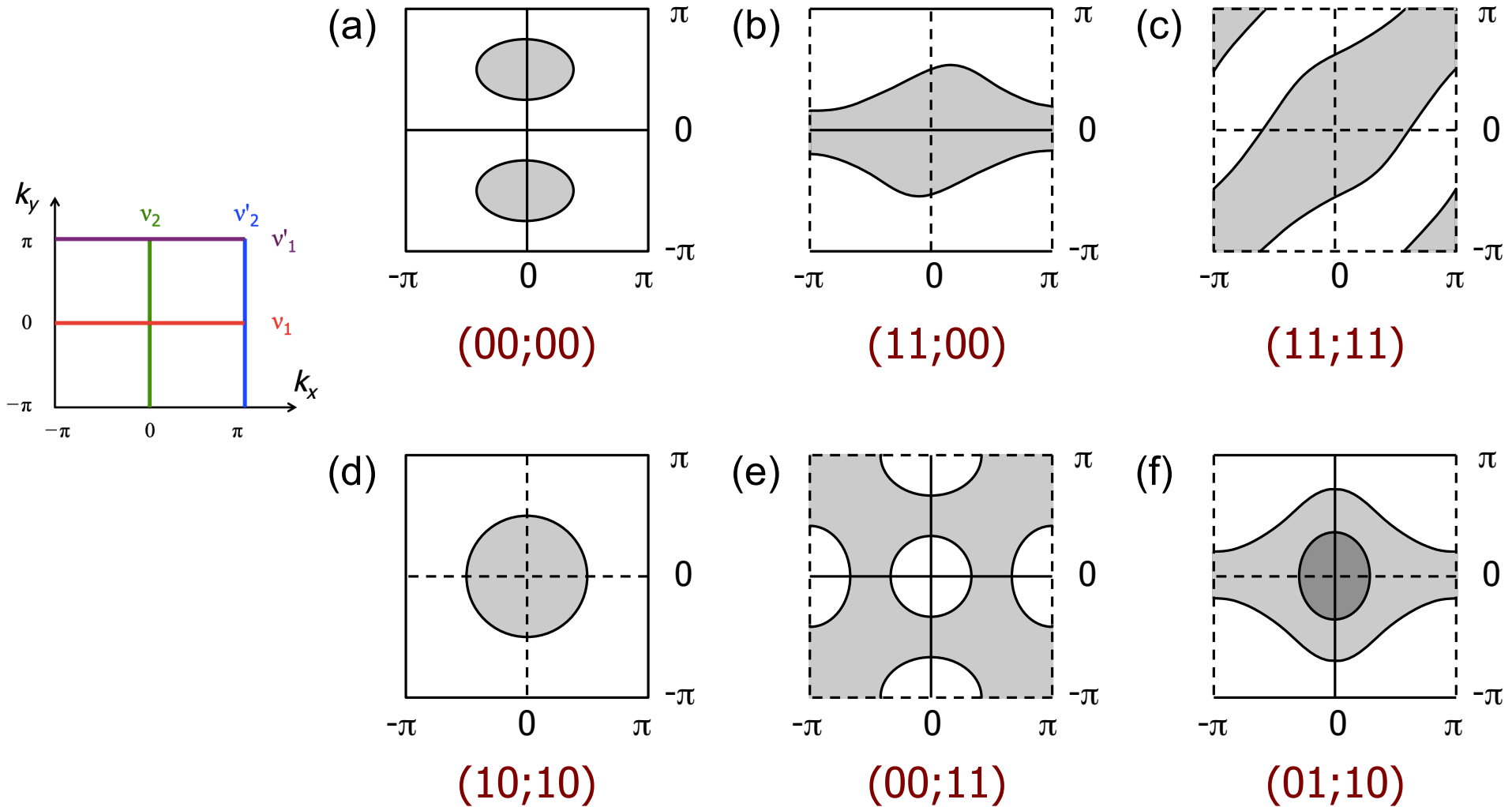
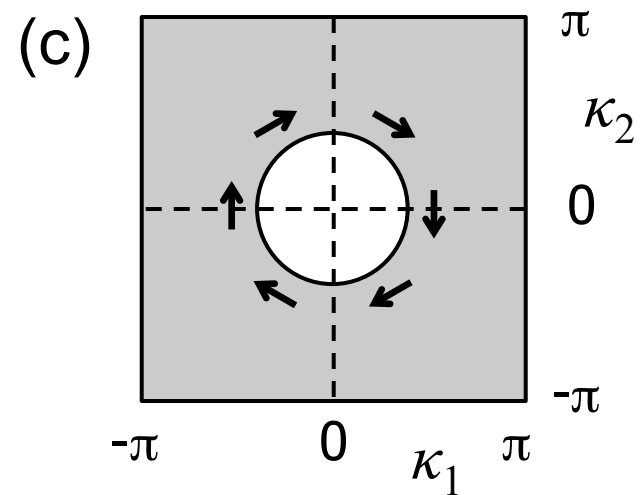
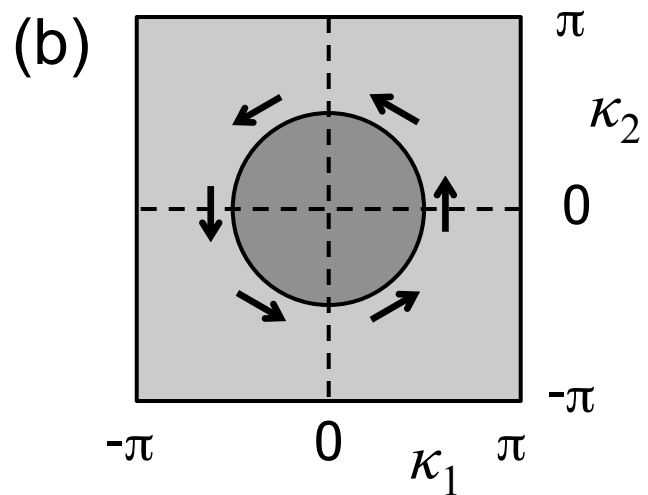
