Berry phases and curvatures, hybrid Wannier centers, and topological insulators

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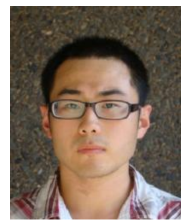

Jiangpeng Liu

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Topological insulators

- *T*-broken QAH insulators (1988-present)
  - QAH = "Quantum anomalous Hall"
  - Also known as "Chern insulators"
  - Integer quantum Hall without B_{macro}
  - 2D (or 3D)
- *T*-conserving insulators (2005-present)
  - 2D: Z_2 topological insulators
  - 3D: strong topological insulators

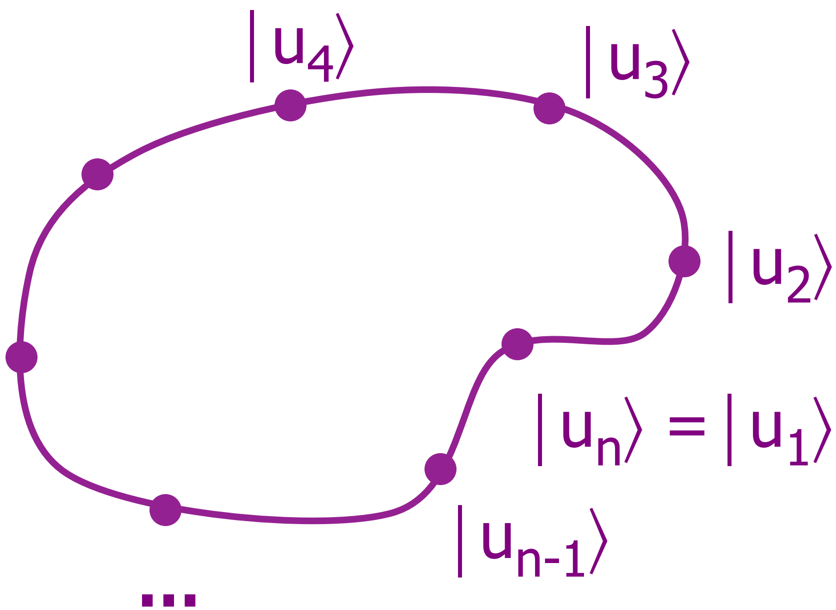
2012:
No known examples!

Several materials known

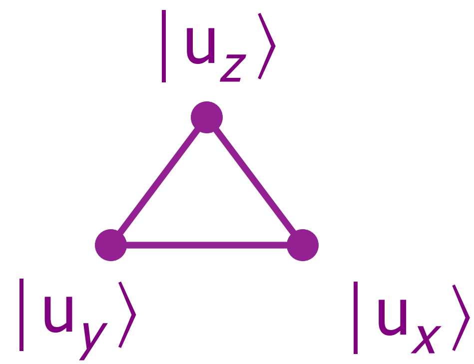
Outline

- Tutorial on Berry phases and curvatures
- 1D charge pump
- 2D quantum anomalous Hall insulator
- TR-invariant insulators (Z_2)
  - 2D ("Quantum spin Hall") insulator
  - 3D "strong" and "weak" topological ins.
- Surface charge and AHC
- Code packages
- Summary

Berry phases



Example:



$$\phi = -\mathrm{Im}\ \ln\left[\langle u_1|u_2\rangle\langle u_2|u_3\rangle\ldots\langle u_{n-1}|u_n\rangle\right]$$

Check: $|\widetilde{u}_2\rangle = e^{i\beta}|u_2\rangle$ has no effect.

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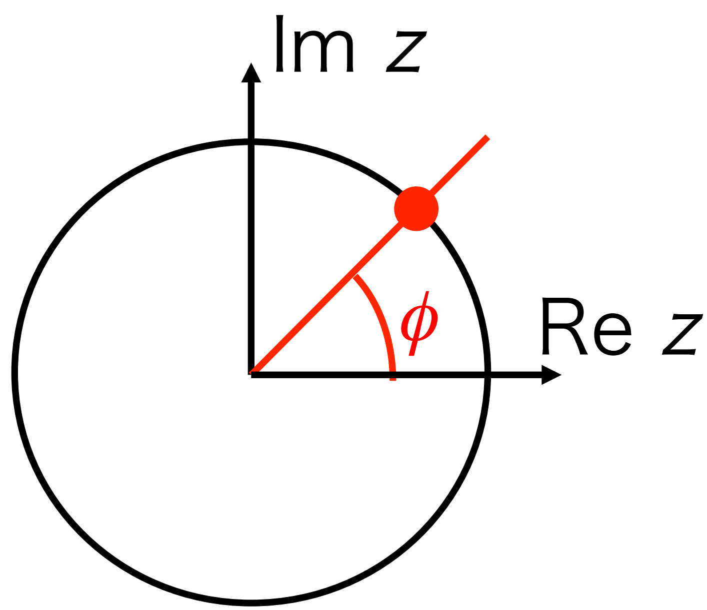
Example

Let $|u_z\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

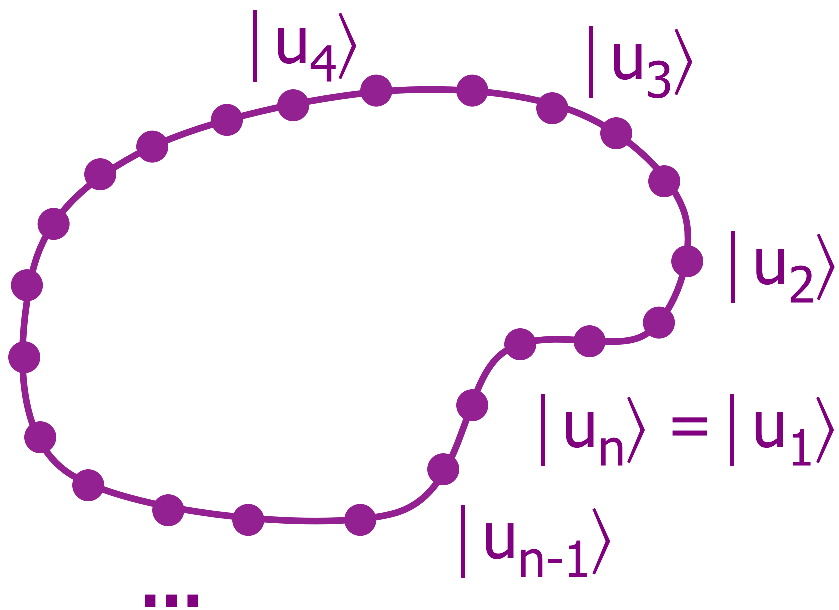
Let $|u_x\rangle = \dfrac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

Let $|u_y\rangle = \dfrac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}$



Then
$$\begin{aligned} \phi &= \mathrm{Arg}\, \langle u_z | u_x \rangle \, \langle u_x | u_y \rangle \, \langle u_y | u_z \rangle \\ &= \mathrm{Arg}\, (1)\,(1+i)\,(1) \\ &= \pi/4 \end{aligned}$$

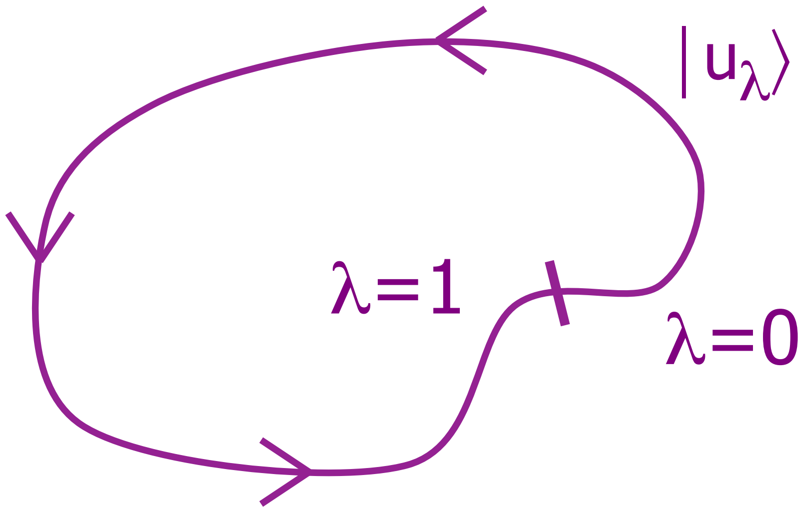
Berry phases



Now take limit that density of points $\rightarrow\infty$

$$\phi = -\mathrm{Im}\ \ln\left[\ \langle u_1|u_2\rangle\ \langle u_2|u_3\rangle \ldots\ \langle u_{n-1}|u_n\rangle\ \right]$$

Berry phases



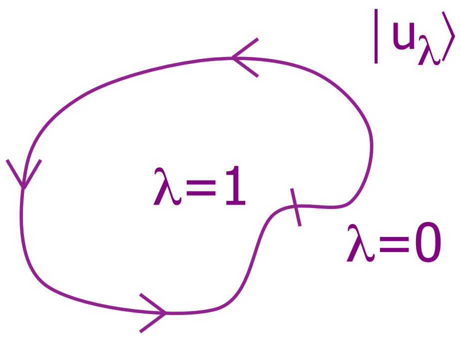
$$\phi = -\mathrm{Im} \oint d\lambda \, \langle u_\lambda | \frac{du_\lambda}{d\lambda} \rangle$$

$$\boxed{\phi = -\mathrm{Im} \oint d\lambda \, \langle u_\lambda | \frac{d}{d\lambda} | u_\lambda \rangle}$$

ϕ is well-defined modulo 2π

$\Rightarrow$ ϕ is a phase

Berry phases



ϕ is well-defined modulo 2π

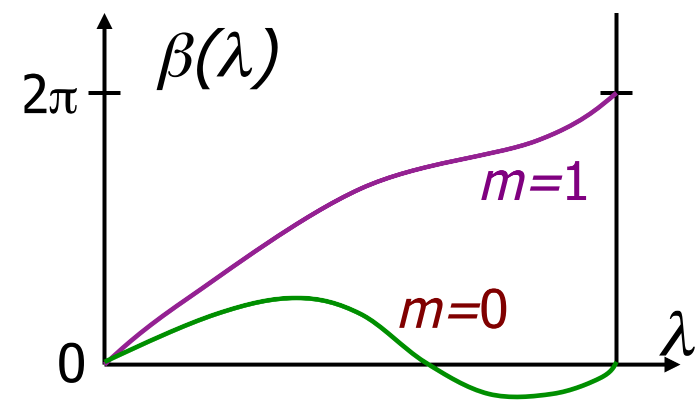
$\Rightarrow$ ϕ is a phase

$$\phi = -\mathrm{Im} \oint d\lambda \, \langle u_\lambda | \frac{d}{d\lambda} | u_\lambda \rangle$$

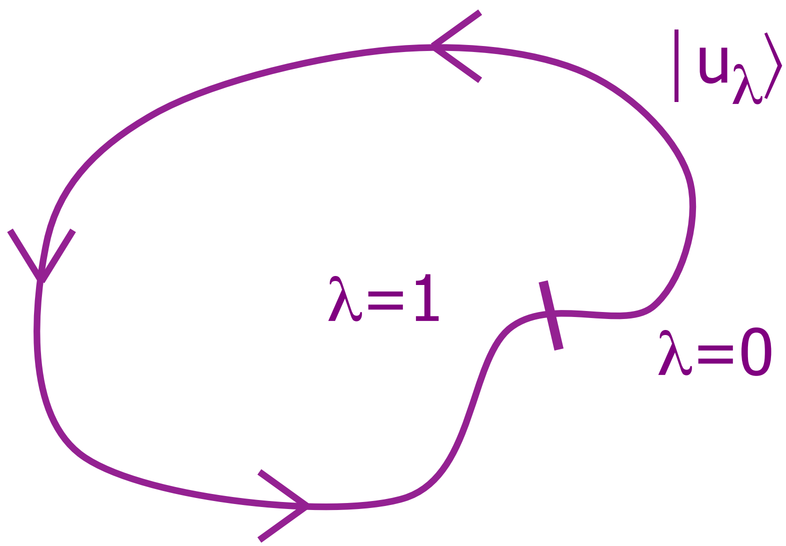
Let

$$|\widetilde{u}_\lambda\rangle = e^{-i\beta(\lambda)} \, |u_\lambda\rangle \text{ with } \beta(1) - \beta(0) = 2\pi m$$

$$\Rightarrow \quad \widetilde{\phi} = \phi + 2\pi m$$



Berry phases



Berry potential

$$A(\lambda) = i\,\langle u_\lambda|\frac{d}{d\lambda}|u_\lambda\rangle$$

Berry phase

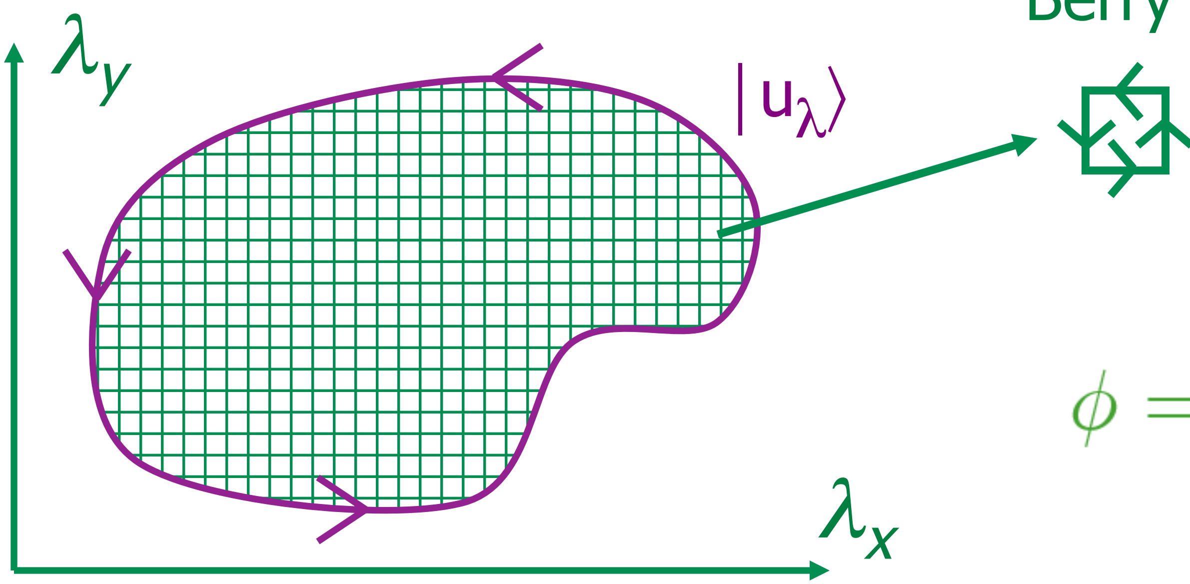
$$\phi = \oint A(\lambda)\,d\lambda$$

Gauge transformation:

$$|\widetilde{u}_\lambda\rangle = e^{-i\beta(\lambda)}\,|u_\lambda\rangle$$

A is gauge-dependent but
ϕ is well-defined modulo 2π

Berry curvature



Berry phase per unit area

$\mathcal{F} = \Delta\phi/\Delta A_\lambda$

$$\phi = \int \mathcal{F}(\lambda)\, dS_\lambda$$

$$\phi = -\mathrm{Im} \oint d\lambda\, \langle u_\lambda | \tfrac{d}{d\lambda} | u_\lambda \rangle$$

$$\mathcal{F} = -2\,\mathrm{Im} \left\langle \frac{du}{d\lambda_x} \middle| \frac{du}{d\lambda_y} \right\rangle$$

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Chern theorem

The integral of the Berry curvature
over any closed 2D manifold
must be $2\pi C$
where C is an integer
known as the Chern number.

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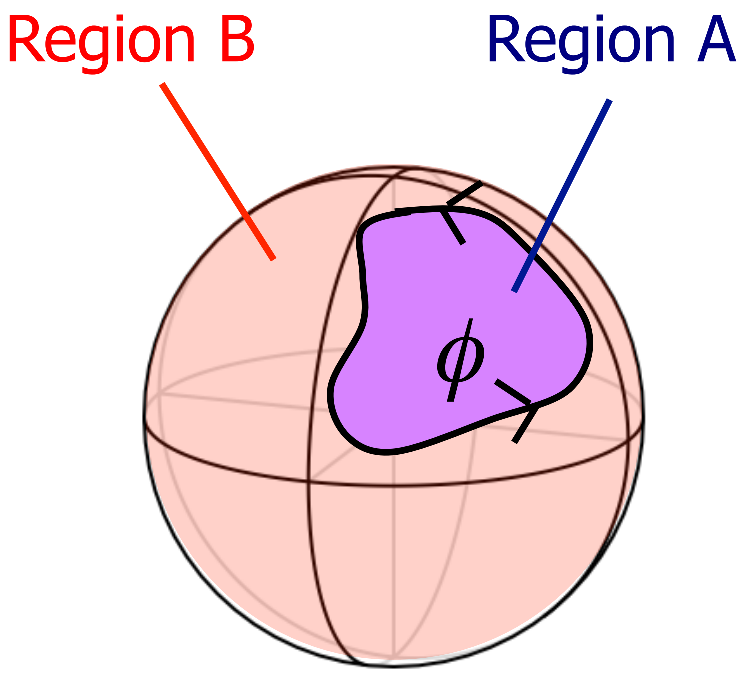
Chern Theorem



Stokes applied to A:

$$\phi = \int_A \mathcal{F}(\lambda)\, dS_\lambda \mod 2\pi$$

Stokes applied to B:

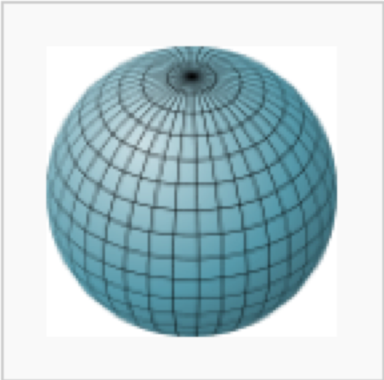
$$\phi = -\int_B \mathcal{F}(\lambda)\, dS_\lambda \mod 2\pi$$

Subtract:

$$0 = \oint \mathcal{F}(\lambda)\, dS_\lambda \mod 2\pi$$

Chern theorem: $\oint \mathcal{F}(\lambda)\, dS_\lambda = 2\pi\, C$

Compare: Gauss-Bonnet Theorem



genus 0

genus 1

genus 2

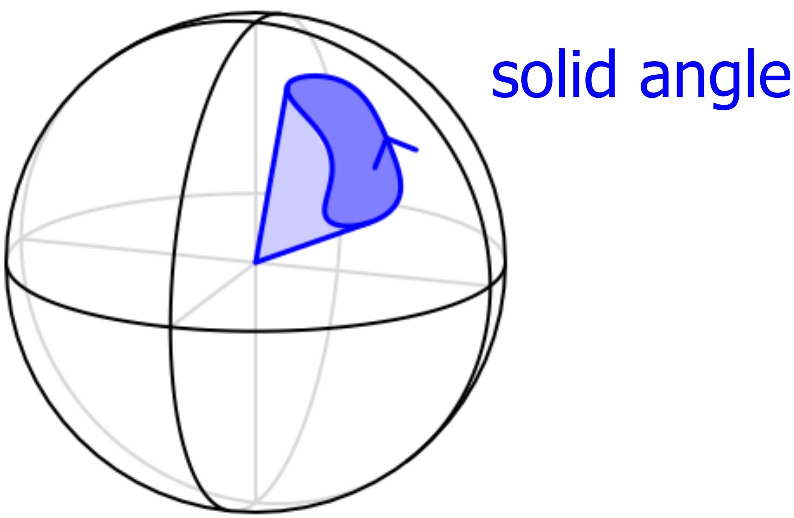
genus 3

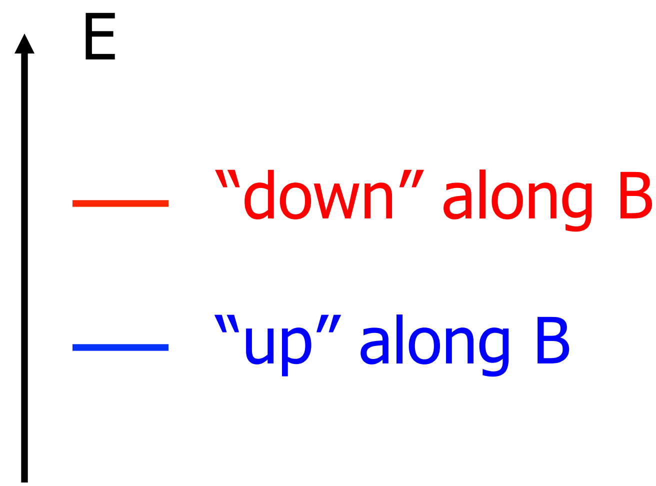
$$\int_S K\,d\sigma = 2\pi\chi(S)$$

Euler characteristic
= 2(1-genus)

Berry phase and curvature

Famous example: Spinor in magnetic field



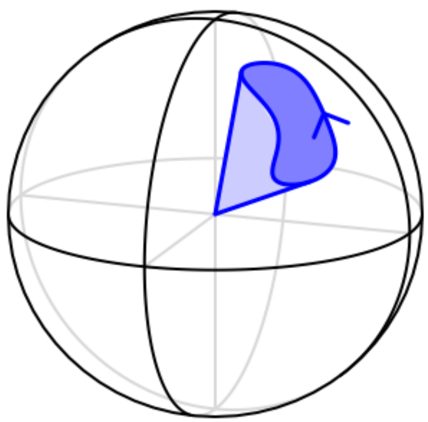


$$\boxed{\phi = -\mathrm{Im} \oint d\lambda \, \langle u_\lambda | \frac{d}{d\lambda} | u_\lambda \rangle}$$