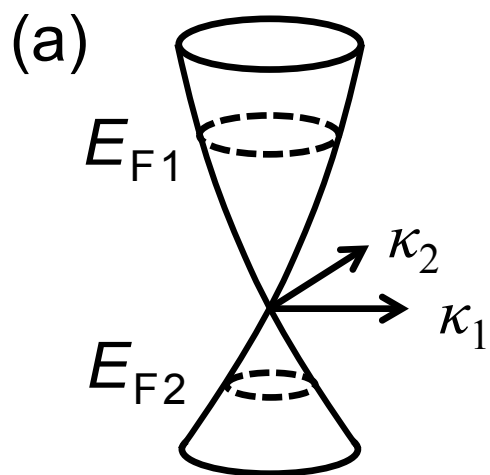
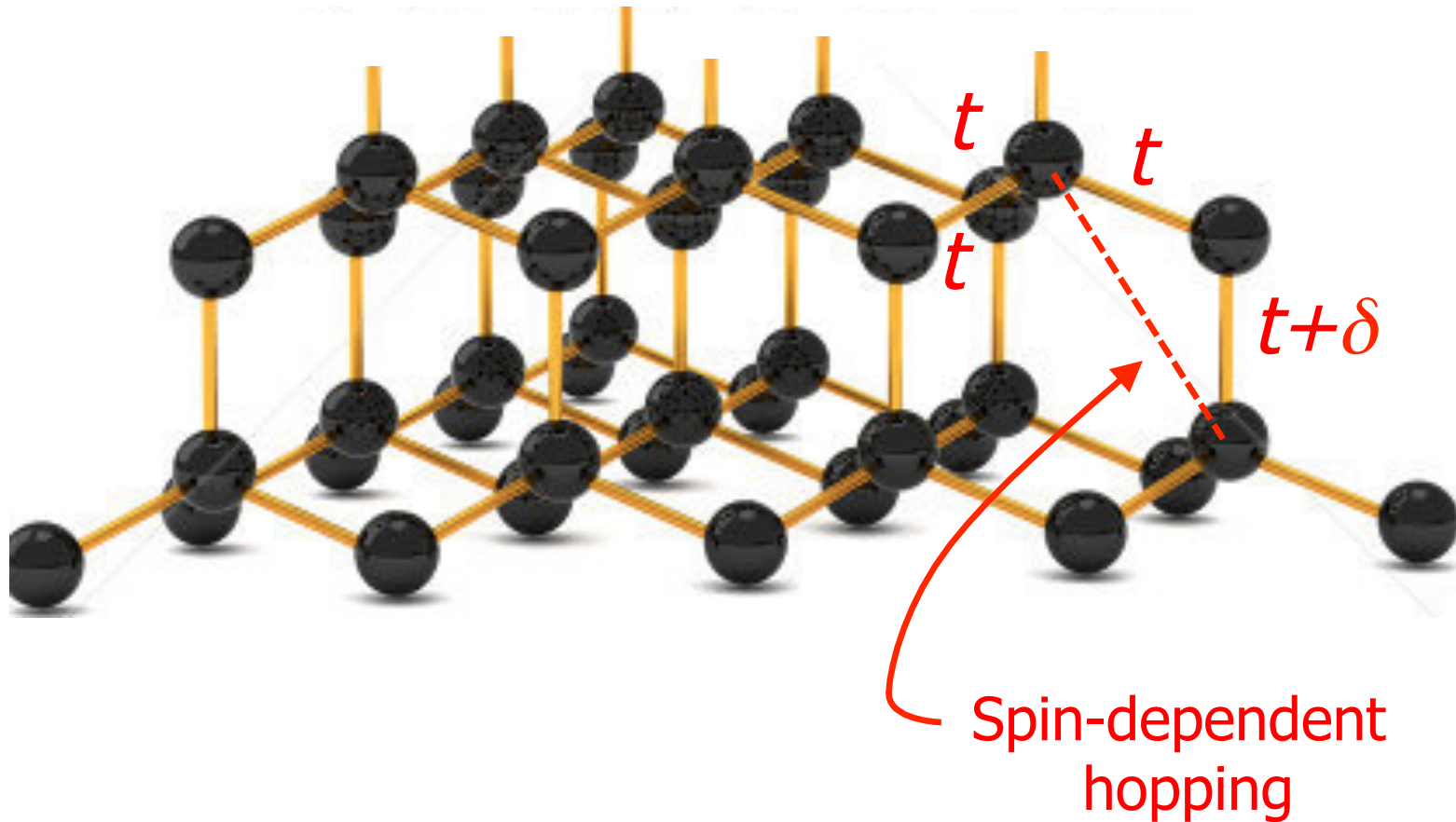