$\boxed{\phi = (\text{solid angle})/2}$

Berry phase and curvature

Symmetry implies $\mathcal{F}$ = const.



$$\int \mathcal{F}(\lambda)\, dS_\lambda = 0,\ 2\pi,\ 4\pi,\ \ldots$$

$$\mathcal{F} = 0,\ ½,\ 1,\ \ldots$$

Change of notation

Berry curvature: $\mathcal{F} \longrightarrow \Omega$

$$\phi = \int \Omega(\lambda)\, dS_\lambda$$

$$\Omega = -2\,\mathrm{Im}\,\left\langle \frac{du}{d\lambda_x} \middle| \frac{du}{d\lambda_y} \right\rangle$$

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Berry phases in crystalline insulators

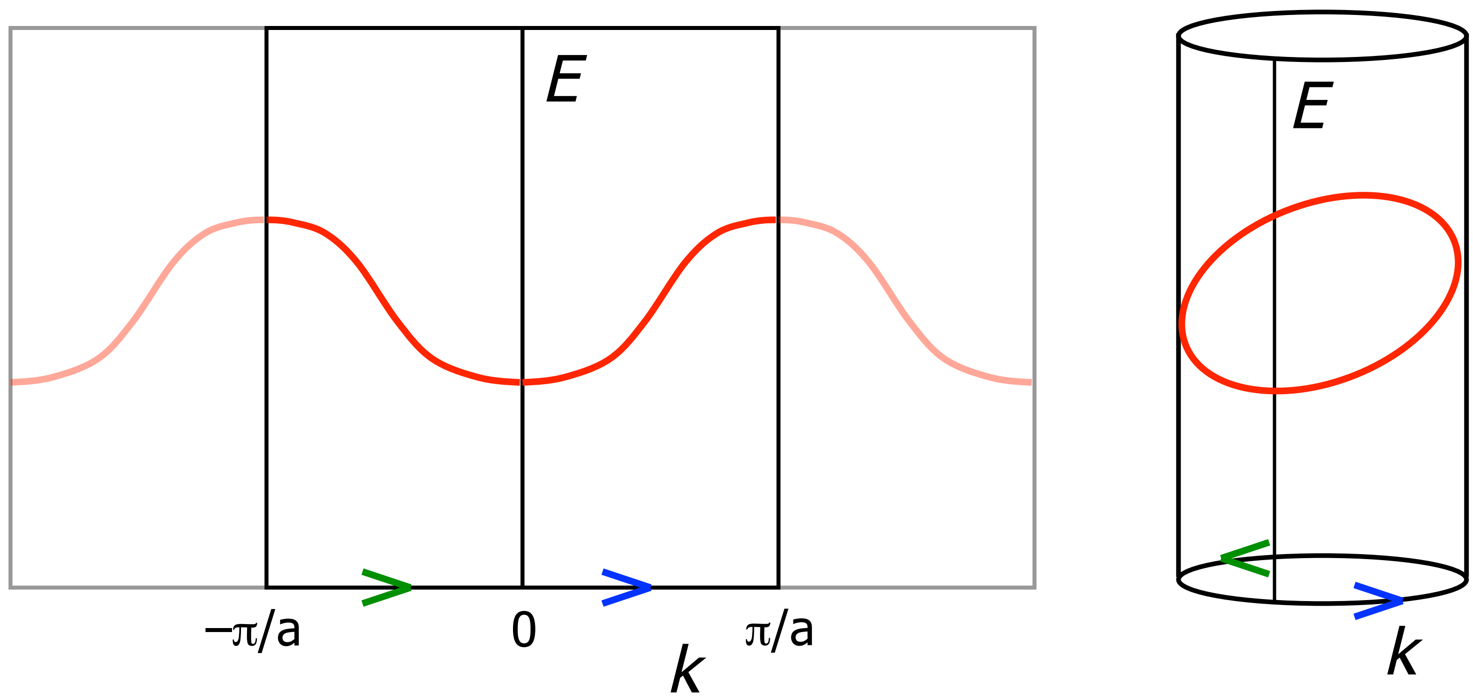
$$(\lambda_x,\lambda_y) \quad \Rightarrow \quad (k,\lambda)$$

General
Parametric
Hamiltonian

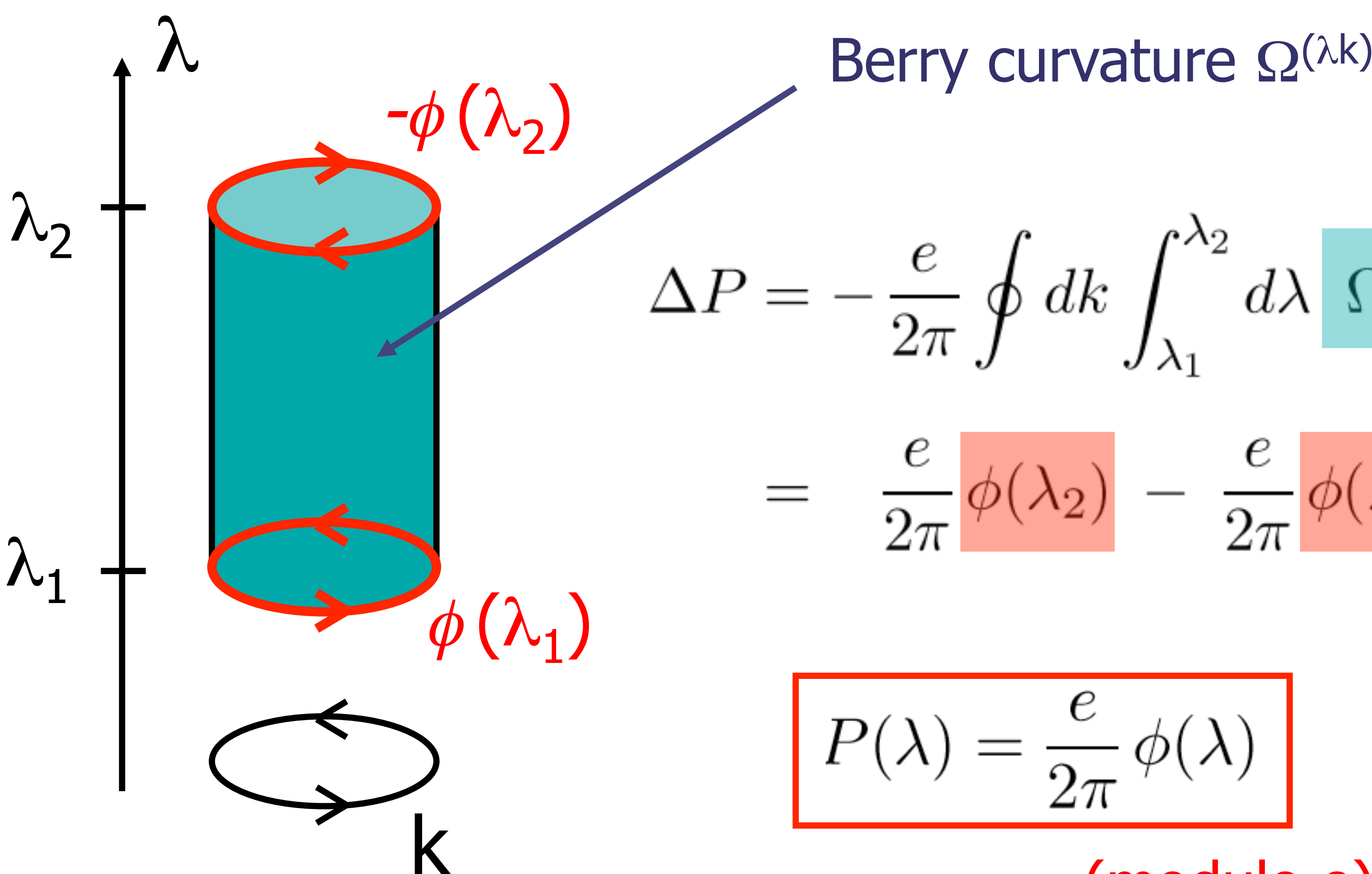
1D insulator
with adiabatic
parameter

1D: BZ is really a loop

- Reciprocal space is really periodic
- Brillouin zone can be regarded as a loop



Parametric 1D Ham. (Open path)



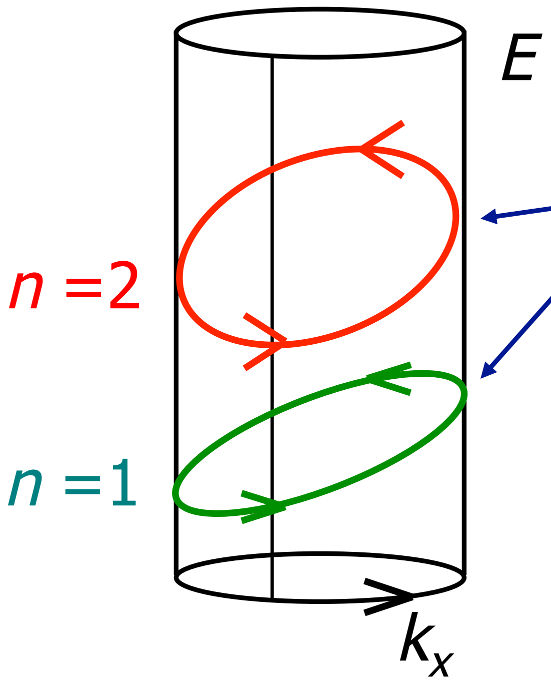
$$\Delta P = -\frac{e}{2\pi}\oint dk \int_{\lambda_1}^{\lambda_2} d\lambda \; \Omega^{(k\lambda)}$$

$$= \quad \frac{e}{2\pi}\phi(\lambda_2) - \frac{e}{2\pi}\phi(\lambda_1)$$

$$\boxed{P(\lambda) = \frac{e}{2\pi}\phi(\lambda)}$$

(modulo e)

1D: Polarization



$$\phi = -\mathrm{Im} \int dk_x \langle u_{\mathbf{k}} | \frac{d}{dk_x} | u_{\mathbf{k}} \rangle$$

$$\boxed{P = \frac{-e}{2\pi} \sum_n^{\mathrm{occ}} \phi_n}$$

King-Smith & V., 1993

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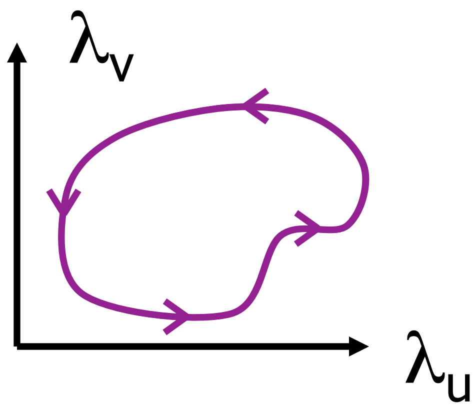
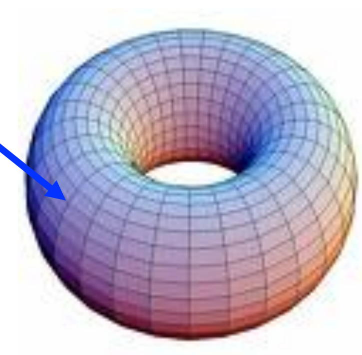
Parametric 1D Ham. (Closed path)



$\Omega\,(k,\lambda)$



(k, λ) space

Under an adiabatic cycle,

$$\Delta P = \frac{e}{2\pi} \oint d\lambda \oint dk \ \ \Omega(k,\lambda)$$

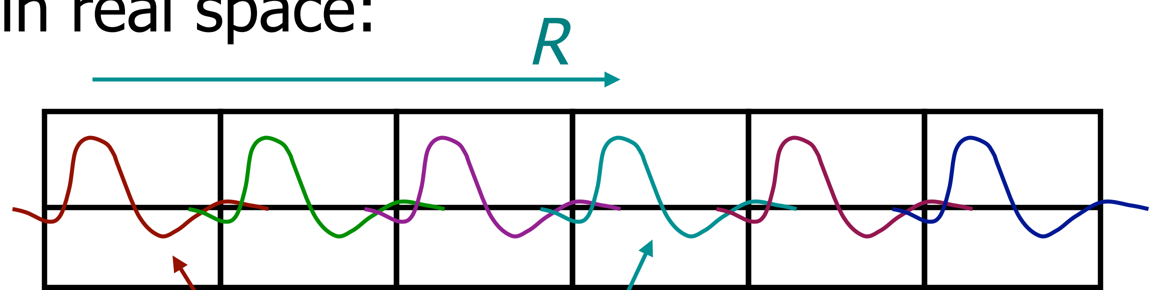
By Chern theorem,

$$\boxed{\Delta P = n\, e}$$

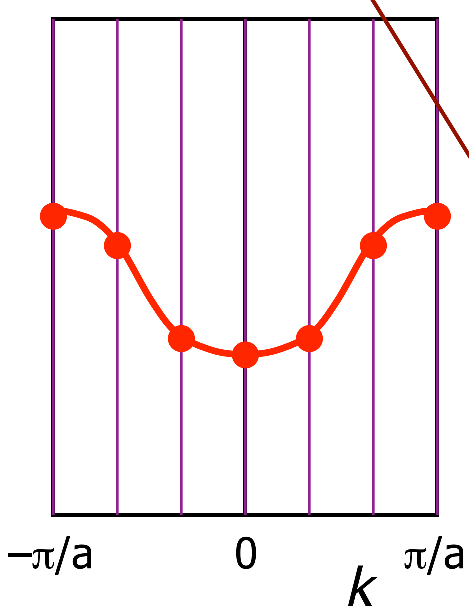
(n = TKNN invariant = integer)

Tutorial on Wannier functions

Crystal in real space:



Brillouin zone in reciprocal space:



$$w_{\mathbf{R}}(\mathbf{r}) = \sum_{\mathbf{k}} \psi_{\mathbf{k}}(\mathbf{r})\, e^{-i\mathbf{k}\cdot\mathbf{R}}\, d\mathbf{k}$$

$$w_0(\mathbf{r}) = \sum_{\mathbf{k}} \psi_{\mathbf{k}}(\mathbf{r})\, d\mathbf{k}$$

Unitary transformation

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Tutorial on Wannier functions

Centers of Wannier functions:

$$|\,w_0\rangle = \frac{V}{(2\pi)^3}\int_{\mathrm{BZ}} d\mathbf{k}\,|\psi_{\mathbf{k}}\rangle$$

$$= \frac{V}{(2\pi)^3}\int_{\mathrm{BZ}} d\mathbf{k}\;e^{i\mathbf{k}\cdot\mathbf{r}}\,|u_{\mathbf{k}}\rangle$$

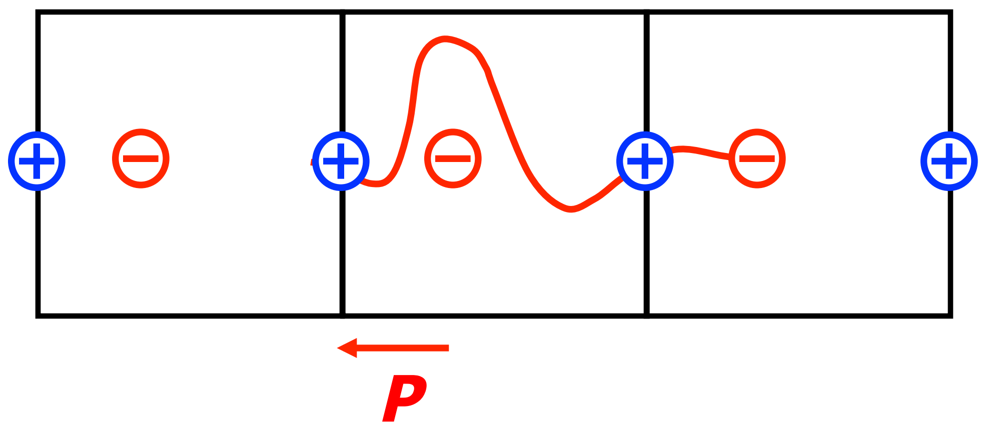
$$\mathbf{r}\,|\,w_0\rangle = \frac{V}{(2\pi)^3}\int_{\mathrm{BZ}} d\mathbf{k}\;\left(\,-\,i\nabla_{\mathbf{k}}\,e^{i\mathbf{k}\cdot\mathbf{r}}\,\right)|u_{\mathbf{k}}\rangle$$

$$= i\,\frac{V}{(2\pi)^3}\int_{\mathrm{BZ}} d\mathbf{k}\;e^{i\mathbf{k}\cdot\mathbf{r}}\left(\,\nabla_{\mathbf{k}}\,|u_{\mathbf{k}}\rangle\,\right)$$

$$\boxed{\langle w_0\,|\,\mathbf{r}\,|\,w_0\rangle = i\,\frac{V}{(2\pi)^3}\int_{\mathrm{BZ}} d\mathbf{k}\;\langle u_{\mathbf{k}}|\,\nabla_{\mathbf{k}}\,|u_{\mathbf{k}}\rangle}$$

Polarization ↔ Wannier centers

Centers of Wannier functions:



$$\langle w_0 \,|\, \mathbf{r} \,|\, w_0 \rangle = i \frac{V}{(2\pi)^3} \int_{\mathrm{BZ}} d\mathbf{k} \, \langle u_\mathbf{k} | \, \nabla_\mathbf{k} \, | u_\mathbf{k} \rangle$$

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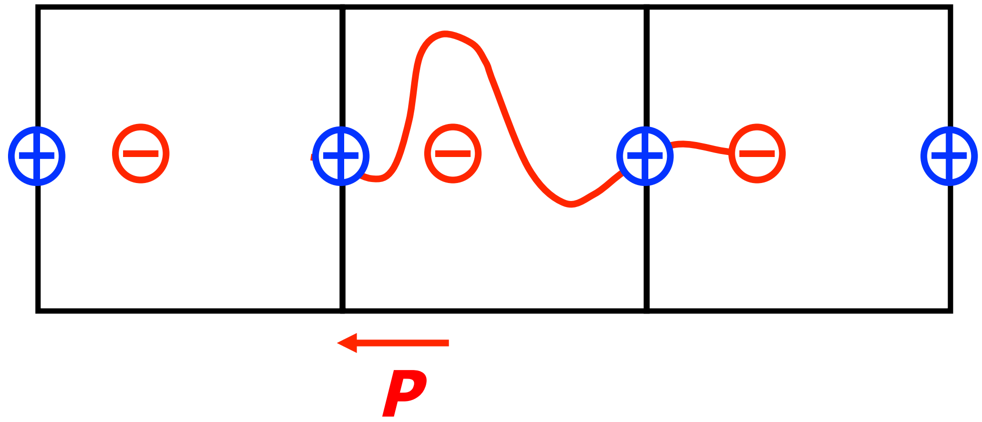
Equivalent def. of Wannier centers (1D)

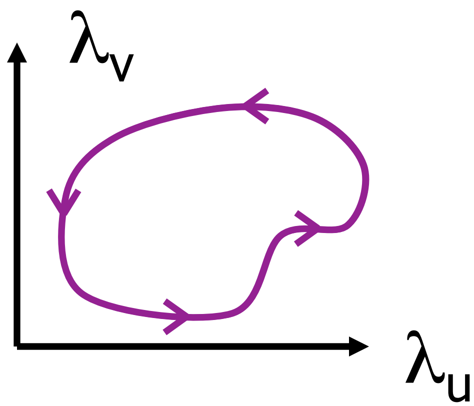
Centers of Wannier functions:

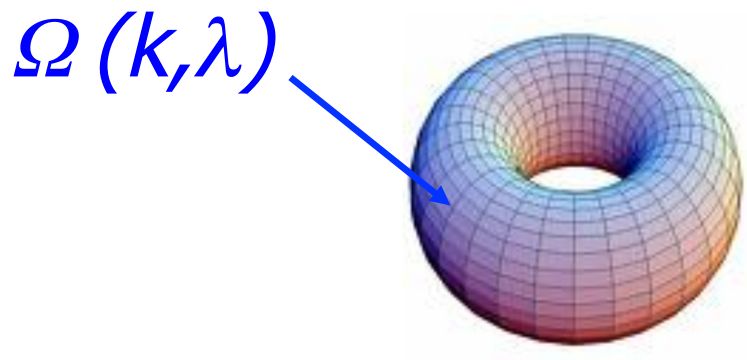


Wannier centers: Eigenvalues of $\mathcal{P}x\mathcal{P}$

$$\mathcal{P} = \sum_n^{\text{occ}} \int dk \, |\psi_{nk}\rangle\langle\psi_{nk}|$$

Parametric 1D Ham. (Closed path)





(k, λ) space

Under an adiabatic cycle,

$$\Delta P = \frac{e}{2\pi} \oint d\lambda \oint dk \;\; \Omega(k,\lambda)$$

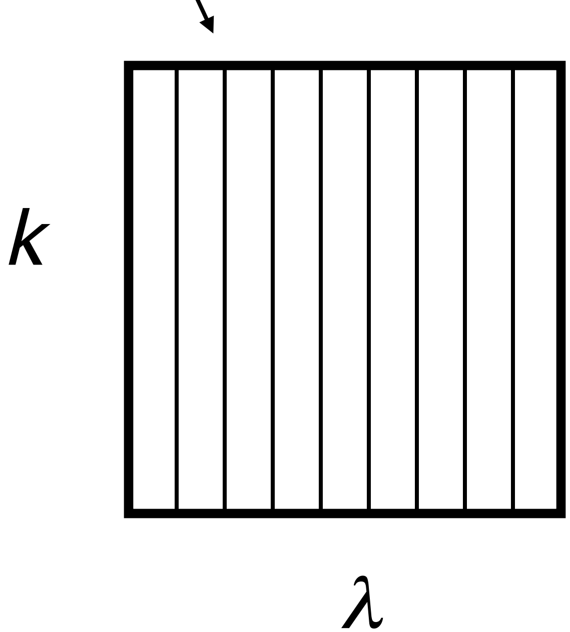
By Chern theorem,

$$\boxed{\Delta P = n\, e}$$

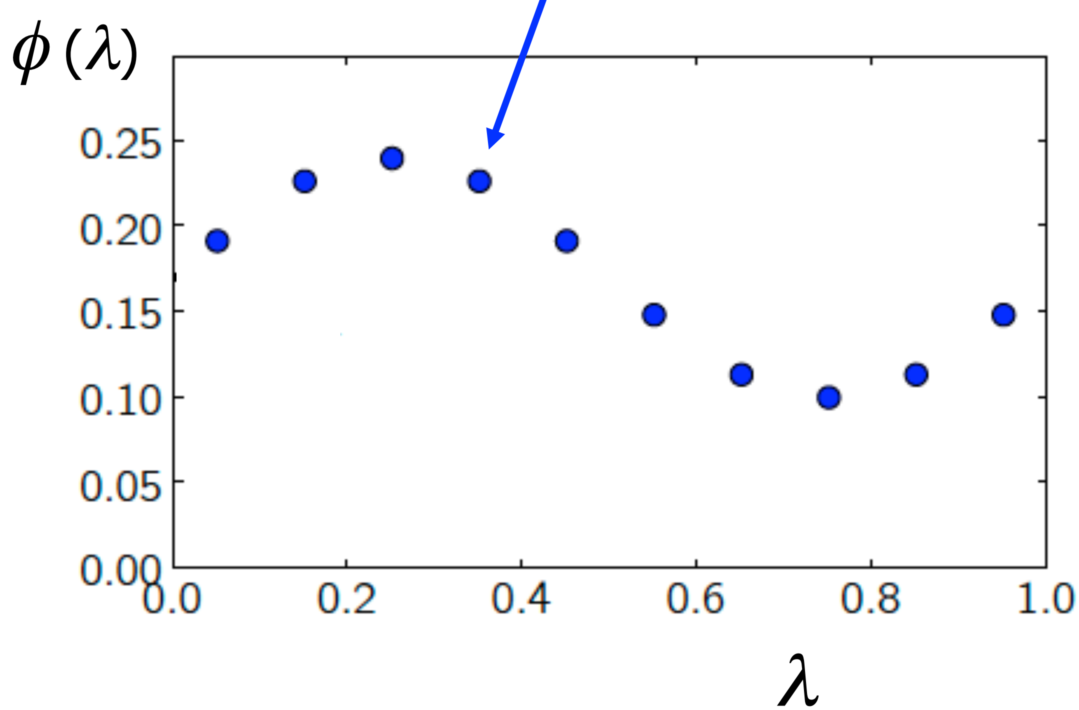
(n = TKNN invariant = integer)

Adiabatic cycle - No pumped charge

$\phi(\lambda)$ = Berry phase at given λ

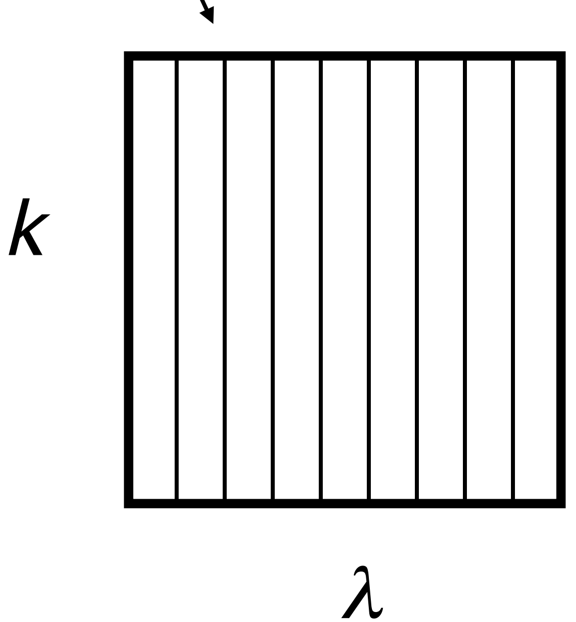


$P(\lambda) \propto \phi(\lambda)$



Adiabatic cycle - Quantum charge pump

$\phi(\lambda)$ = Berry phase at given λ



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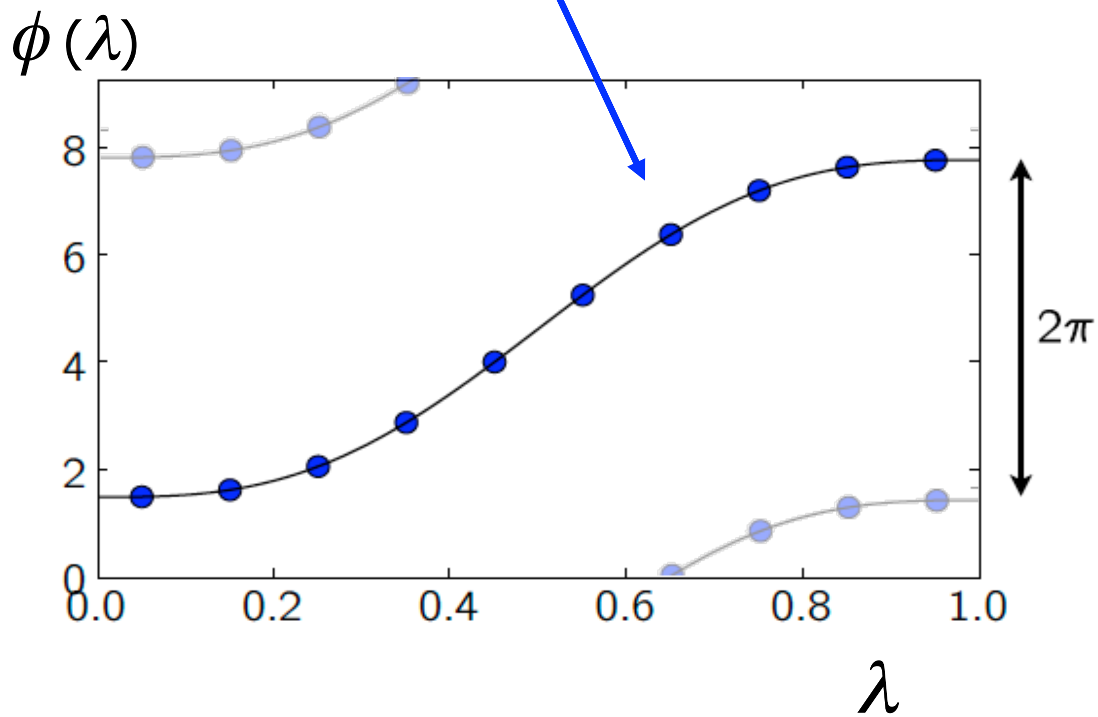
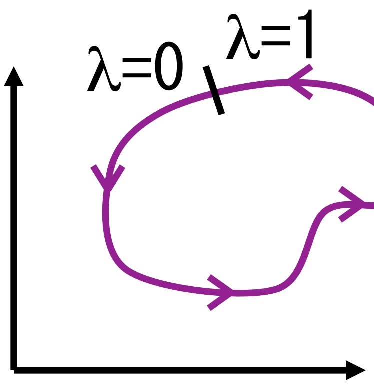
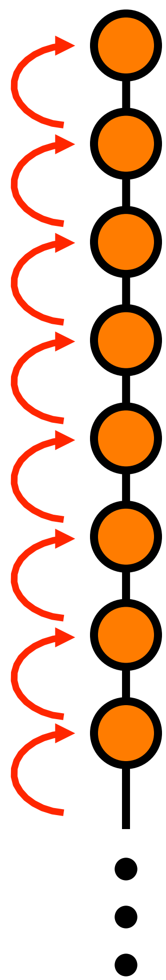
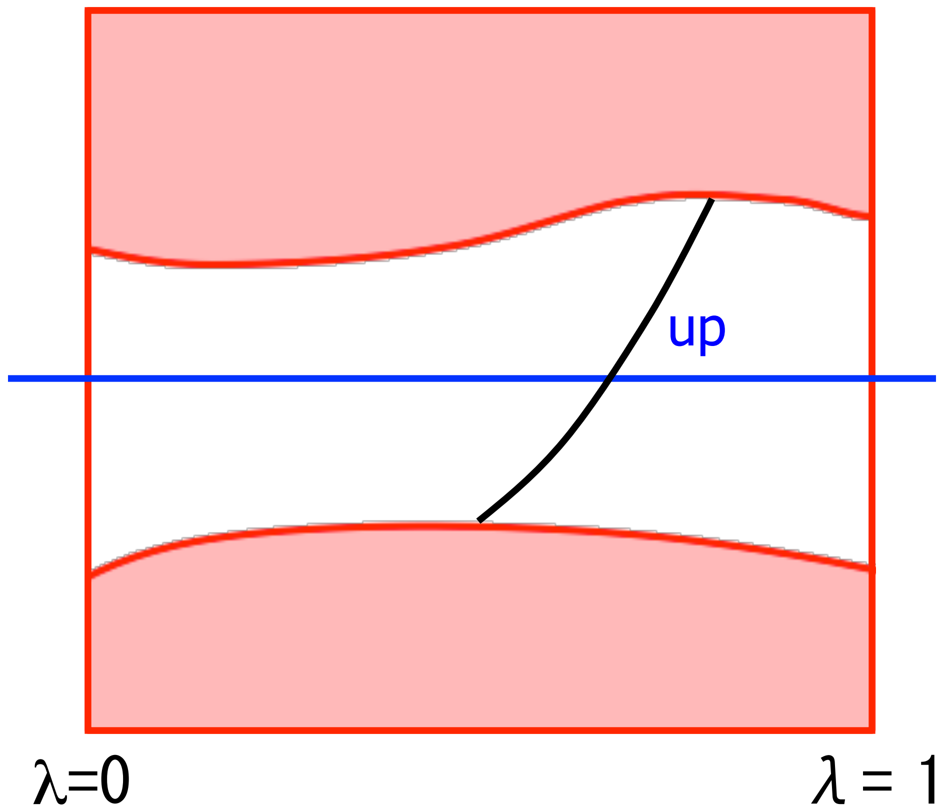


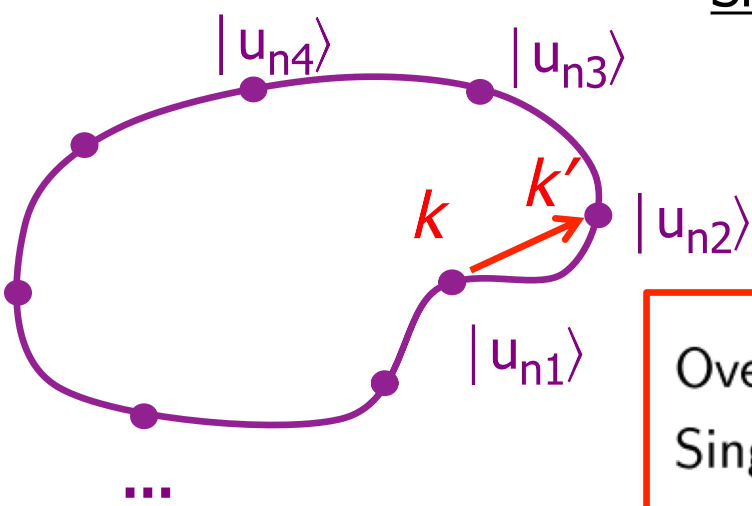
Semi-infinite chain: cyclic evolution







Multi-band Berry phases



Single band:

$$\phi = -\text{Im}\ \ln\ [\ \langle u_1|u_2\rangle\ \langle u_2|u_3\rangle \ldots\ \langle u_{n-1}|u_n\rangle\ ]$$

Overlap matrix: $M_{mn}^{(k,k')} = \langle u_{mk}|u_{nk'}\rangle$

Singular value decomposition: $M = U\Sigma V^\dagger$

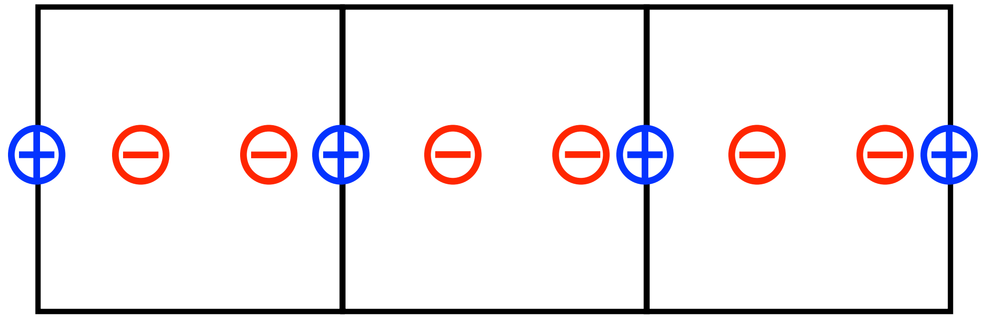
Unitary rotation: $W = UV^\dagger$

Diagonalize $[\ W^{(1,2)}\ W^{(2,3)} \ldots W^{(N,1)}\ ] \implies \begin{pmatrix} e^{i\phi_1} & & \\ & e^{i\phi_2} & \\ & & \ddots \end{pmatrix}$

ϕ_j = Berry phases ("Wilson loop eigenvalues")

Multi-band Berry phases

Centers of Wannier functions:



Wannier centers: Eigenvalues of $\mathcal{P}x\mathcal{P}$

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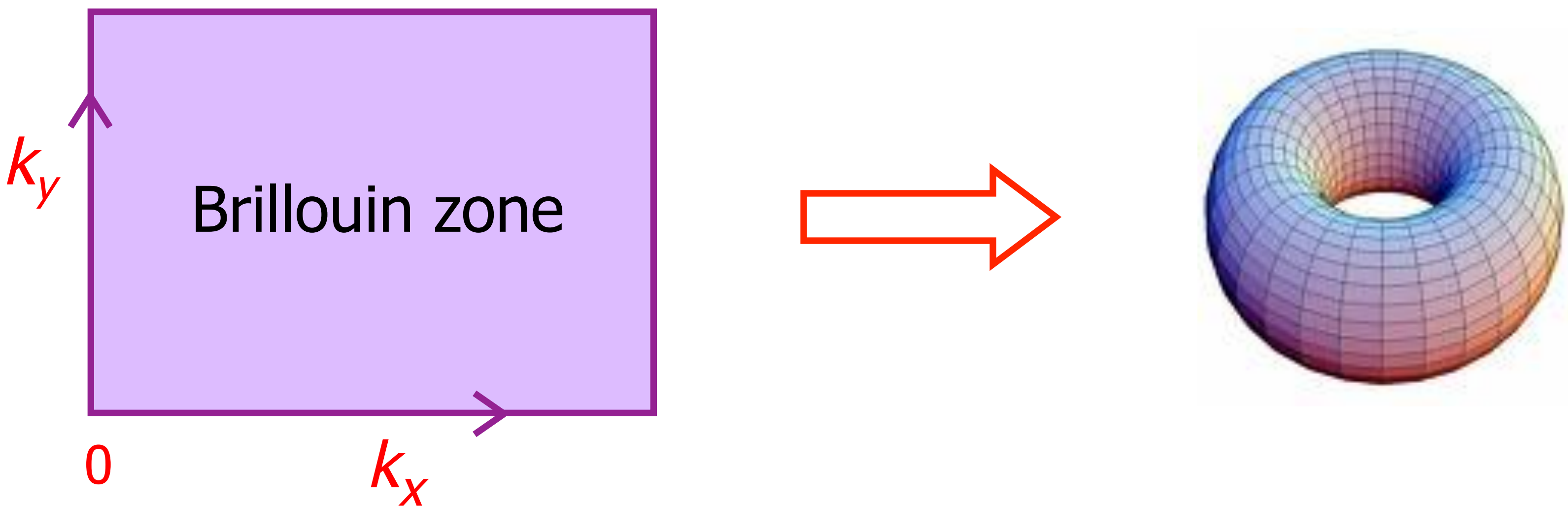
$$(k, \lambda) \quad \Rightarrow \quad (k_x, k_y)$$

1D insulator with adiabatic parameter

2D insulator

2D Crystal



Brillouin zone is closed manifold
(2-torus)

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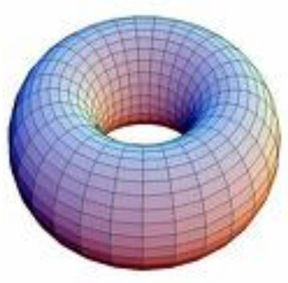
Chern Theorem in 2D BZ



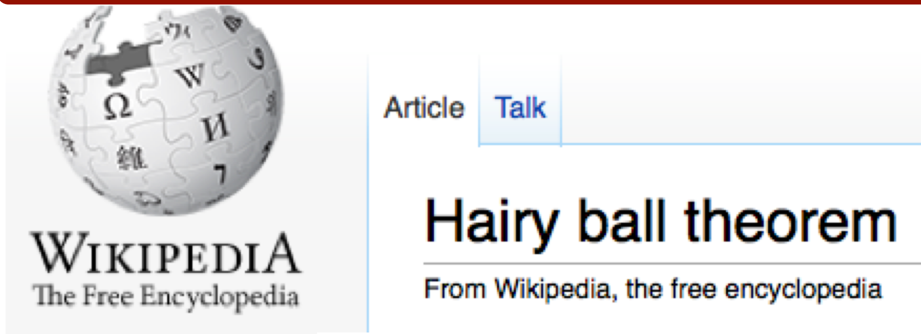
Chern theorem: $$\int_{BZ} \Omega_z(\mathbf{k})\, d^2k = 2\pi C$$

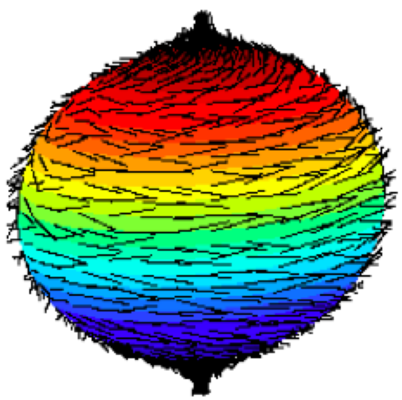
Where C is an integer!

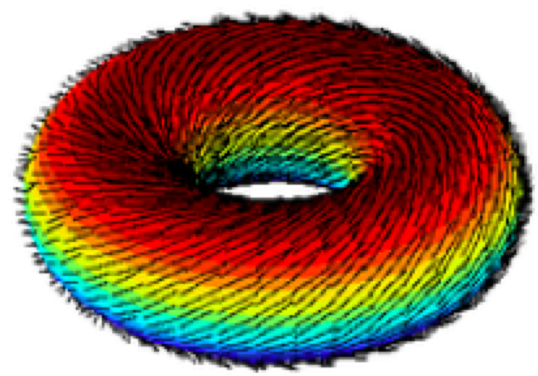
Application to 2D crystals:

- Each Bloch band $\psi_{nk}(r)$ has Chern integer C_n
- Insulating 2D crystal has total Chern invariant C
- Is there a Wannier representation?

Hairy ball theorem





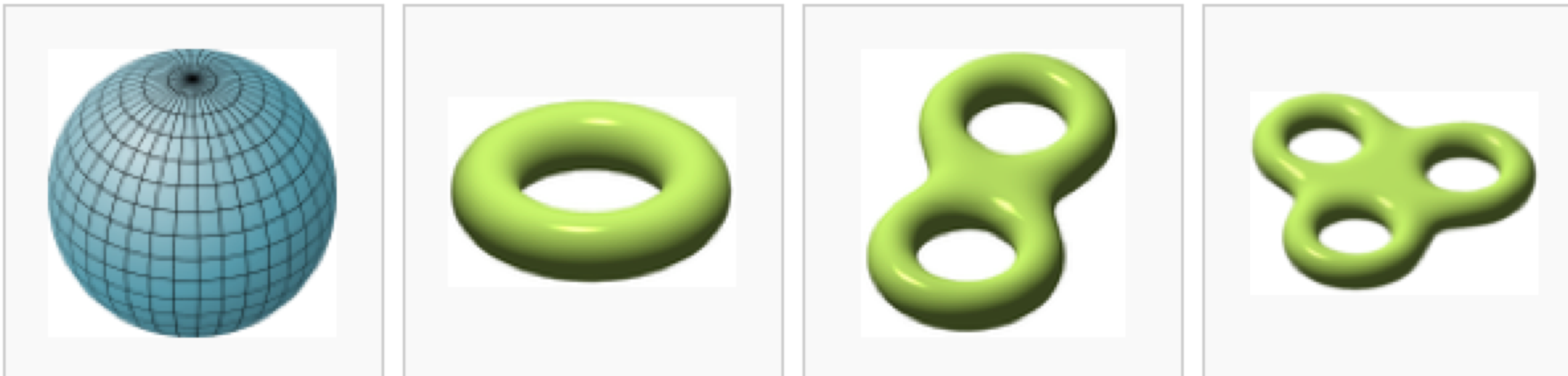


$\chi \neq 0$: Cannot comb

$\chi = 0$: Can comb

Analogy: Combing hair ➔ Choose smooth gauge

Compare: Gauss-Bonnet Theorem

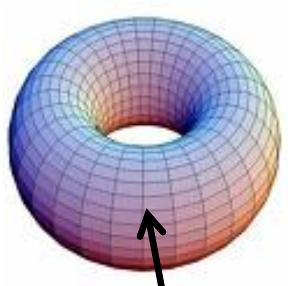


$\chi = 2$ $\chi = 0$ $\chi = -2$ $\chi = -4$

$$\boxed{\int_S K\, d\sigma = 2\pi\chi(S)}$$

Euler characteristic
= 2(1-genus)

Wannier representability



Chern theorem: $\int_{\mathrm{BZ}} \Omega_z(\mathbf{k})\, d^2k = 2\pi C$

Change of gauge:

$$|u_{n\mathbf{k}}\rangle \longrightarrow e^{-i\beta(\mathbf{k})}|u_{n\mathbf{k}}\rangle$$

Is it possible to make a gauge choice such that $|u_{n\mathbf{k}}\rangle$ is everywhere smooth in k?