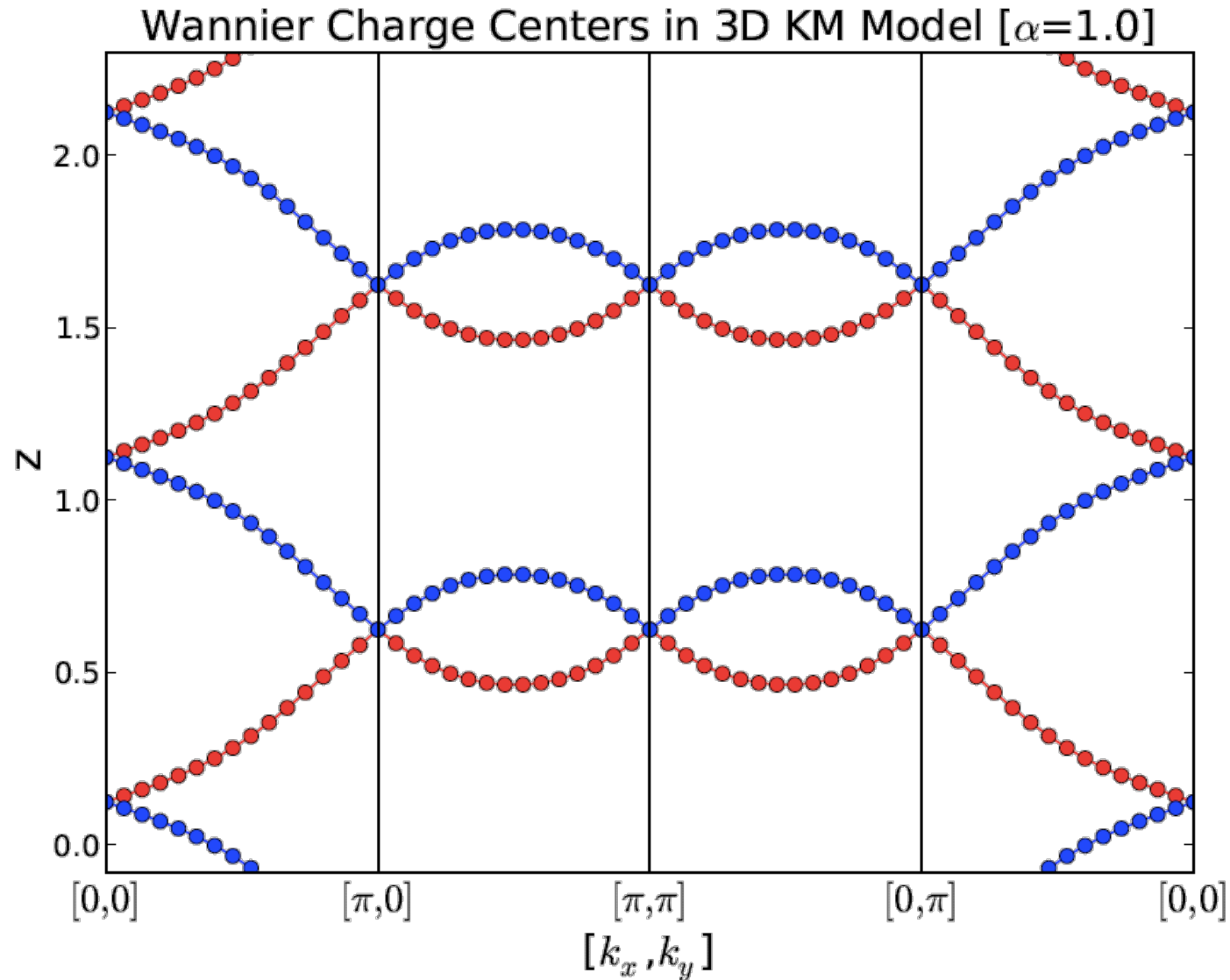
Fig. 5.18



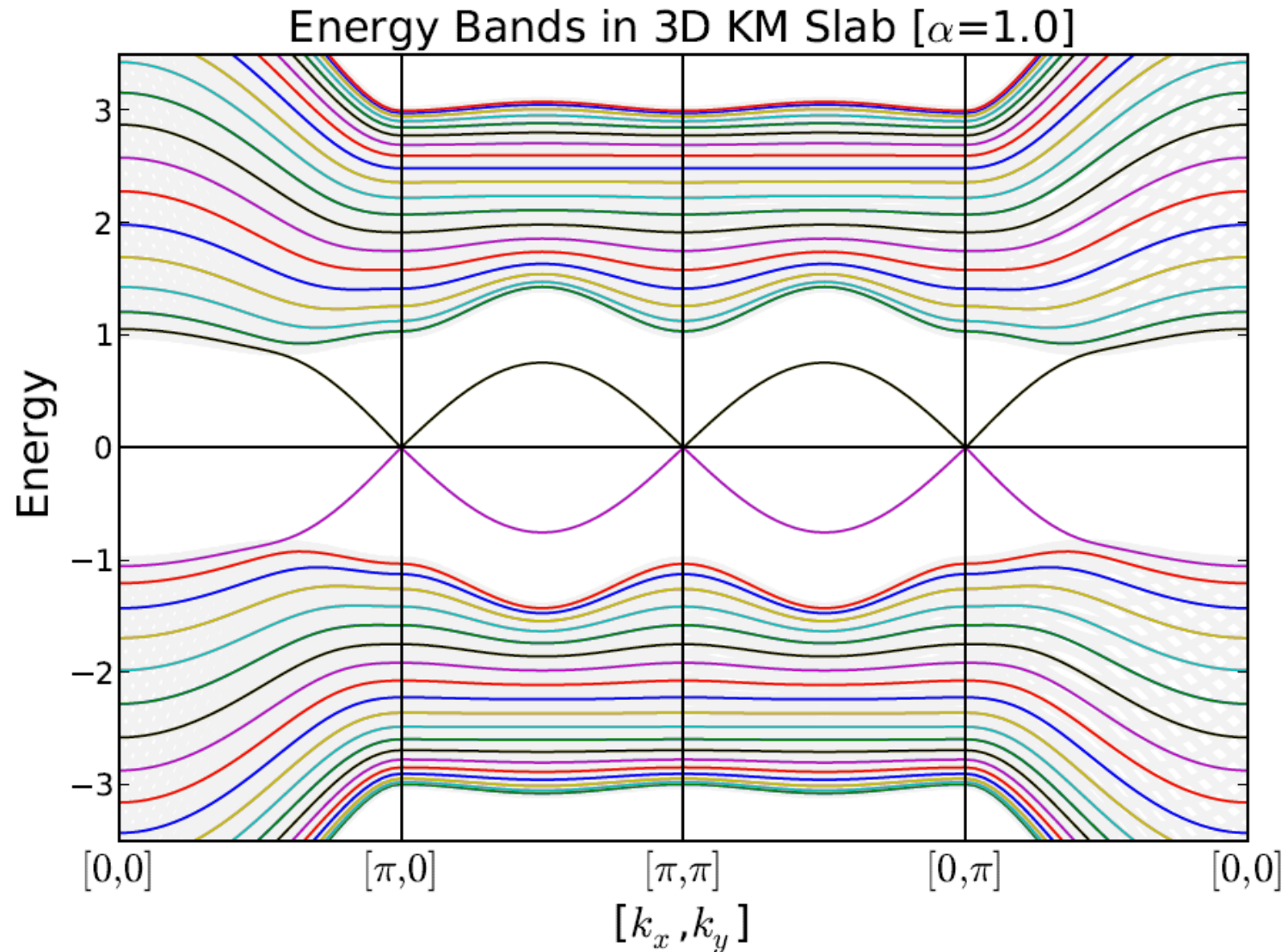
3D Kane-Mele model



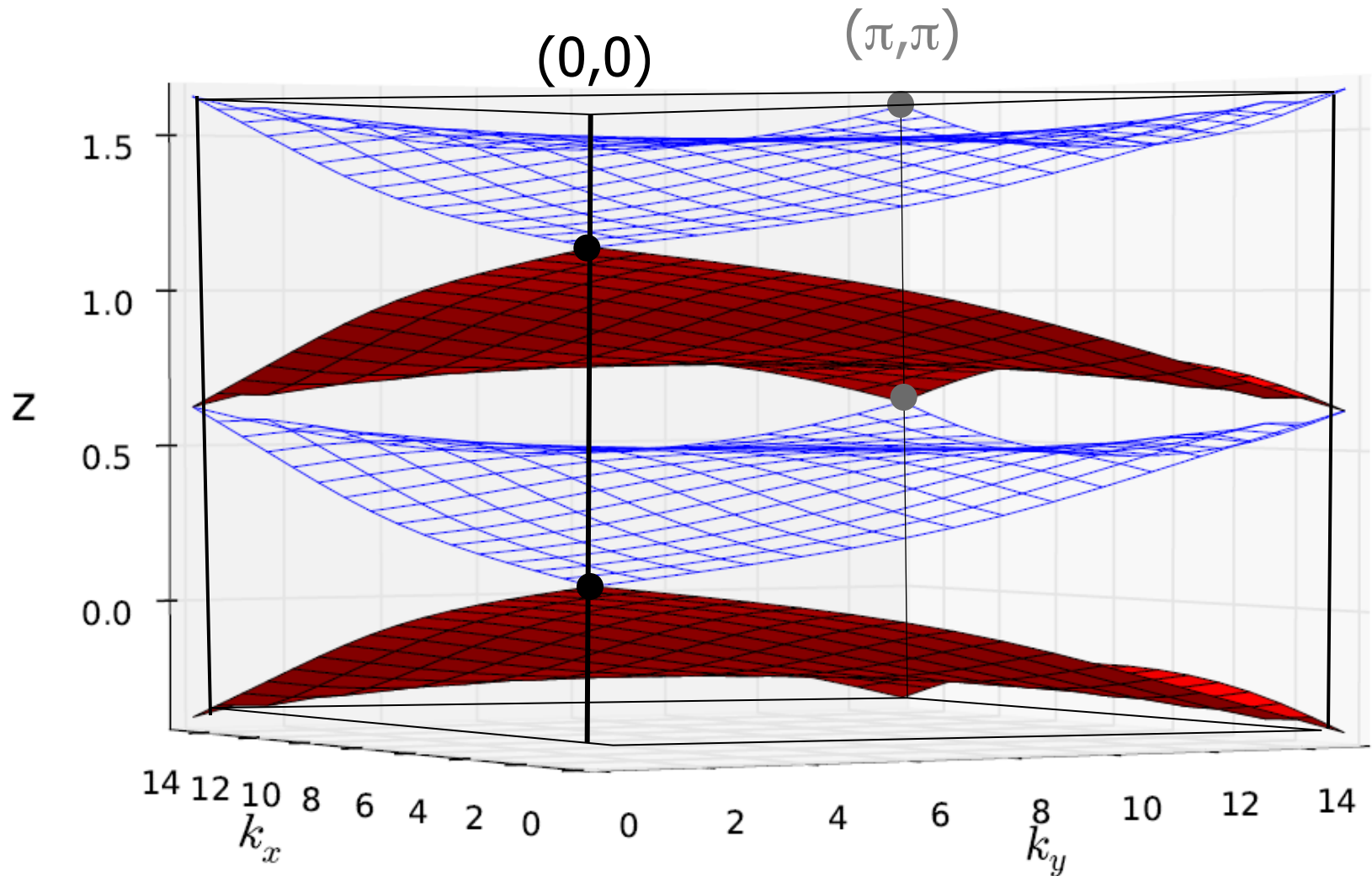
Hybrid WF sheets



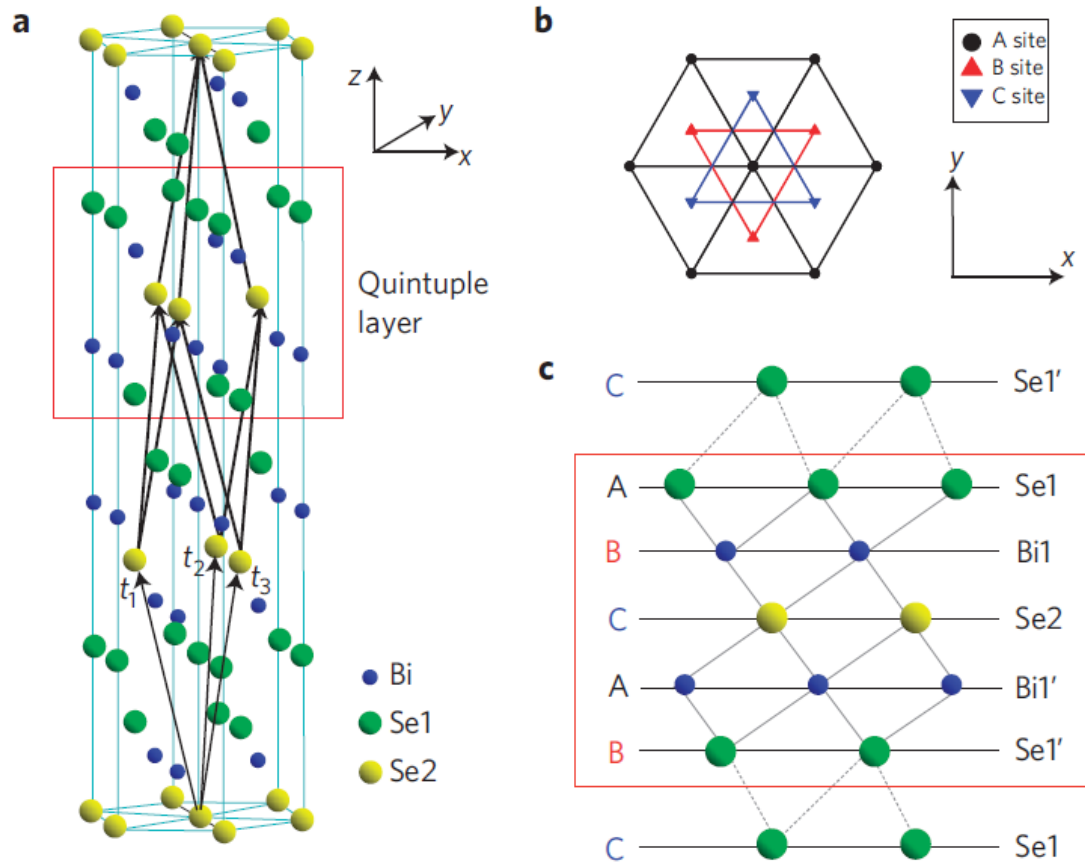
Surface energy bands