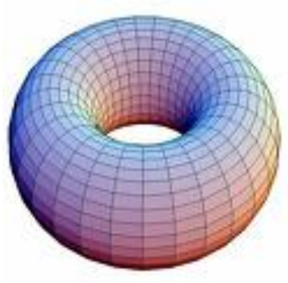
If so, Fourier transform ➔ localized Wannier functions

Answer:

If C=0, yes!

Otherwise, no! Gauge discontinuity (vortex) must exist!

Chern Theorem in 2D BZ



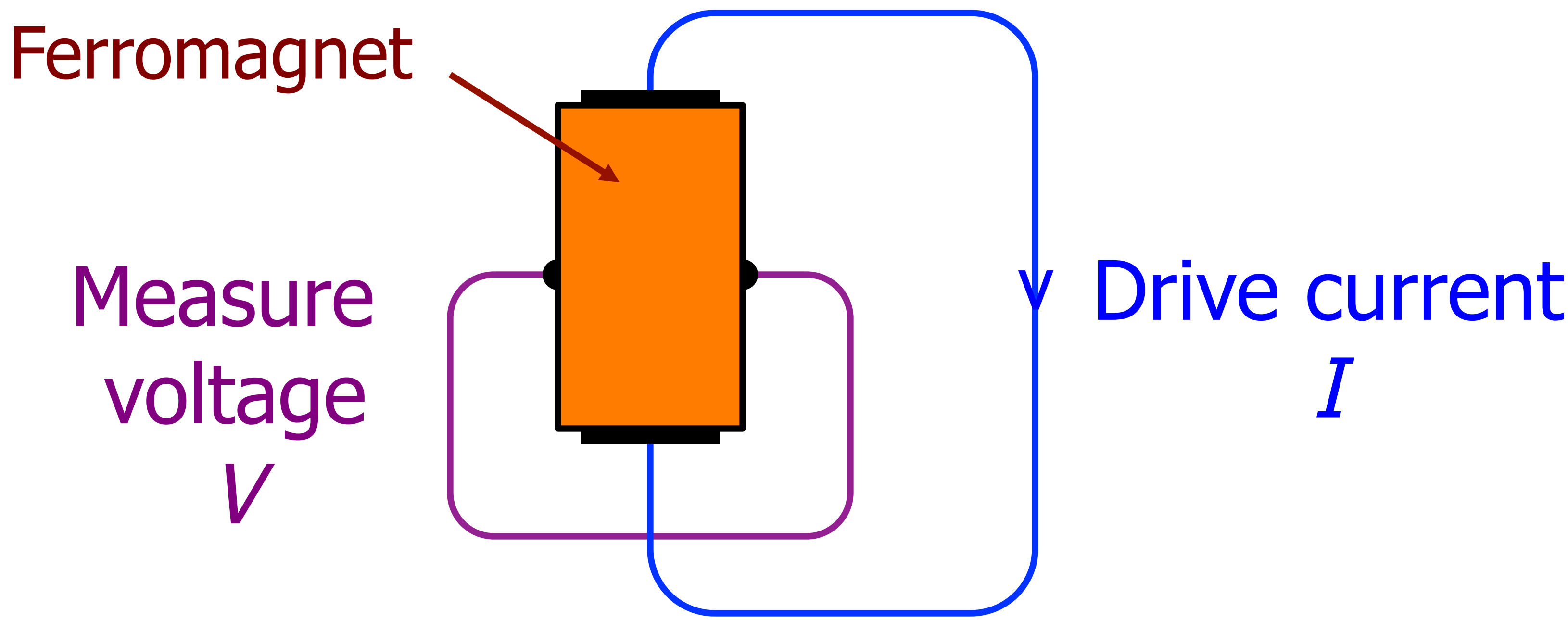
Chern theorem: $$\int_{BZ} \Omega_z(\mathbf{k})\, d^2k = 2\pi C$$

Where C is an integer!

Application to 2D crystals:

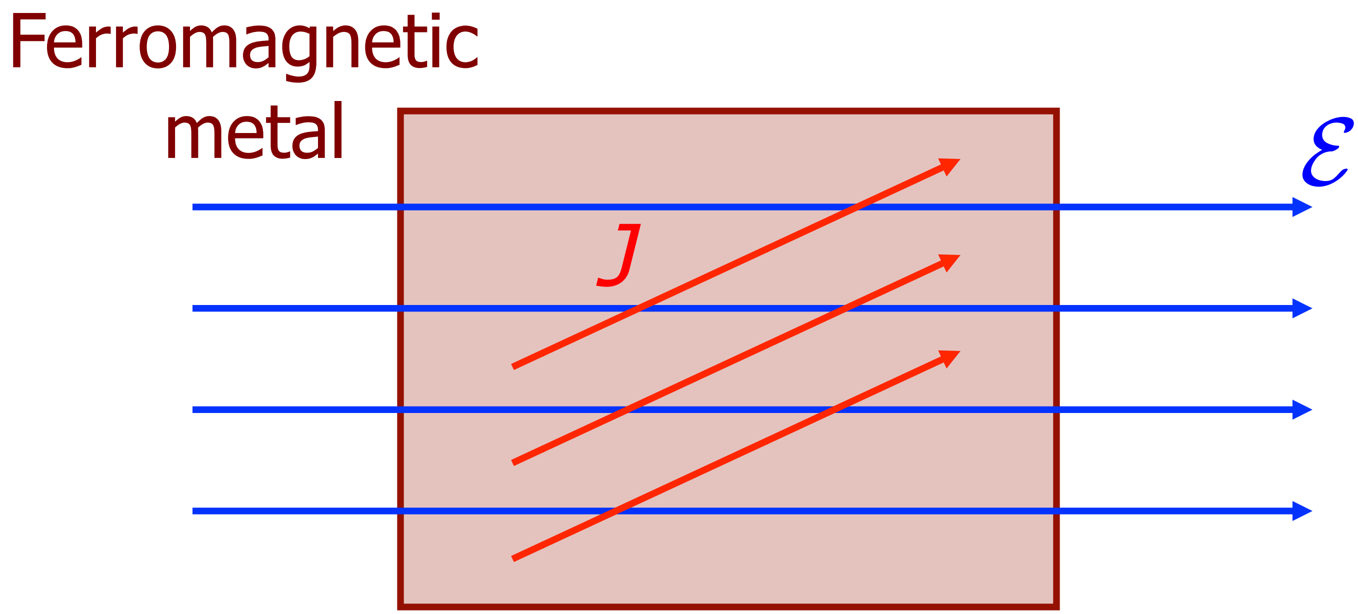
- Each Bloch band $\psi_{nk}(r)$ has Chern integer C_n
- Insulating 2D crystal has total Chern invariant C
- Physical significance?

Anomalous Hall conductivity (AHC)



Measure σ_{xy} in *absence* of B-field

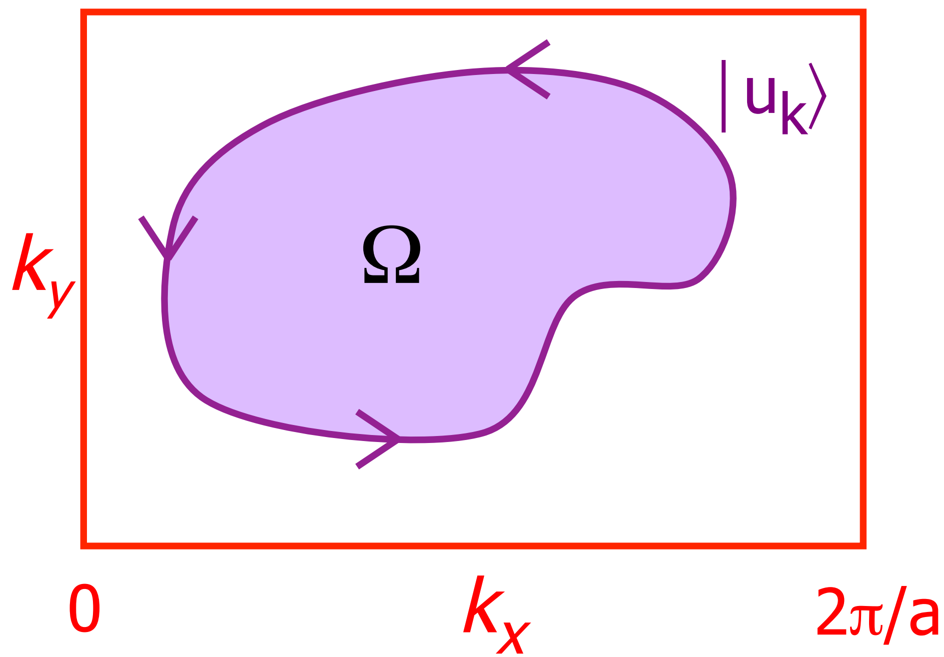
Anomalous Hall effect



$$\sigma_{xy} \neq 0$$

No external B field

Berry curvature in the Brillouin zone



$$\boxed{\Omega_z(\mathbf{k}) = -2\mathrm{Im}\left\langle \frac{du}{dk_x} \middle| \frac{du}{dk_y} \right\rangle}$$

$$\phi = \int_{\mathrm{FS}} \Omega_z(\mathbf{k})\, d^2k$$

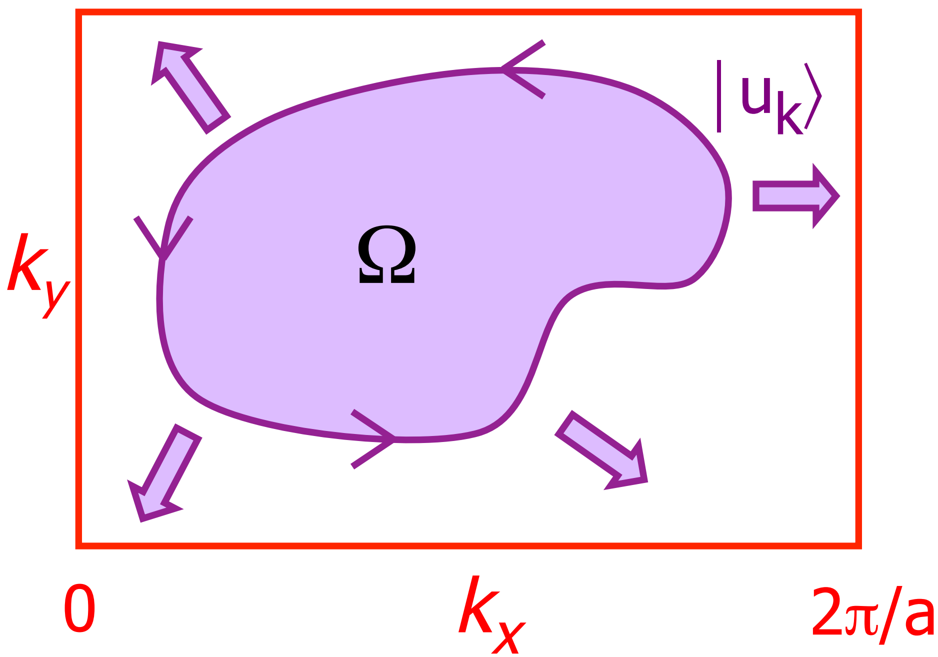
Metal

Anomalous Hall conductivity: $\boxed{\sigma_{xy} = \frac{-e^2}{2\pi h}\phi}$

Karplus and Luttinger; Sundaram and Niu

RUTGERS

Berry curvature in the Brillouin zone



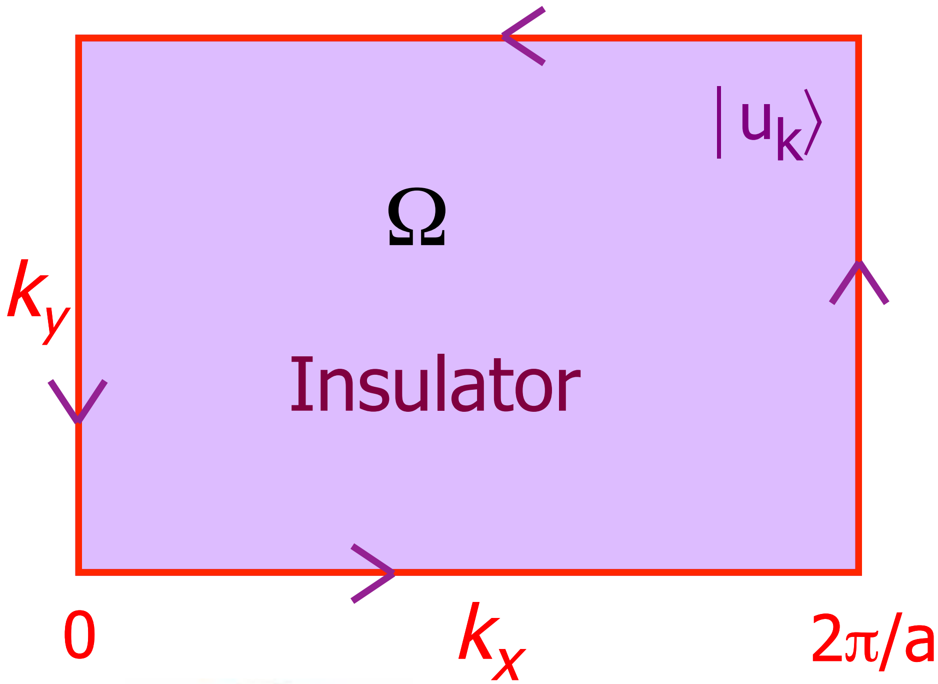
$$\Omega_z(\mathbf{k}) = -2\mathrm{Im}\left\langle \frac{du}{dk_x} \middle| \frac{du}{dk_y} \right\rangle$$

$$\phi = \int_{\mathrm{FS}} \Omega_z(\mathbf{k})\, d^2k$$

Anomalous Hall conductivity:

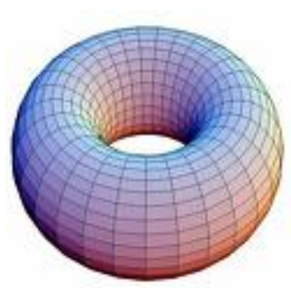
$$\sigma_{xy} = \frac{-e^2}{2\pi h}\,\phi$$

Berry curvature in the Brillouin zone



$$\Omega_z(\mathbf{k}) = -2\,\mathrm{Im}\left\langle \frac{du}{dk_x} \middle| \frac{du}{dk_y} \right\rangle$$

$$\phi = \int_{BZ} \Omega_z(\mathbf{k})\, d^2k = 2\pi C$$



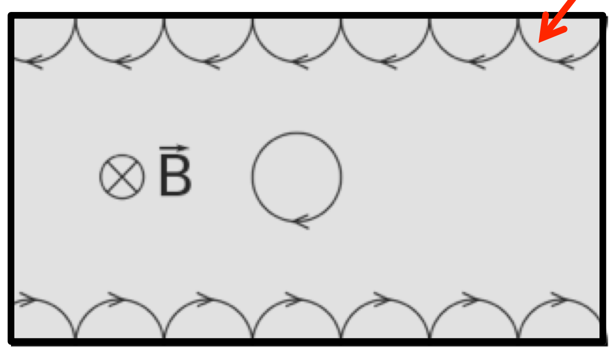
Quantum Anomalous Hall: $\boxed{\sigma_{xy} = \frac{-e^2}{h} C}$

"Chern number" or "TKNN invariant"

2D Quantum Hall to QAH insulator

- Quantum Hall effect

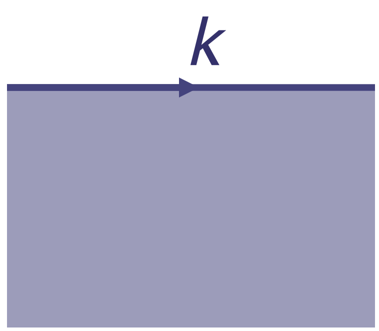
Skipping orbits (edge states)

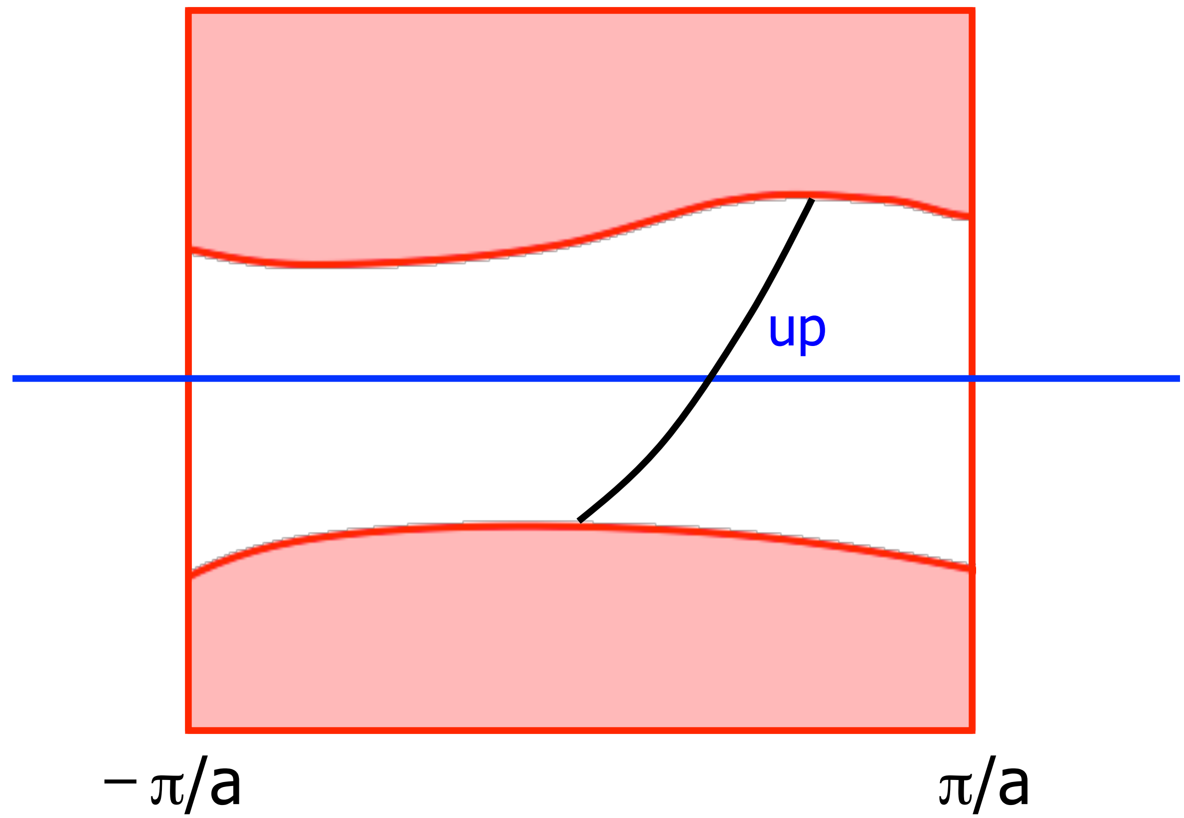


$\sigma_{xy} = e^2/h$ exactly !

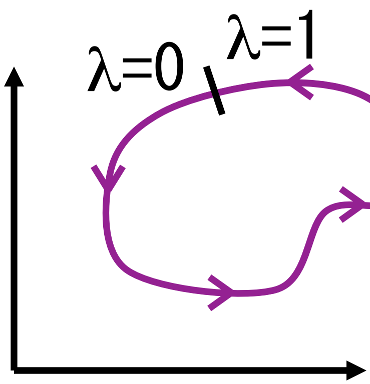
- Quantum anomalous Hall effect
  - In crystal with broken time-reversal symmetry
  - No external magnetic field
  - In principle, at room temperature

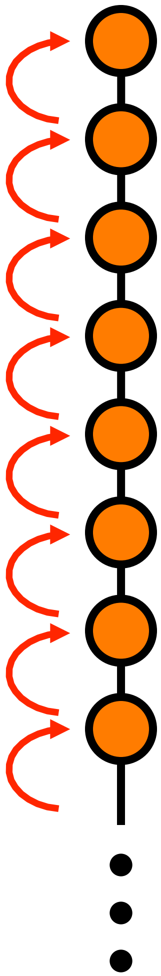
Edge states: 2D QAH insulator

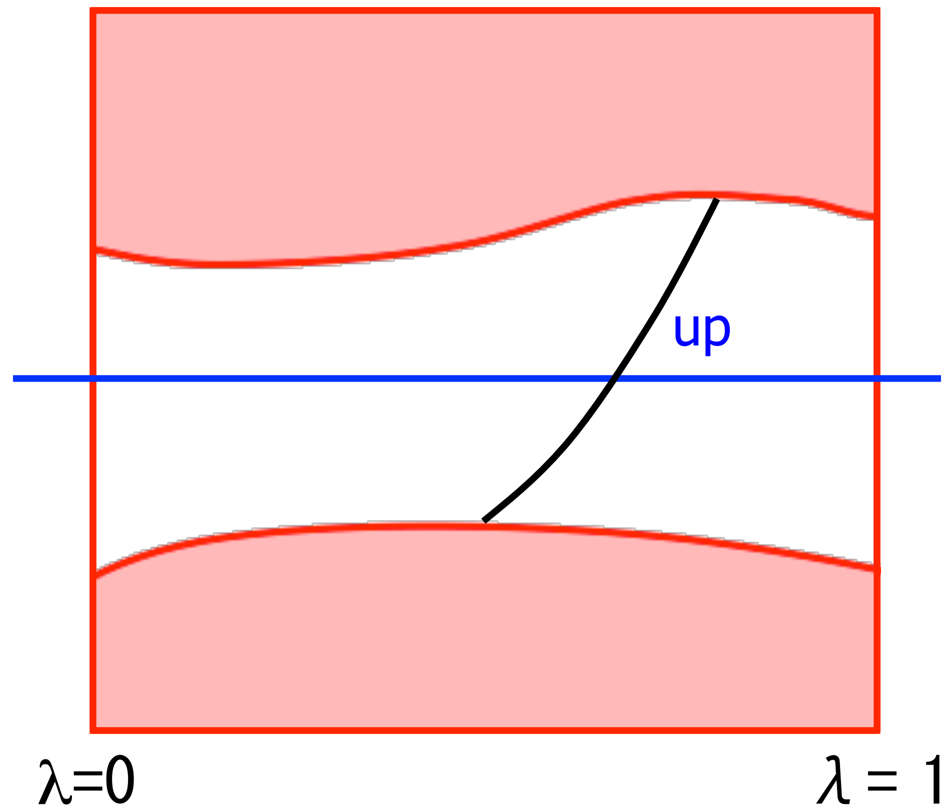




Semi-infinite chain: cyclic evolution







Surface vs. bulk indicator?