Hybrid WF sheets

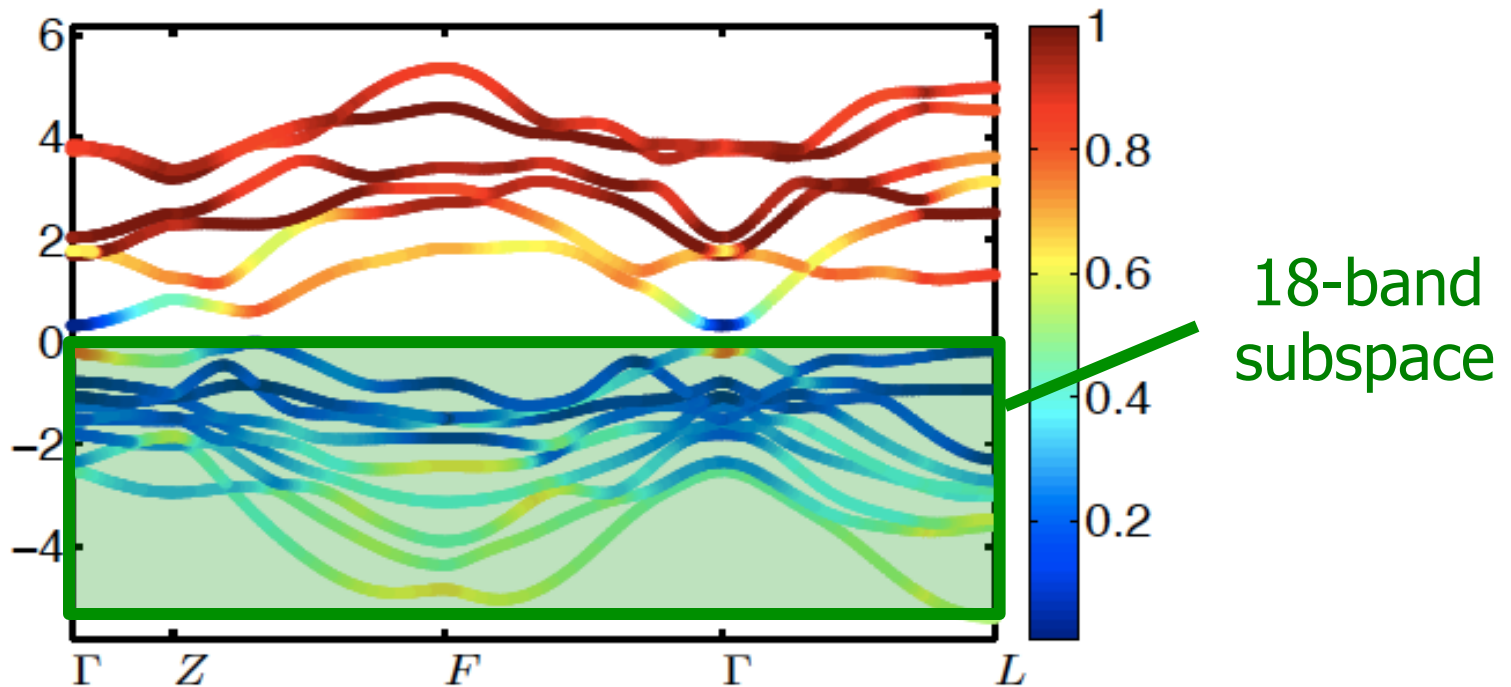


First-principles calculation: Bi_2Se_3



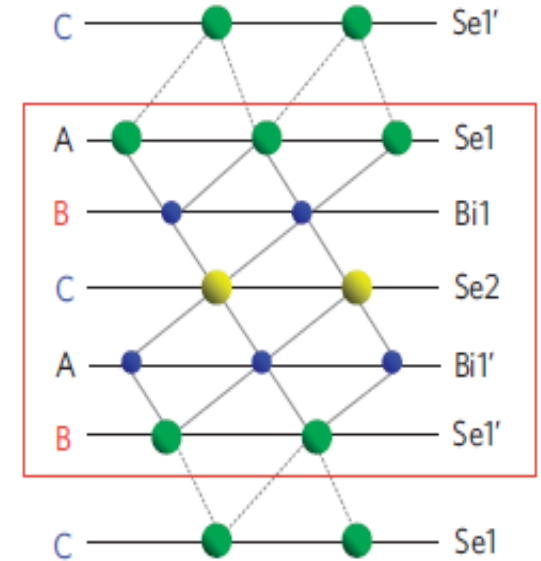
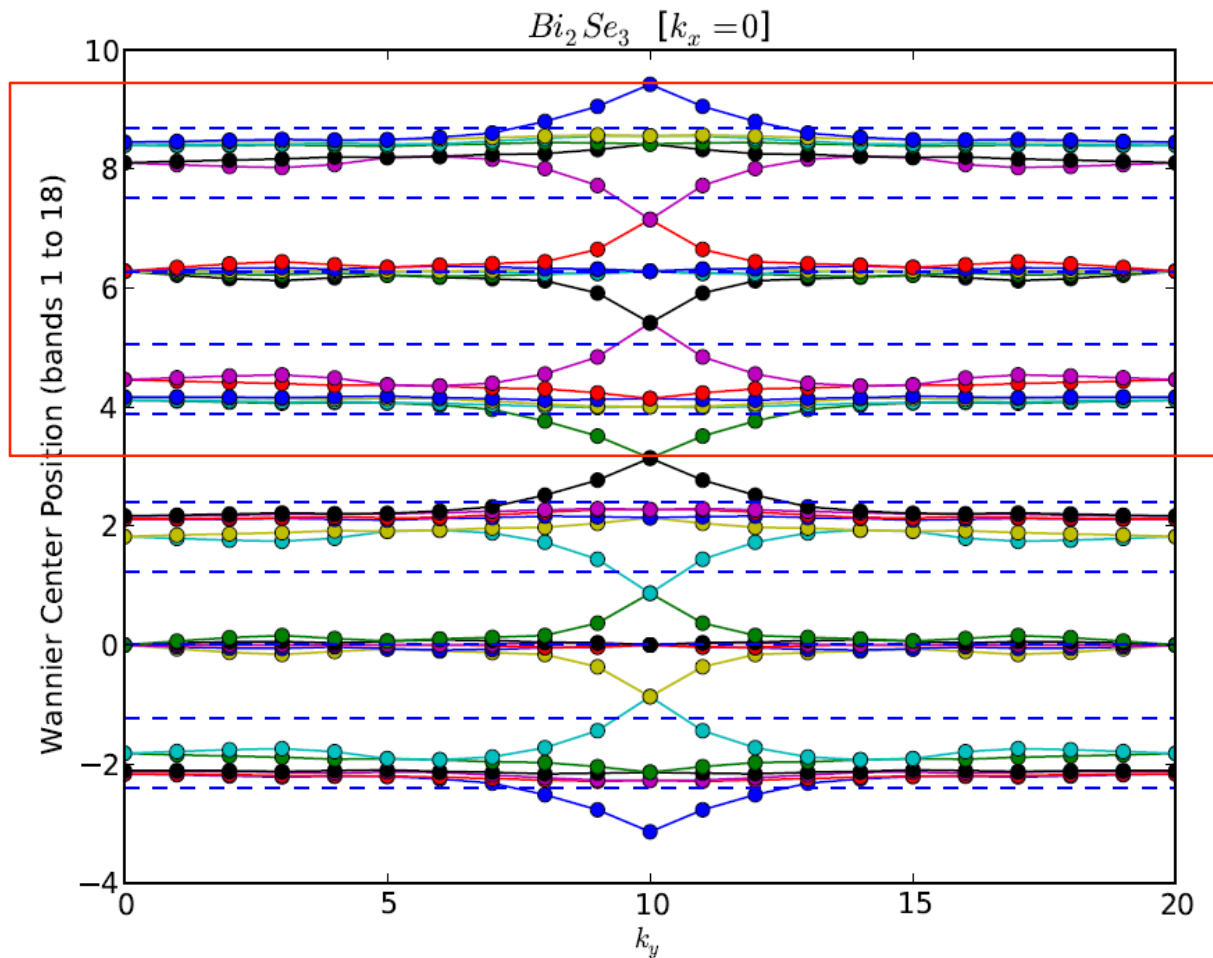
H. Zhang et al., Nature Physics **5**, 2009