- Counting surface states is a surface indicator
- Can we find a bulk indicator that works in a similar way?
- Yes! Hybrid Wannier centers!
  - Bloch-like in k_x
  - Wannier-like along y
  - Plot y locations vs. k_x

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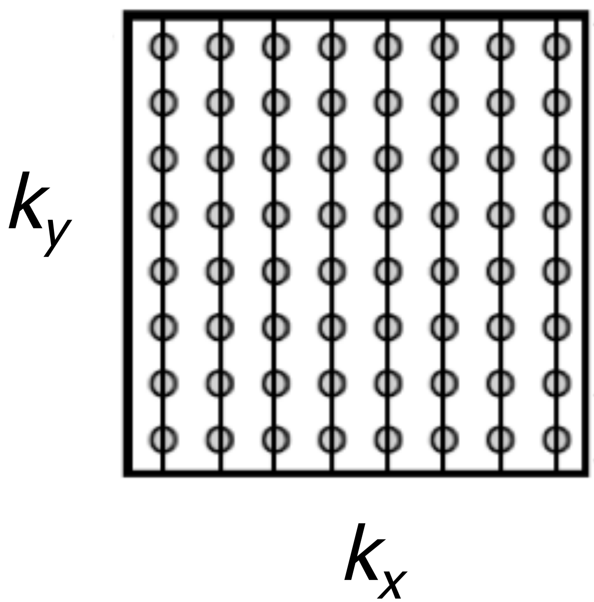
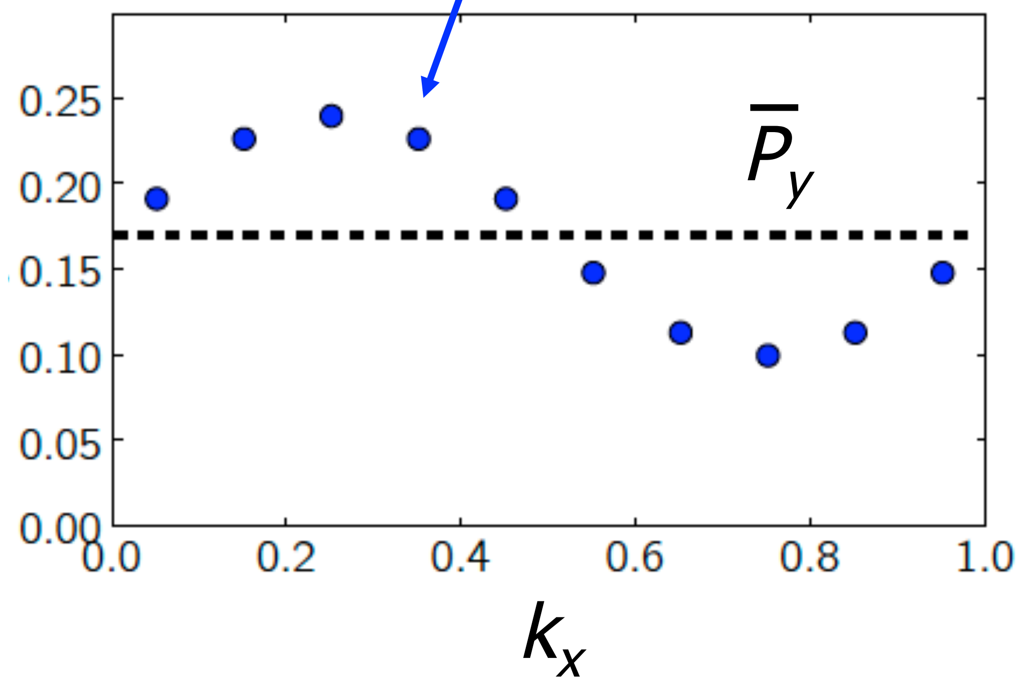
String Berry phases for normal band

$$\phi\,(k_x) = -\mathrm{Im}\,\ln\left[\,\langle u_1|u_2\rangle\,\langle u_2|u_3\rangle \ldots \langle u_{n-1}|u_n\rangle\,\right]$$



$P_y(k_x) \propto \phi\,(k_x)$



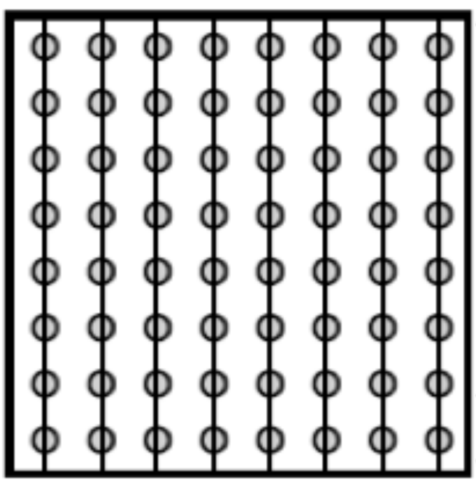
RUTGERS

String Berry phases in QAH band

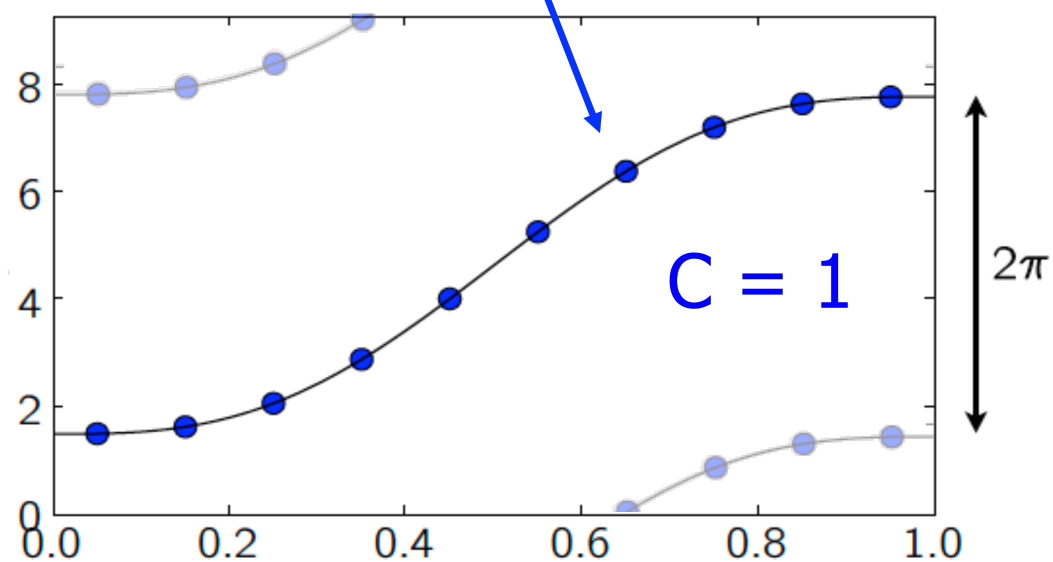
$$\phi(k_x) = -\mathrm{Im}\ \ln\left[\langle u_1|u_2\rangle\langle u_2|u_3\rangle\ldots\langle u_{n-1}|u_n\rangle\right]$$

$P_y(k_x) \propto \phi(k_x)$

k_y

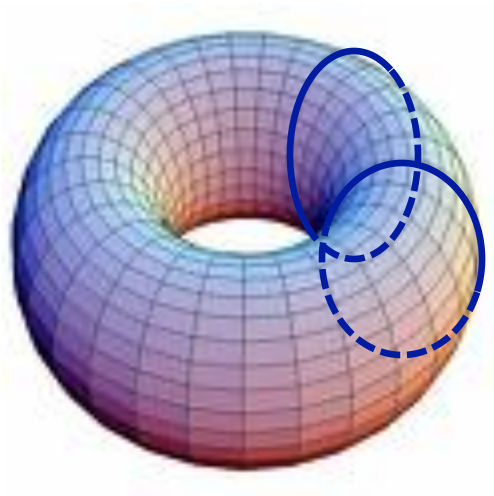


k_x



k_x

Hybrid Wannier functions



Even if $C \neq 0$:

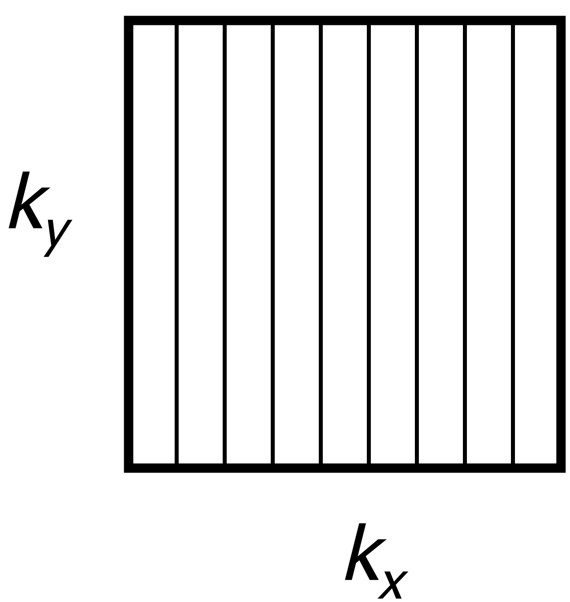
- Choose smooth gauge on one loop
- Compute Berry phases (hybrid Wannier centers)
- Repeat as a function of position on the torus
- There is no topological obstruction!

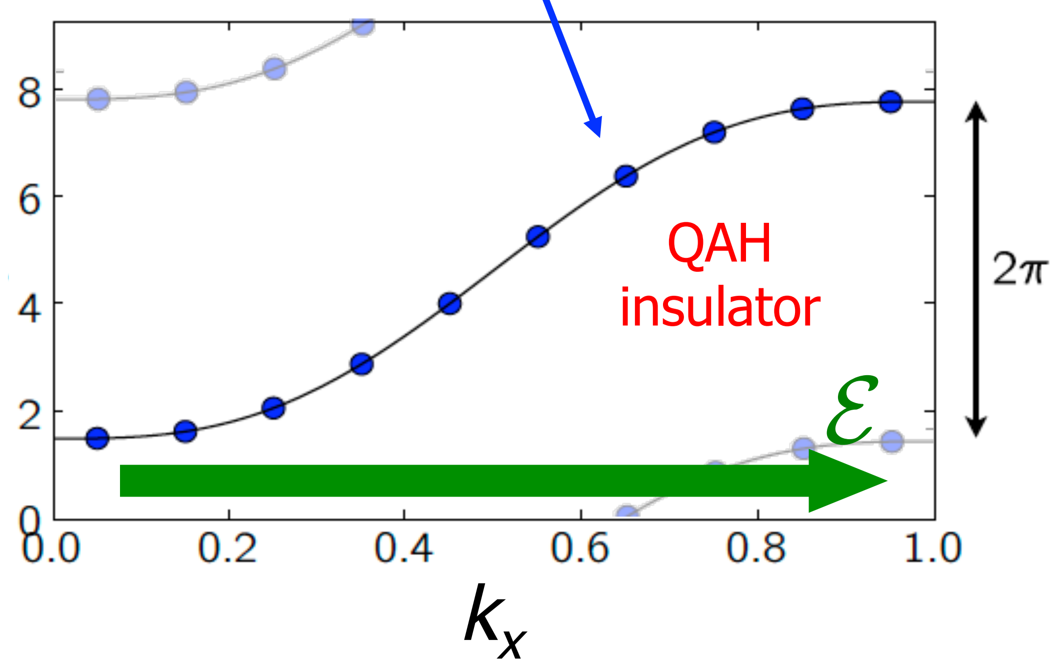
2D QAH insulator

$\phi(k_x)$ = Berry phase along y at given k_x

= "Hybrid Wannier centers"

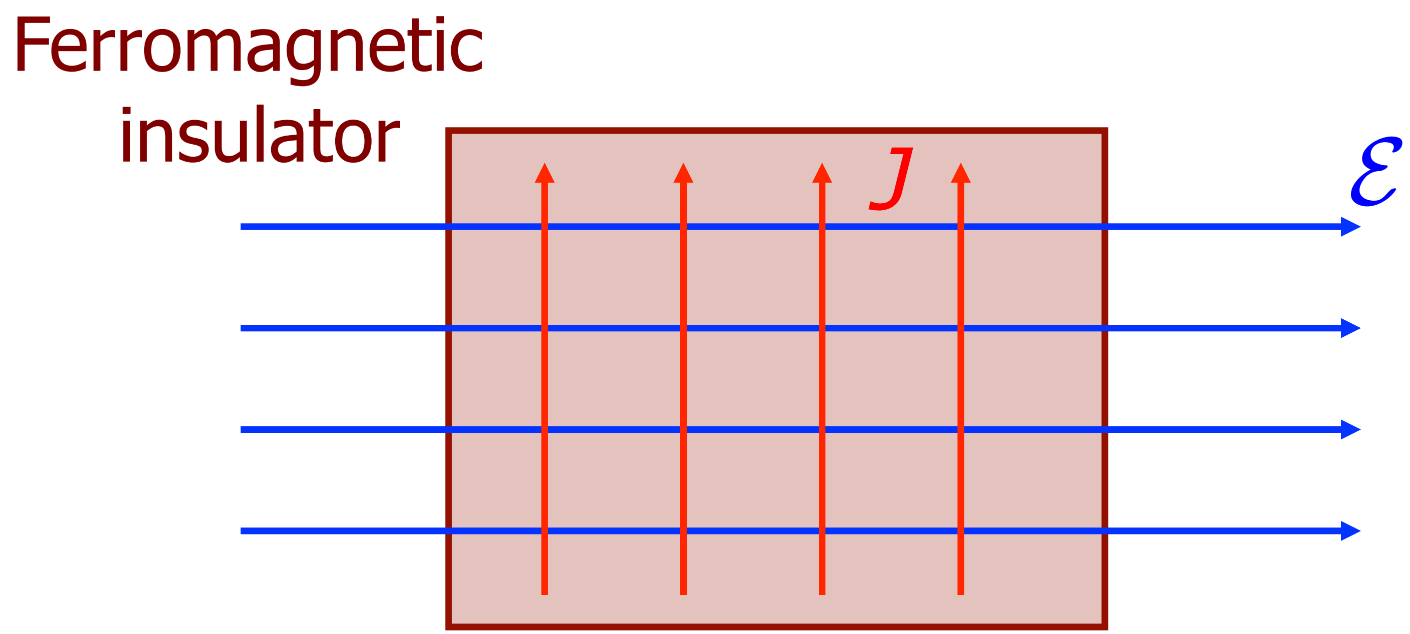
$P_y(k_x) \propto \phi(k_x)$





Explains $\sigma_{xy} = e^2/h$

Quantum anomalous Hall effect



$\sigma_{xy} \neq 0$

Like integer quantum Hall, but no B_{ext}

Tight-binding models for 2D QAH insulators

VOLUME 61, NUMBER 18 PHYSICAL REVIEW LETTERS 31 OCTOBER 1988

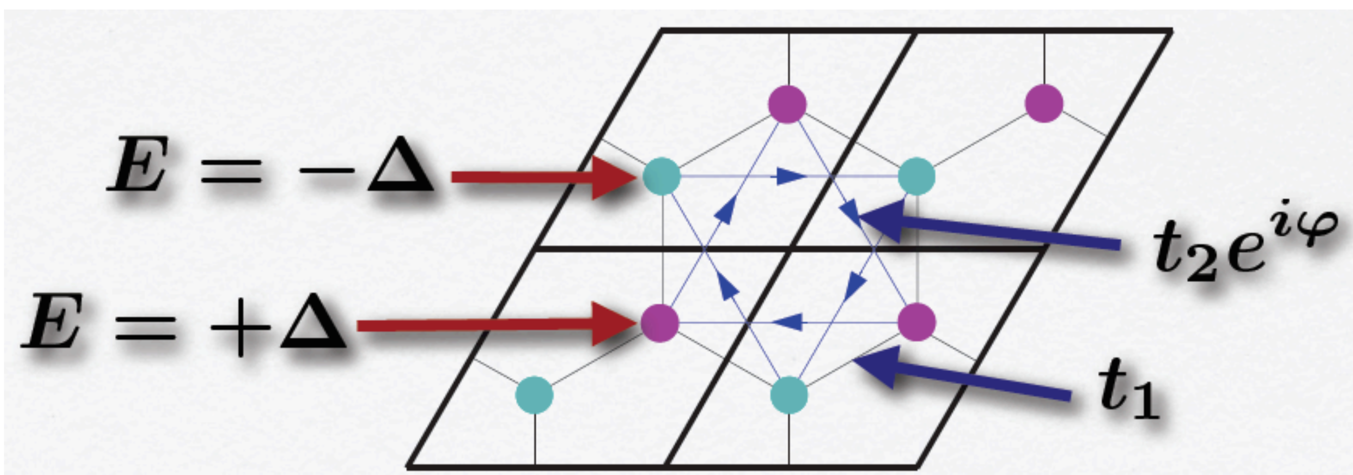
Model for a Quantum Hall Effect without Landau Levels: Condensed-Matter Realization of the "Parity Anomaly"

F. D. M. Haldane

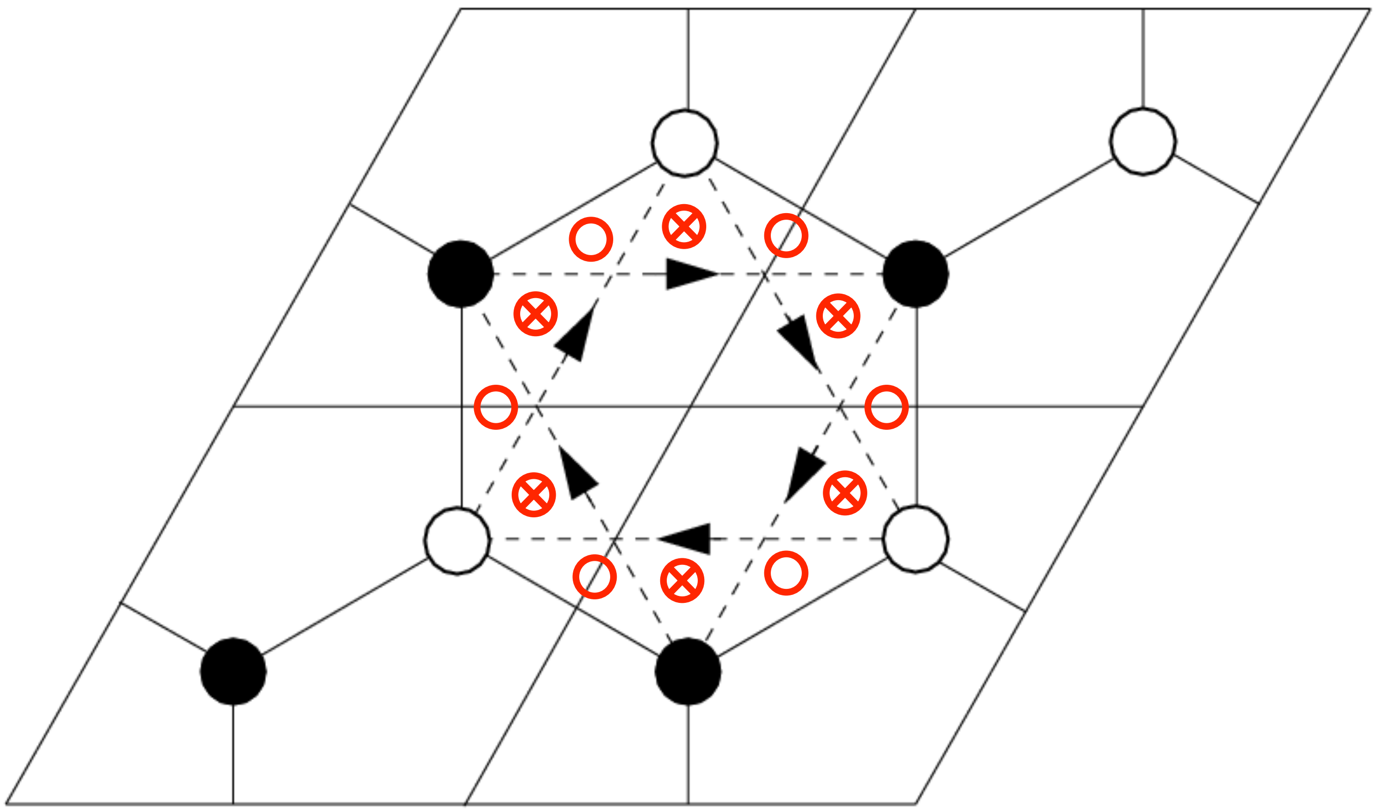
Department of Physics, University of California, San Diego, La Jolla, California 92093

(Received 16 September 1987)

A two-dimensional condensed-matter lattice model is presented which exhibits a nonzero quantization of the Hall conductance σ^{xy} in the *absence* of an external magnetic field. Massless fermions *without spectral doubling* occur at critical values of the model parameters, and exhibit the so-called "parity anomaly" of (2+1)-dimensional field theories.