First-principles calculation: Bi_2Se_3



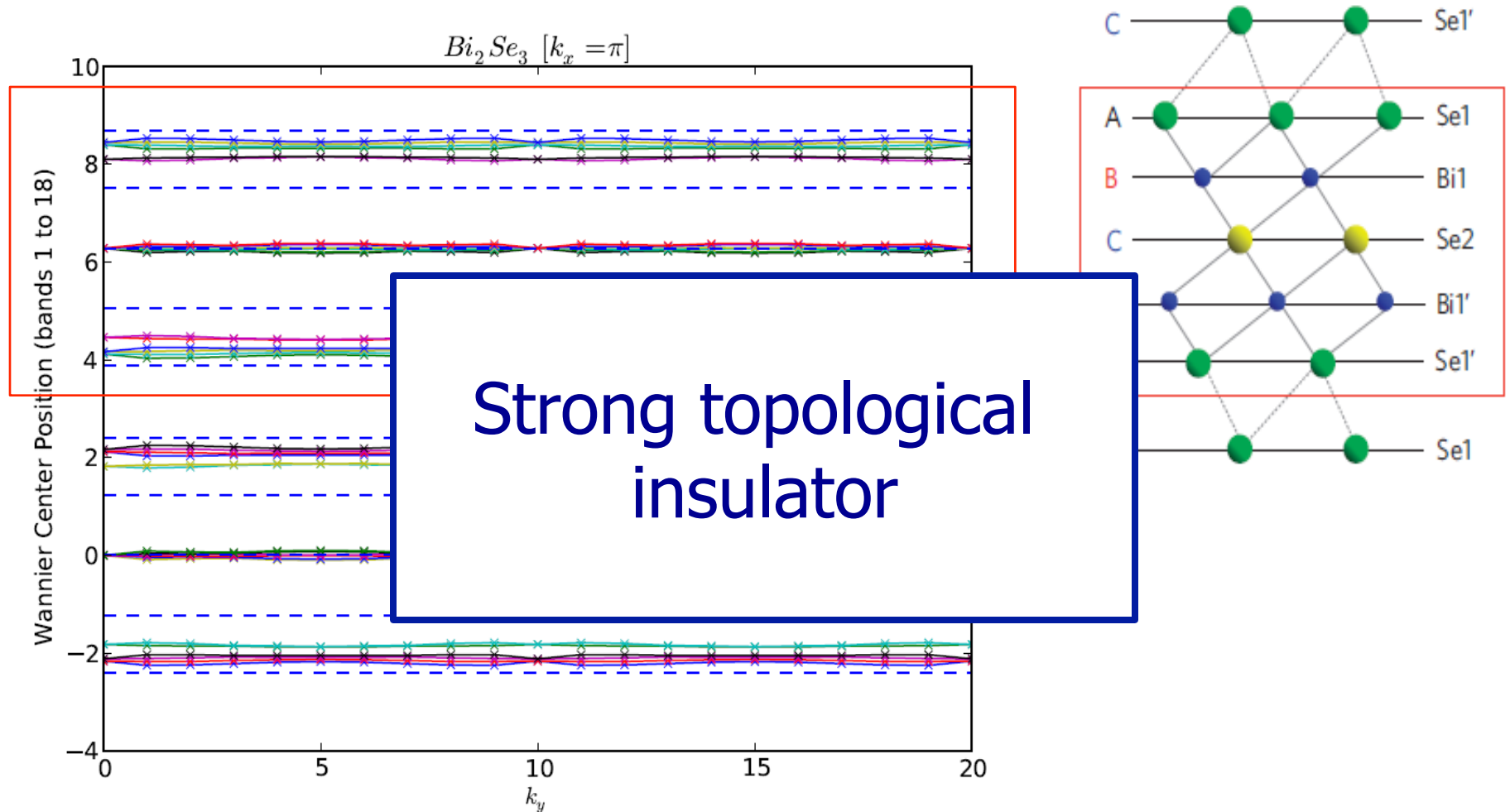
bulk bandstructure of Bi_2Se_3 projected onto Bi 6p orbitals

First-principles Bi_2Se_3 Wannier centers



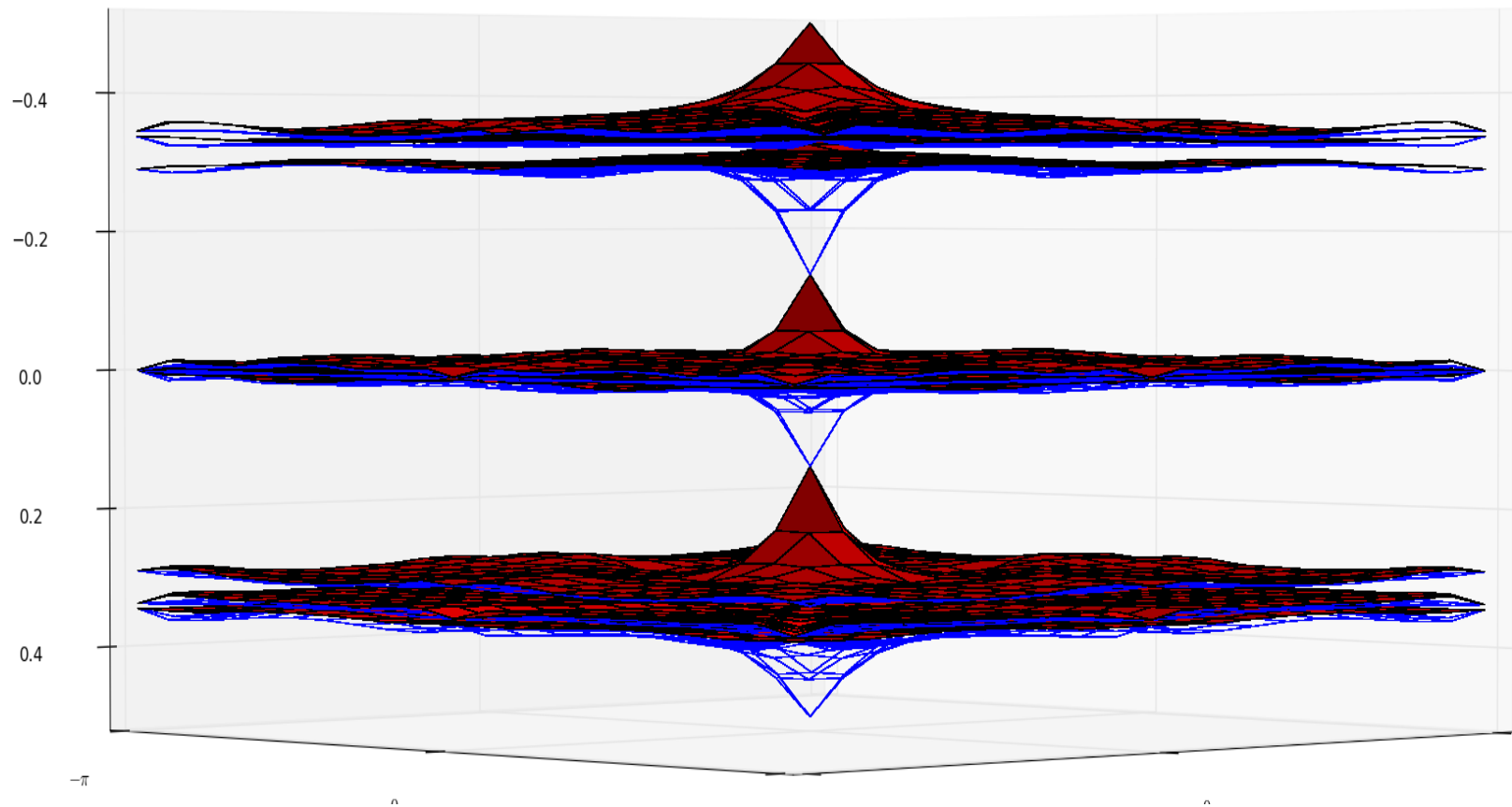
$$\mathbf{v}_{1a} = \mathbf{v}(k_x=0) = (-)$$

First-principles Bi_2Se_3 Wannier centers



$$\mathbf{v}_{1b} = \mathbf{v}(k_x = \pi) = (+)$$

First-principles Bi_2Se_3 Wannier centers



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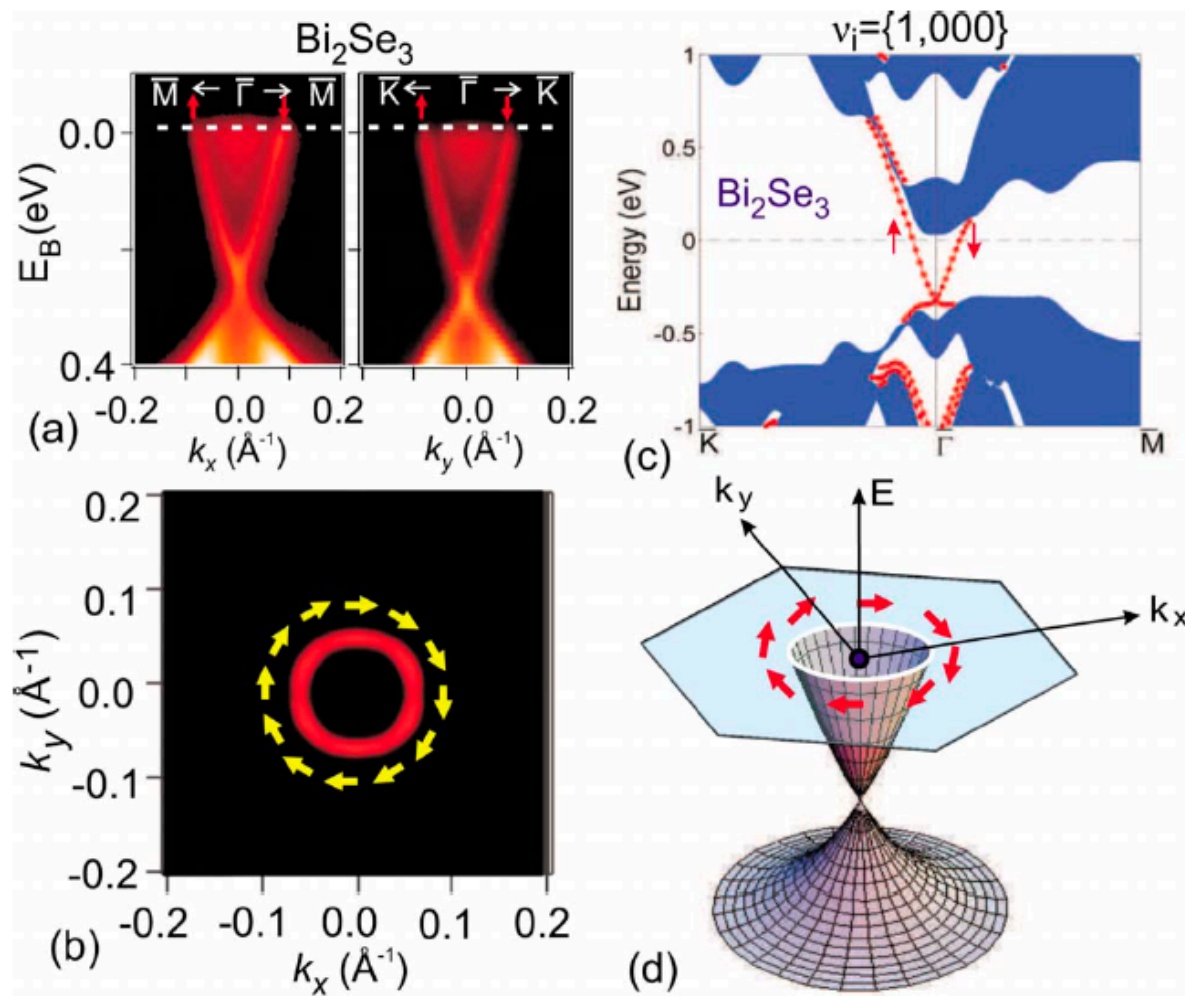


Figure from Hasan and Kane, RMP, 2010

(Adapted from Xia et al., 2008; Hsieh, Xia, Qian, Wray, et al., 2009a; and Xia, Qian, Hsieh, Wray, et al., 2009)