Flux tubes in Haldane model



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QAH insulators

- "QAH insulator" = "Chern insulator"
- Quantized Hall conductance even in the absence of macroscopic magnetic fields
- Quite possibly at room temperature
- Usefulness:
  - Metrology?
  - Magnetoelectric coupling?

Can QAH insulators be found?

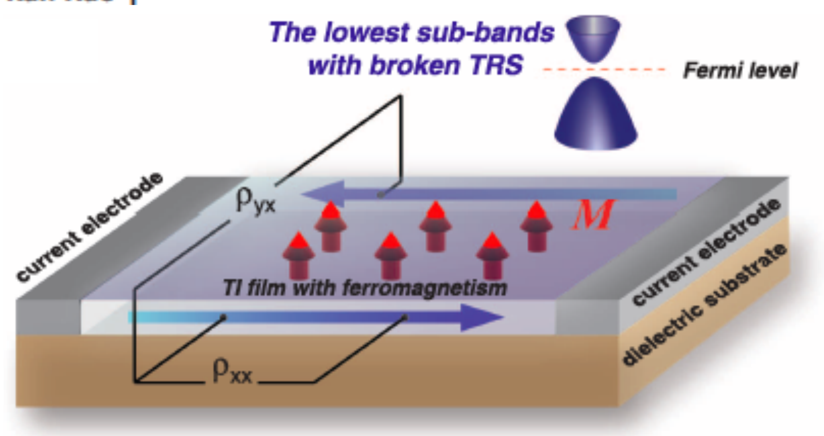
- Requirements
  - Spontaneously broken TR (FM or FiM)
  - Insulator
  - Strong spin-orbit splitting
- Prefer gap > 0.2 eV (Q Hall at T_{room})
- Proposals
  - Magnetically doped TR-invariant TI's
  - Magnetic adatoms on graphene
  - 2D adlayer on a magnetic insulator

Magnetic doping: Claim for QAH

www.sciencemag.org SCIENCE VOL 340 12 APRIL 2013

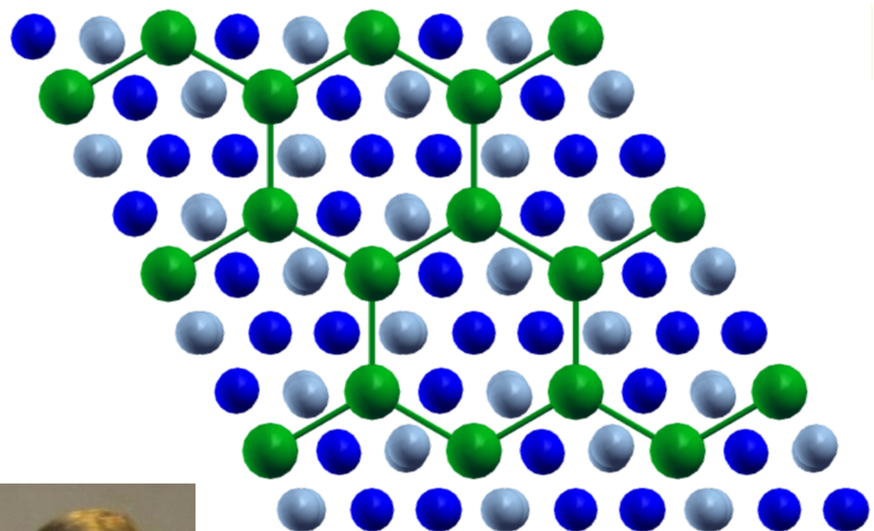
Experimental Observation of the Quantum Anomalous Hall Effect in a Magnetic Topological Insulator

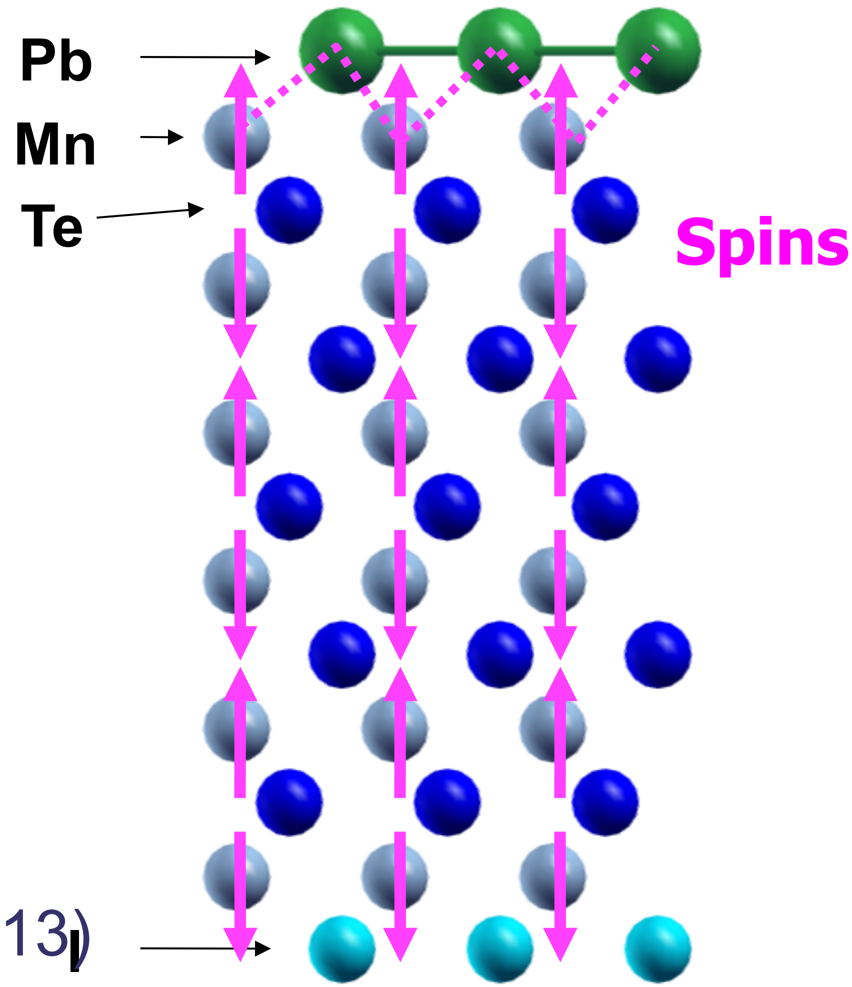
Cui-Zu Chang,[1,2*] Jinsong Zhang,[1*] Xiao Feng,[1,2*] Jie Shen,[2*] Zuocheng Zhang,[1] Minghua Guo,[1] Kang Li,[2] Yunbo Ou,[2] Pang Wei,[2] Li-Li Wang,[2] Zhong-Qing Ji,[2] Yang Feng,[1] Shuaihua Ji,[1] Xi Chen,[1] Jinfeng Jia,[1] Xi Dai,[2] Zhong Fang,[2] Shou-Cheng Zhang,[3] Ke He,[2]† Yayu Wang,[1]† Li Lu,[2] Xu-Cun Ma,[2] Qi-Kun Xue[1]†



Observed below ~1K

Another approach (Friday seminar)





Kevin Garrity & D.V.

Phys. Rev. Lett. **110**, 116802 (2013)

Outline

- Tutorial on Berry phases and curvatures
- 1D charge pump
- 2D quantum anomalous Hall insulator
- TR-invariant insulators (Z_2)
  - 2D ("Quantum spin Hall") insulator
  - 3D "strong" and "weak" topological ins.
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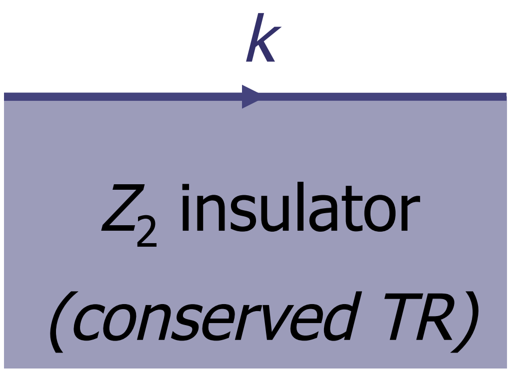
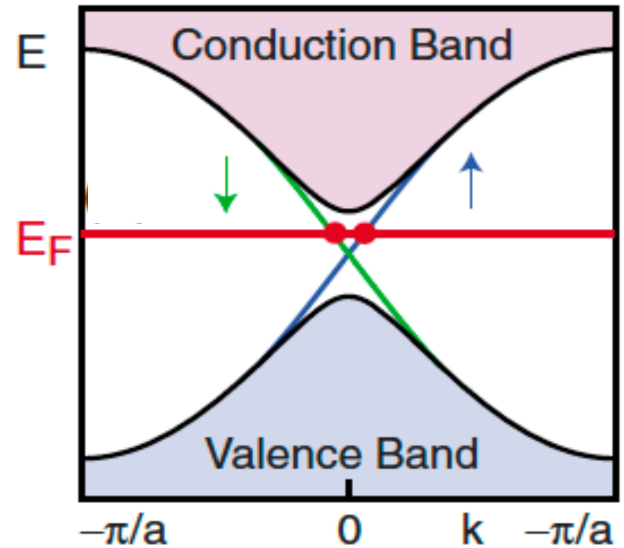
- Summary

2D Z_2 topological insulator (QSH)

QSH = Quantum spin Hall





***Colloquium*: Topological insulators**

M. Z. Hasan*

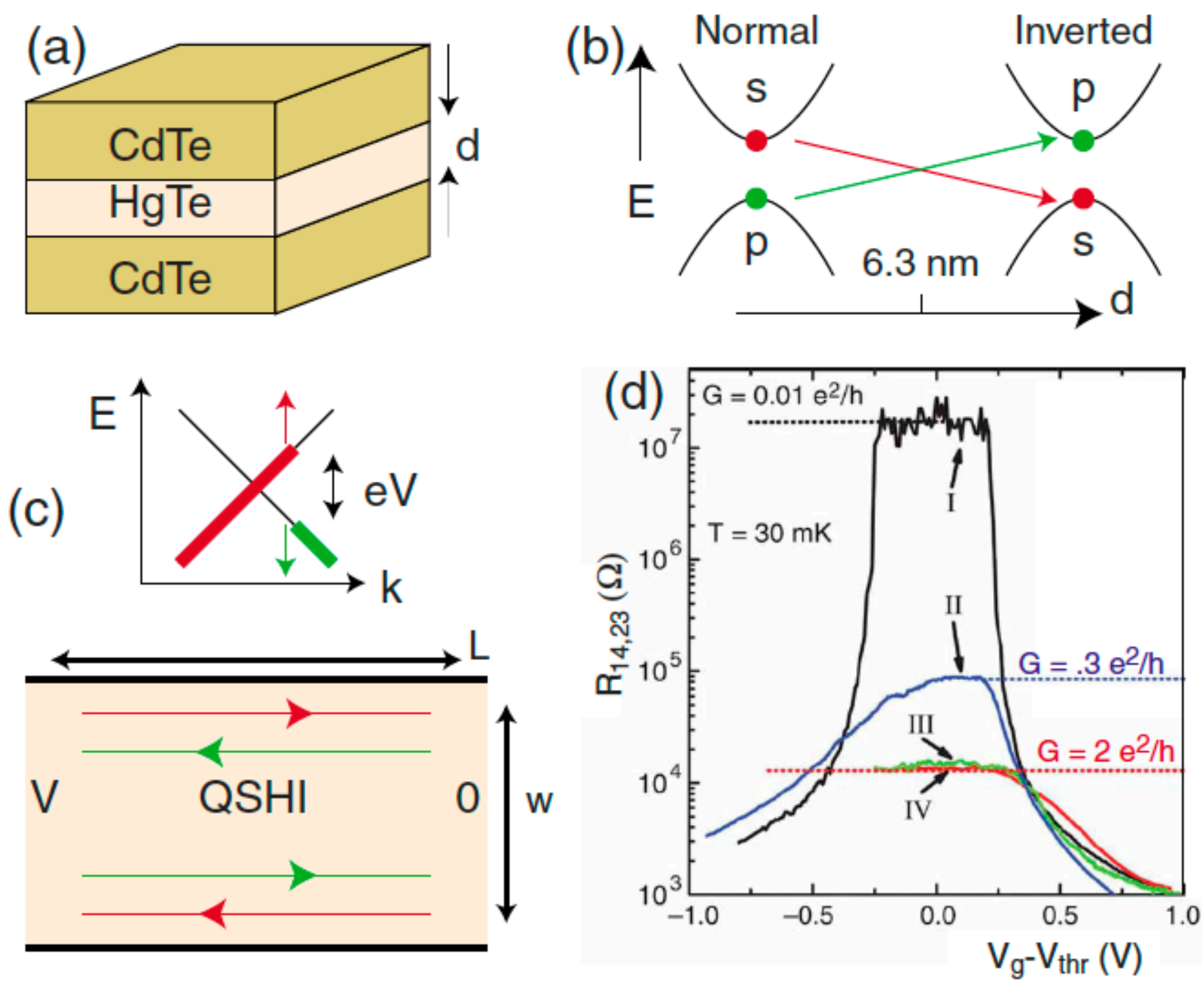
Joseph Henry Laboratories, Department of Physics, Princeton University, Princeton, New Jersey 08544, USA

C. L. Kane†

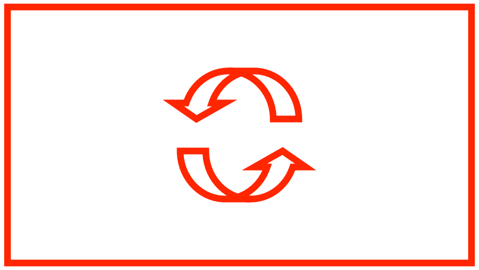
Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, Pennsylvania 19104, USA

(Published 8 November 2010)

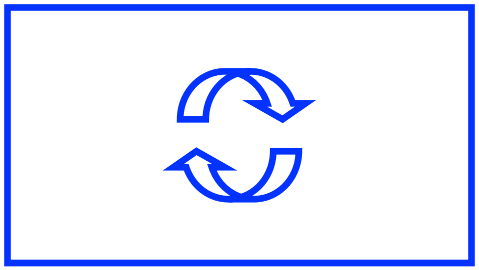
2D Z_2 topological insulator (QSH)



Z_2 Topological Insulator ("Quantum spin Hall")

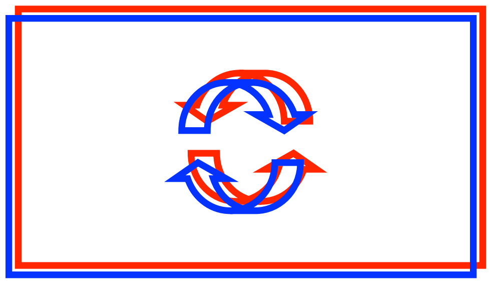


Spin up, $C = +1$



Spin down, $C = -1$

Z_2 Topological Insulator ("Quantum spin Hall")



Spin up, $C = +1$

Spin down, $C = -1$

Then turn on spin-orbit coupling (SOC):

- Obeys T symmetry
- Total $C = 0$
- Z_2 invariant is odd

Meaning of Z and Z_2

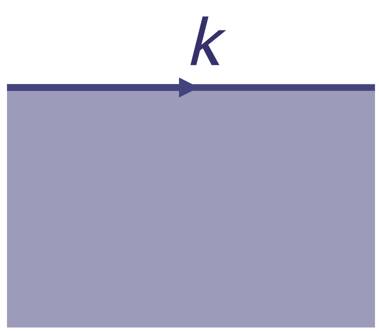
- Z = group of integers under addition

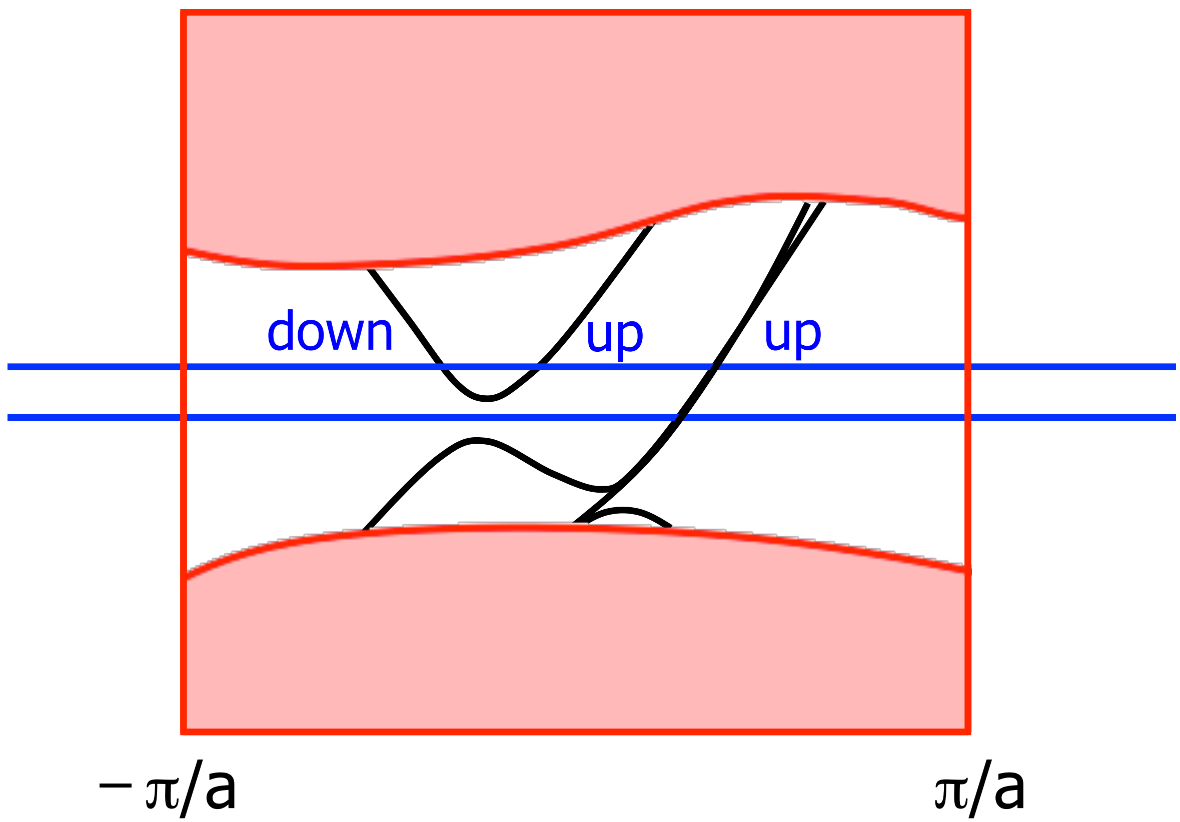
- $Z_2 = \{0,1\}$ under addition (mod 2)

Or equivalently,

- $Z_2 = \{+,-\}$ under multiplication

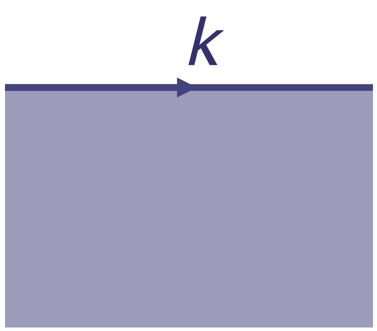
Edge states: 2D QAH insulator

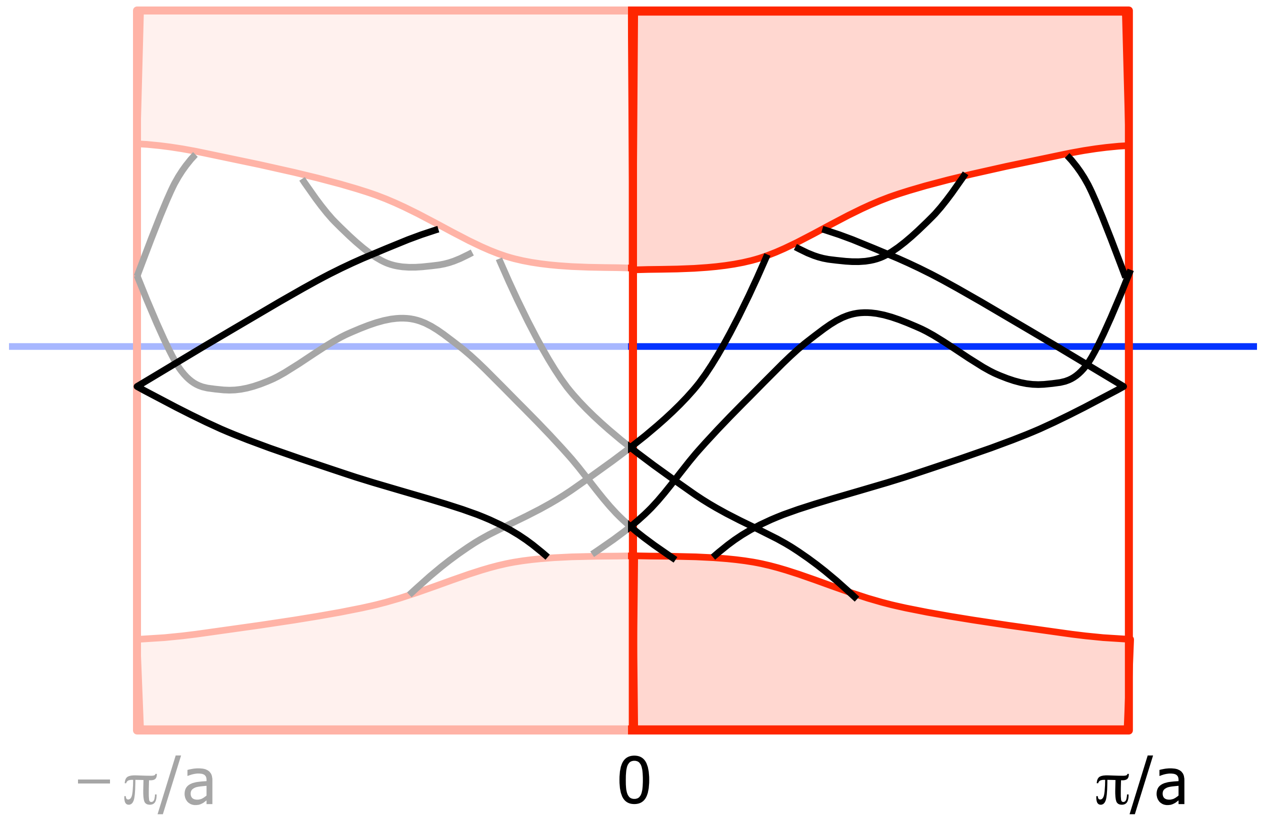




$$Z = N_{\mathrm{up}} - N_{\mathrm{down}} = \text{Invariant}$$

Edge states: 2D TR-invariant insulator





$Z_2 = N_{\mathrm{cross}}$ (mod 2) = Invariant

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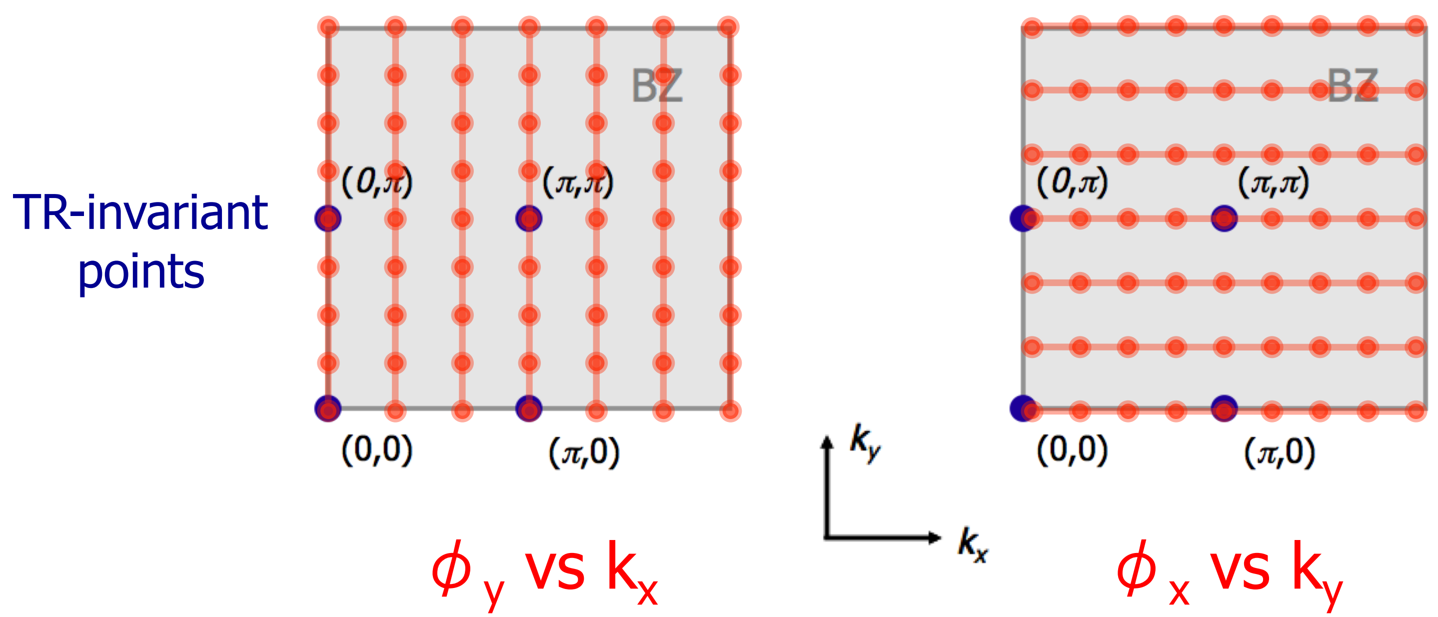
Surface vs. bulk indicator?

- Counting surface states is a surface indicator
- Can we find a bulk indicator that works in a similar way?
- Yes! Wannier centers again!

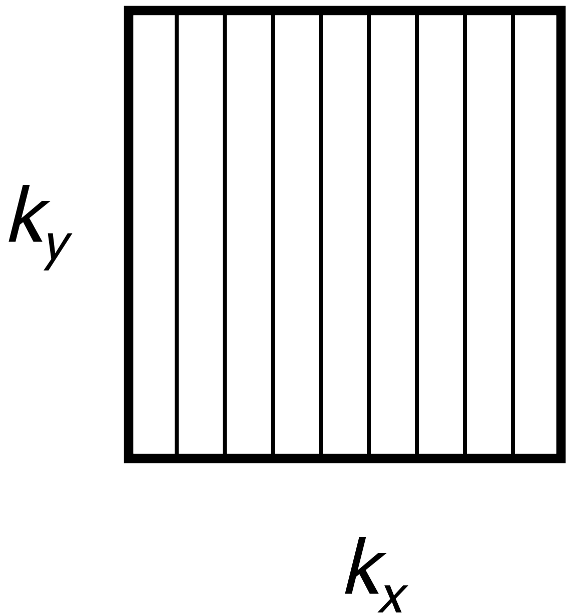
Surface vs. bulk indicator?

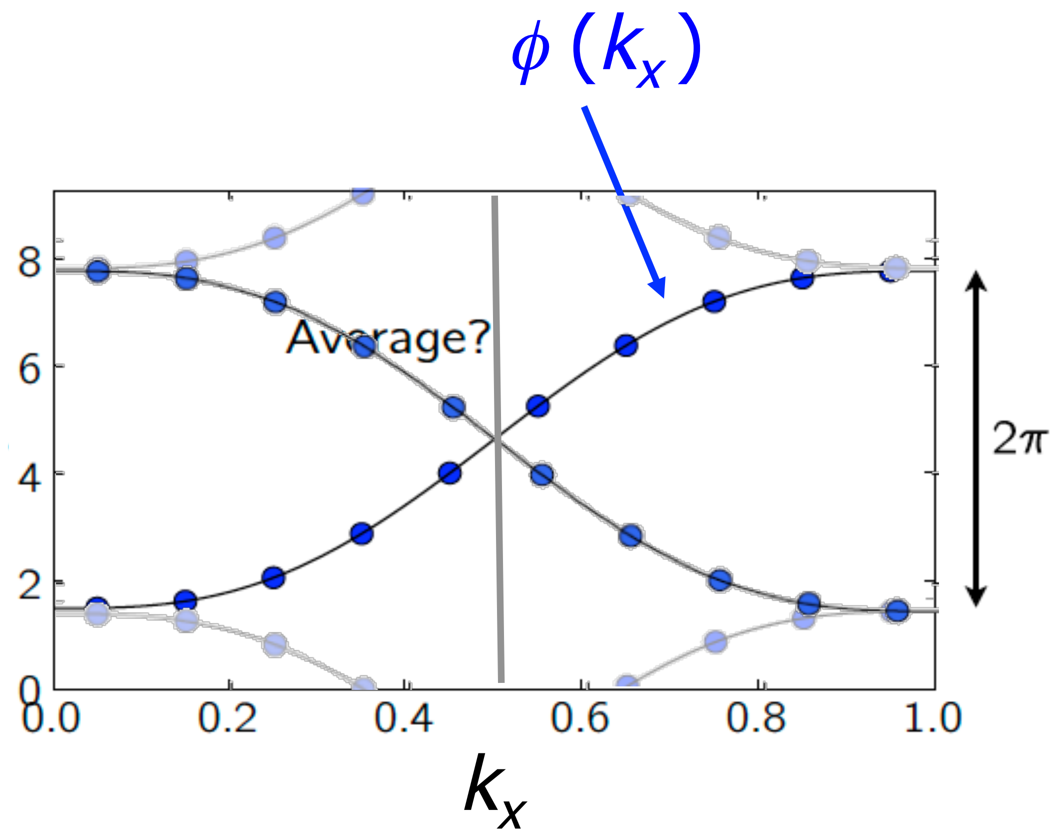
- Yes! Wannier centers again!



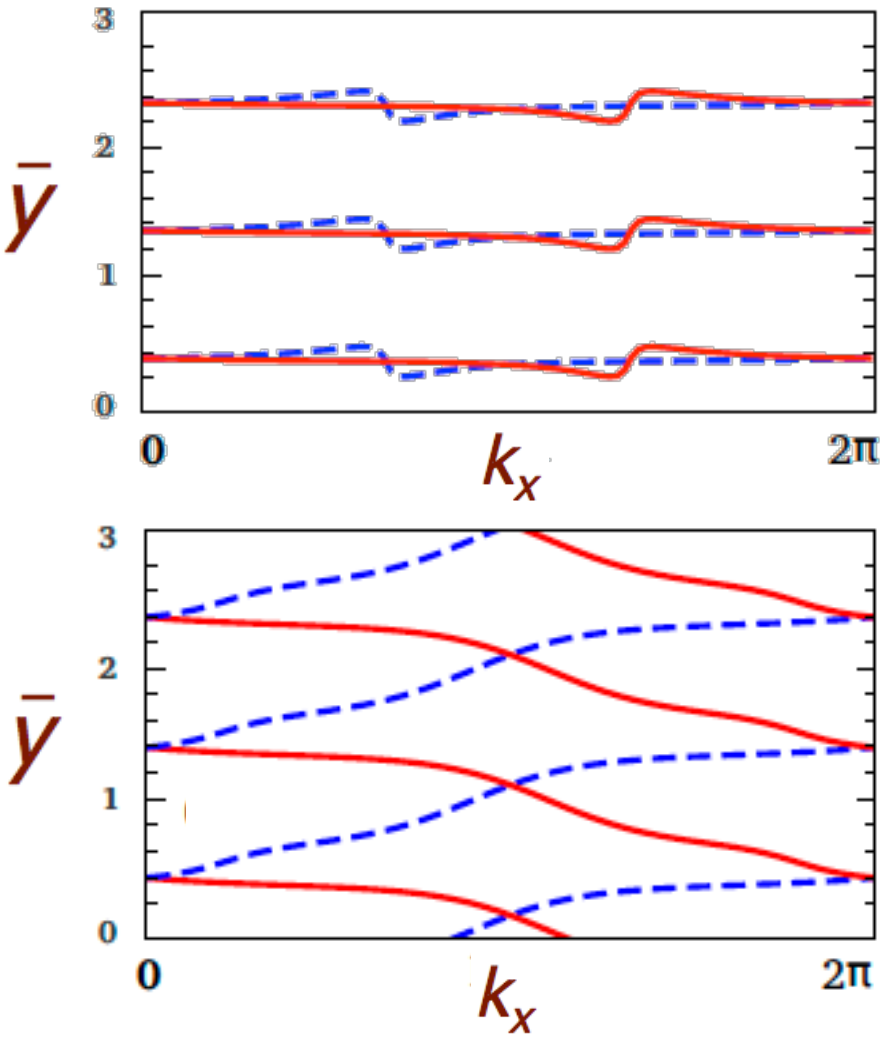
![Rutgers logo]

Z_2 insulator: Hybrid WF centers $\bar{y}(k_x)$





Z_2 insulator: Hybrid WF centers $\bar{y}\,(k_x)$



Normal

Kane-Mele tight-binding model

Z_2-odd

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Method for computing Z_2 invariants

PHYSICAL REVIEW B **83**, 235401 (2011)

Computing topological invariants without inversion symmetry

Alexey A. Soluyanov* and David Vanderbilt†
Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854-0849, USA

Alexei
Soluyanov

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Closely related work

PHYSICAL REVIEW B **84**, 075119 (2011)

Equivalent expression of $\mathbb{Z}_2$ topological invariant for band insulators using the non-Abelian Berry connection

Rui Yu,[1] Xiao Liang Qi,[2] Andrei Bernevig,[3] Zhong Fang,[1] and Xi Dai[1]

[1] *Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China*
[2] *Department of Physics, Stanford University, Stanford, California 94305, USA*
[3] *Department of Physics, Princeton University, Princeton, New Jersey 08540, USA*

(Received 12 January 2011; revised manuscript received 2 June 2011; published 8 August 2011)

We introduce an expression for the $\mathbb{Z}_2$ topological invariant of band insulators using the non-Abelian Berry connection. Our expression can identify the topological nature of a general band insulator *without* any of the gauge-fixing problems that plague the concrete implementation of previous invariants. This expression can be derived from the "partner switching" of the Wannier function center during time-reversal pumping and is thus equivalent to the Z_2 topological invariant proposed by Kane and Mele. Using our expression, we have recalculated the Z_2 topological index for several topological insulator material systems and obtained consistent results with the previous studies.

DOI: 10.1103/PhysRevB.84.075119 PACS number(s): 71.10.Pm, 71.15.Mb

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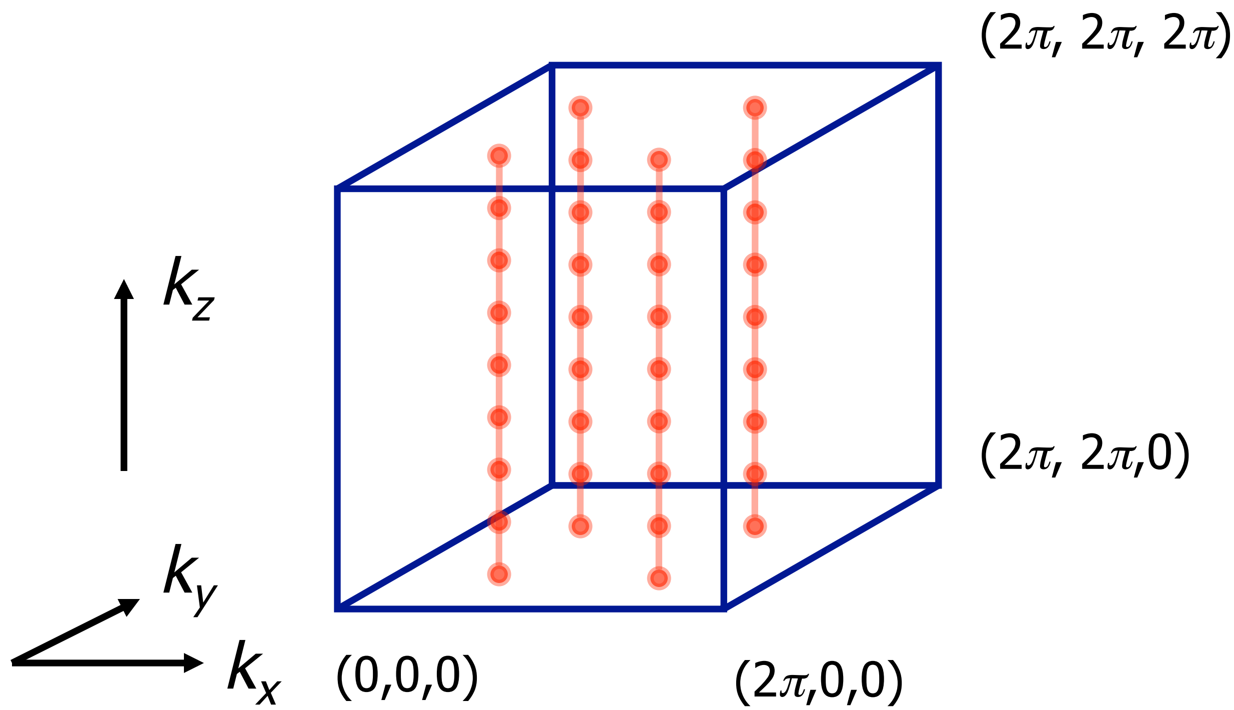
$$(k_x, k_y) \quad \Rightarrow \quad (k_x, k_y, k_z)$$

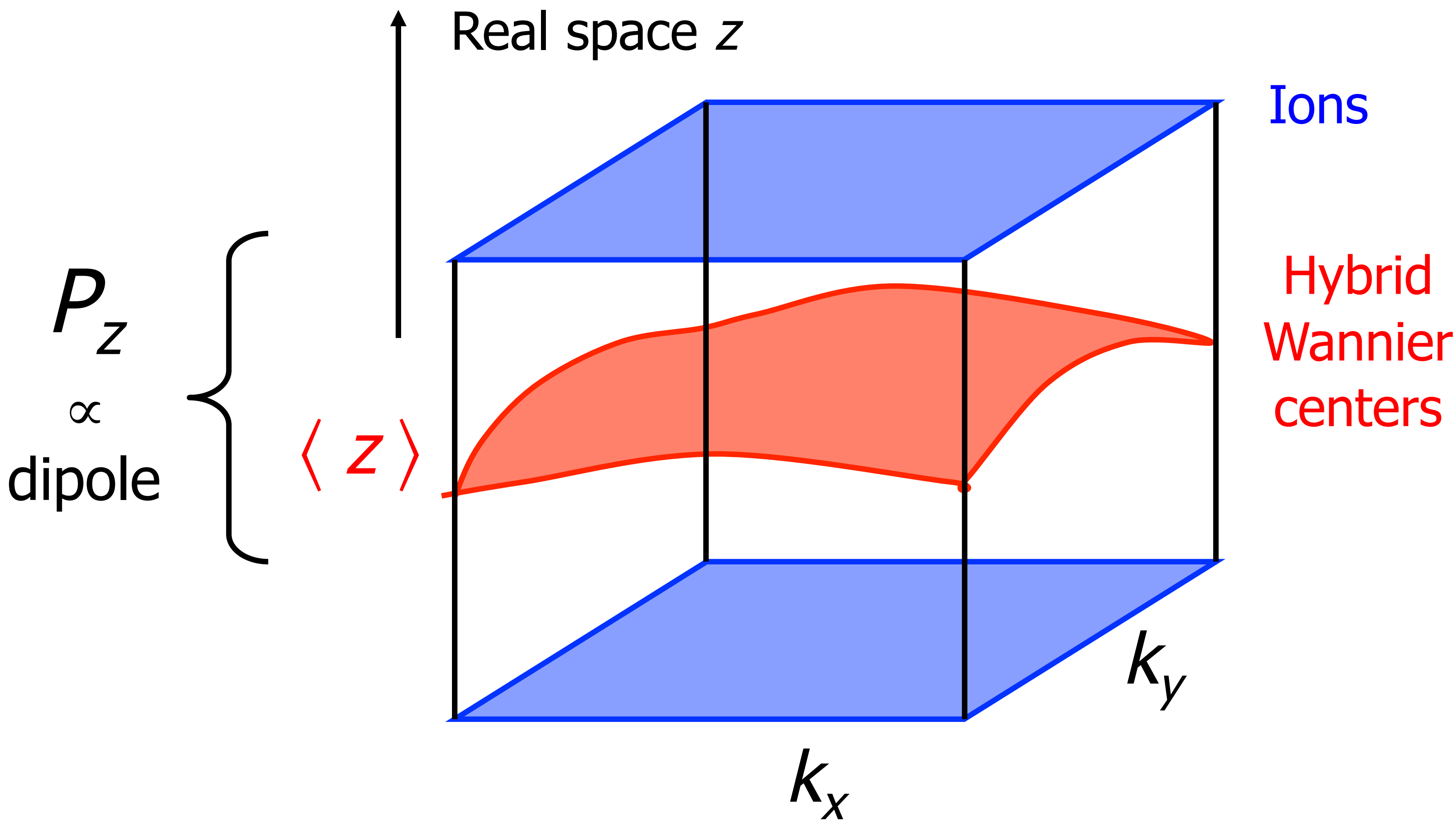
2D insulator

3D insulator

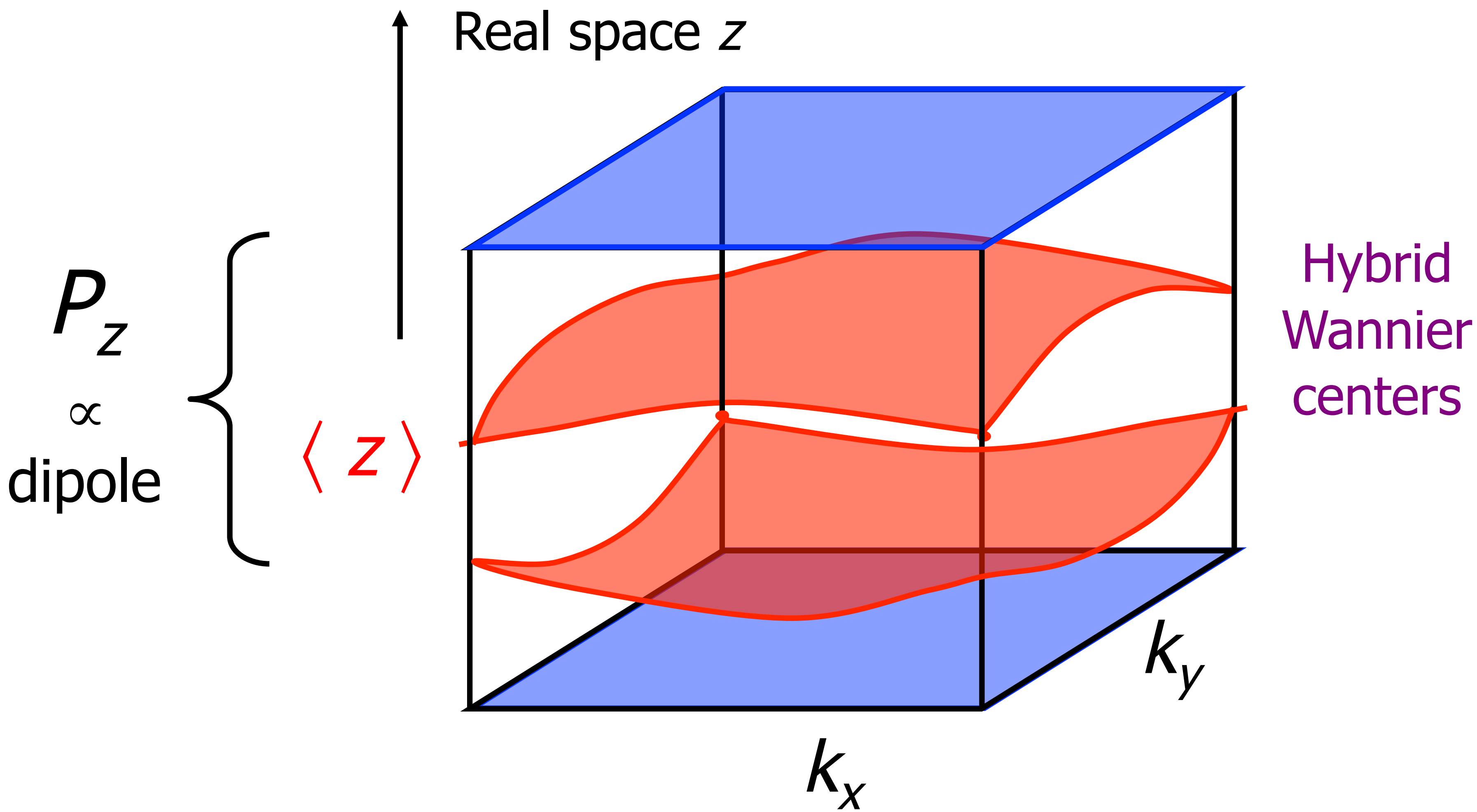
Polarization in 3D



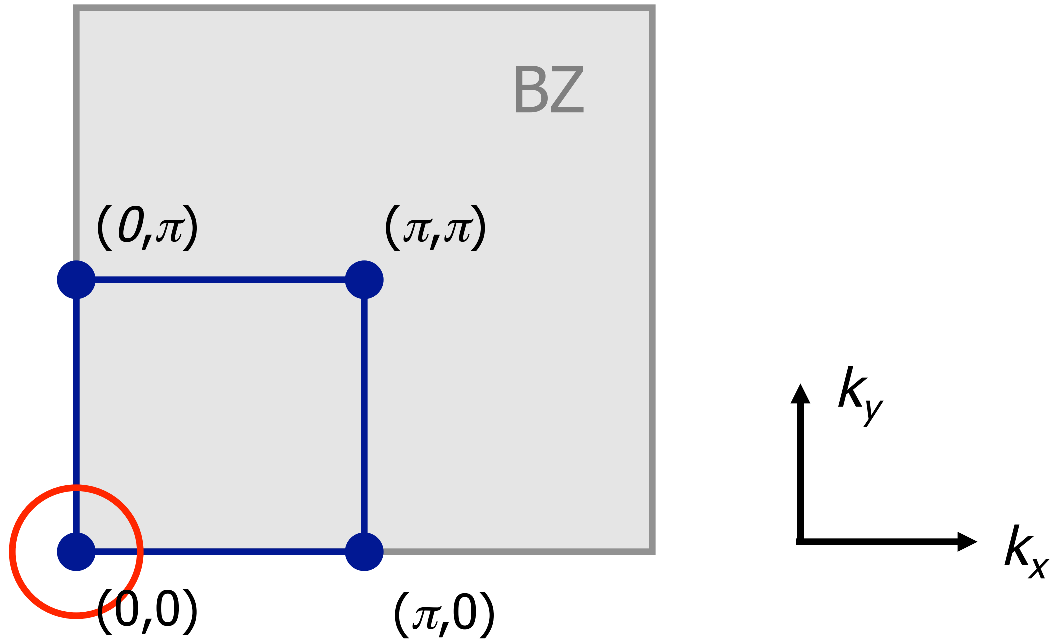
Polarization in 3D



Polarization in 3D: Multiband case



TR symmetry: 2D QSH insulator

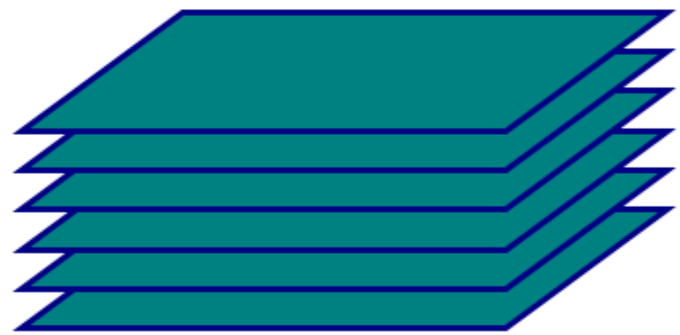


4 T-invariant points in k-space

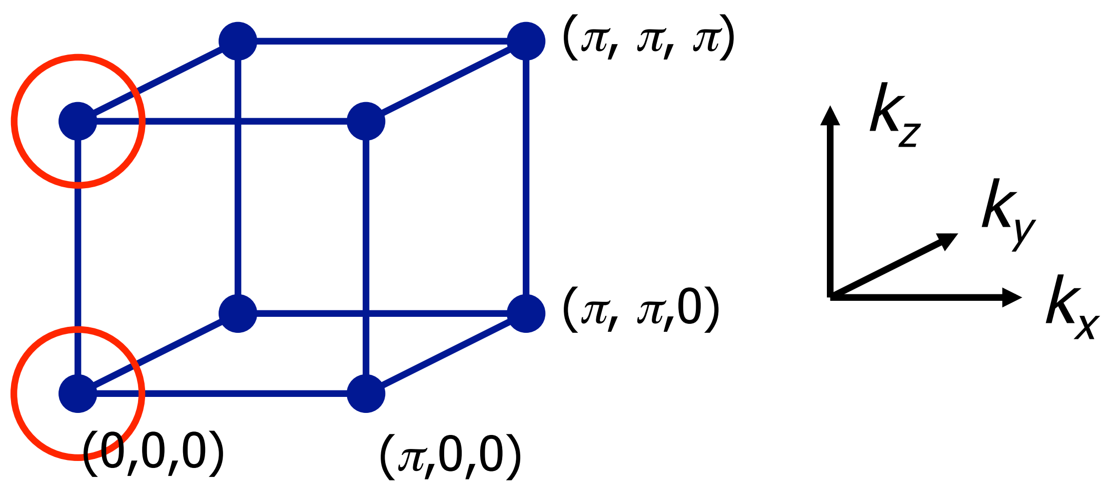
3D weak topological insulator

Real space:

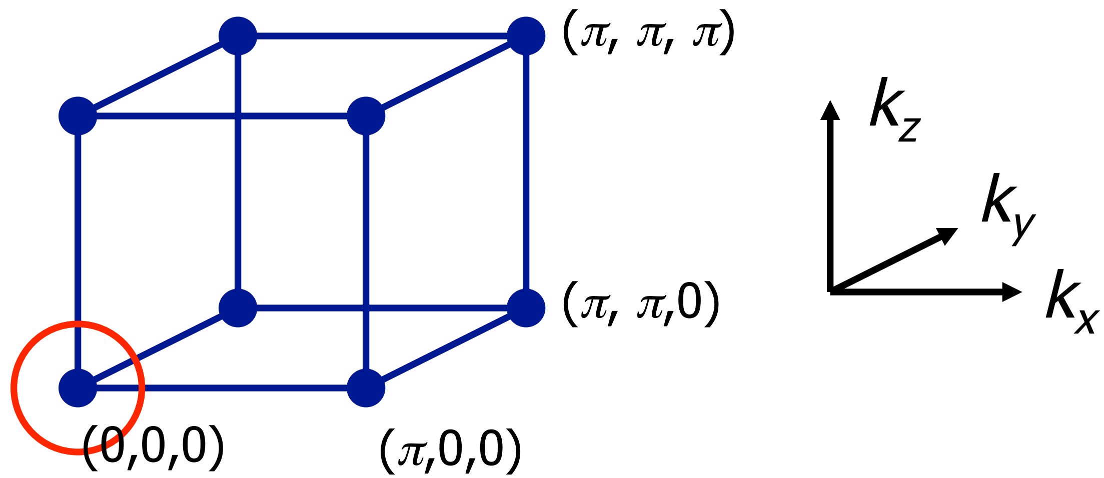
Stack Z_2-odd layers



Reciprocal space:

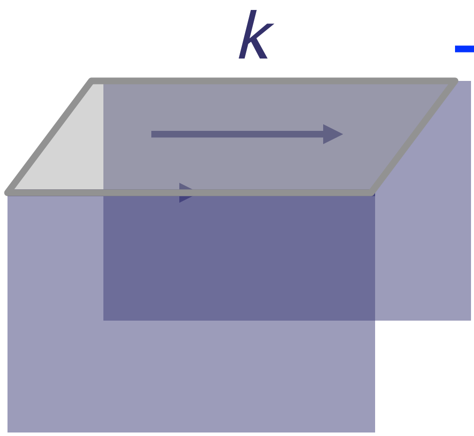


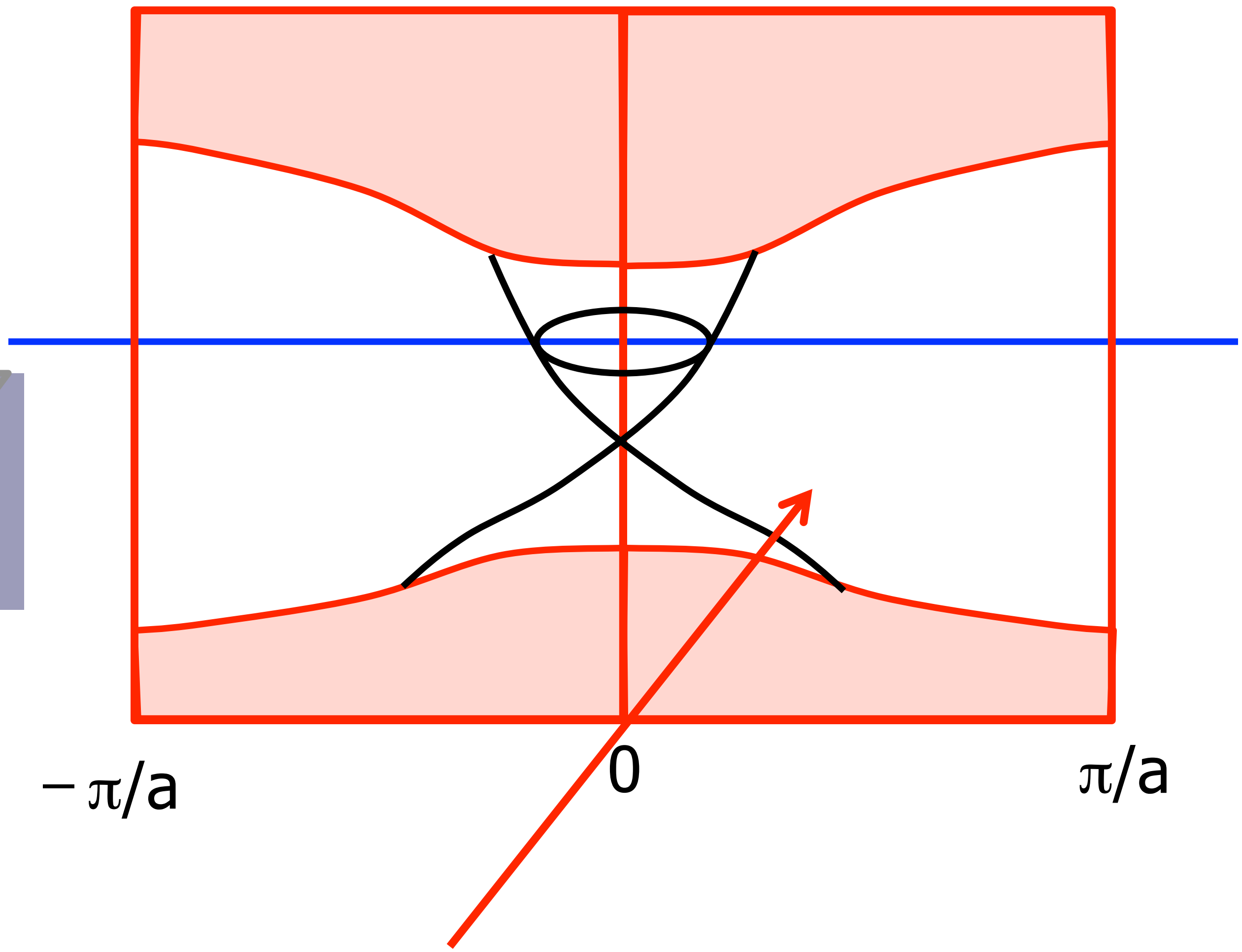
3D strong topological insulator (STI)



Inversion of spin-orbit labels at just one of (or at an odd number of) the 8 *T*-invariant points in k-space

3D strong topological insulator (STI)





3D strong topological insulator

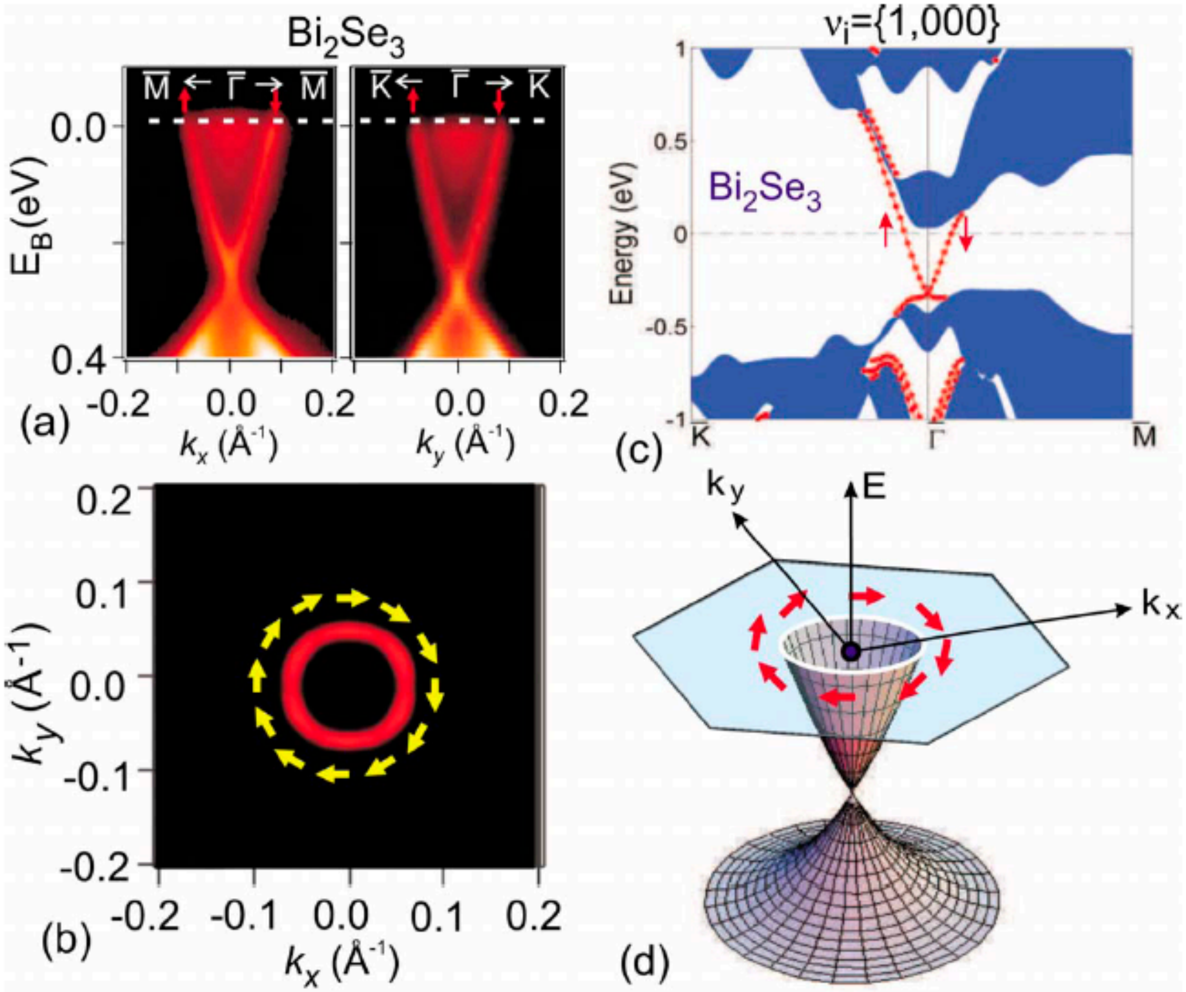


Figure from Hasan and Kane, RMP, 2010
(Adapted from Xia et al., 2008; Hsieh, Xia, Qian, Wray, et al., 2009a; and Xia, Qian, Hsieh, Wray, et al., 2009)

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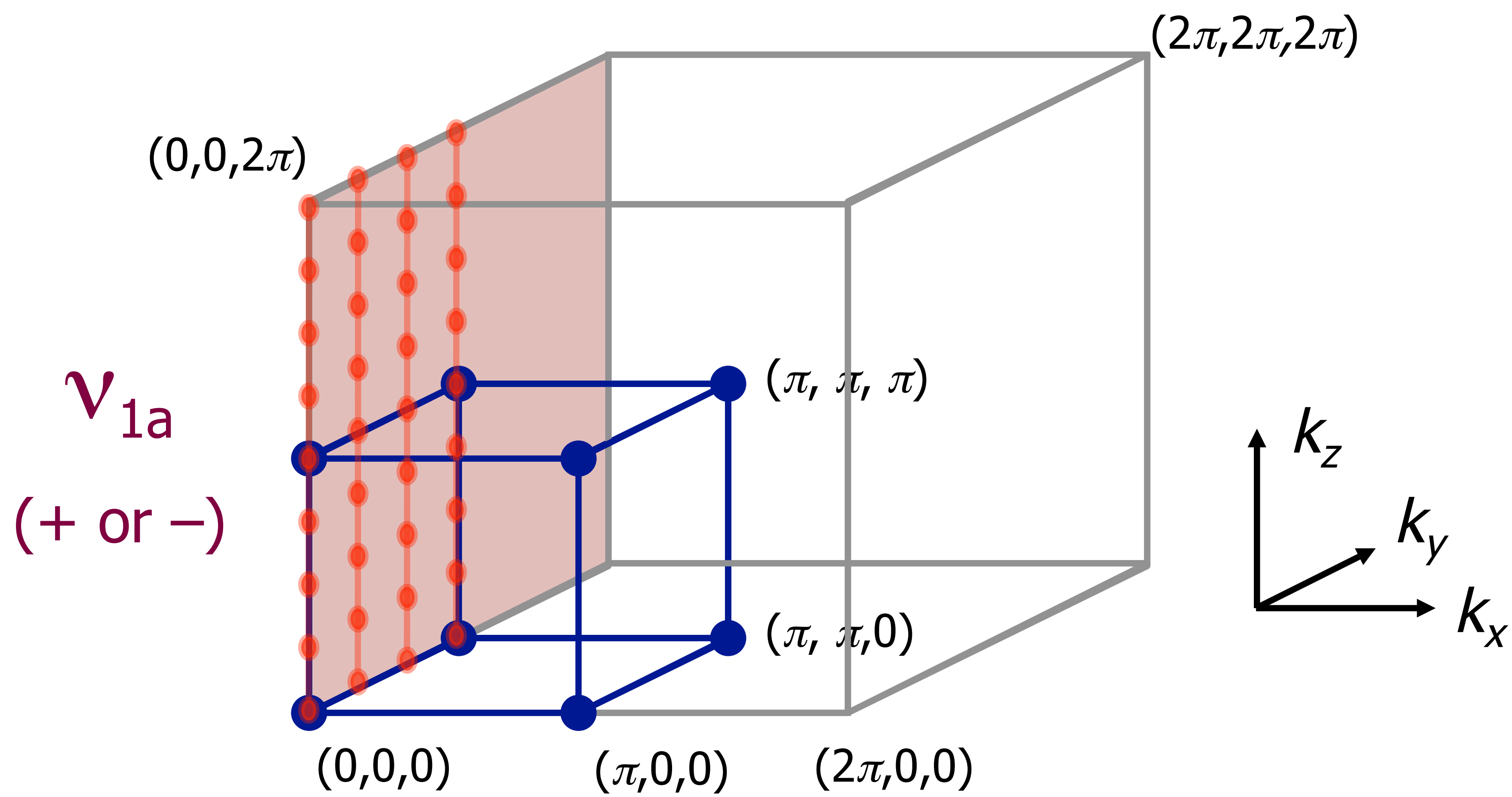
Surface vs. bulk indicator?

- Counting surface Dirac cones is a surface indicator
- Can we find a bulk indicator that works in a similar way?
- Yes! Wannier centers again!

3D Brillouin zone of TR-invariant ins.



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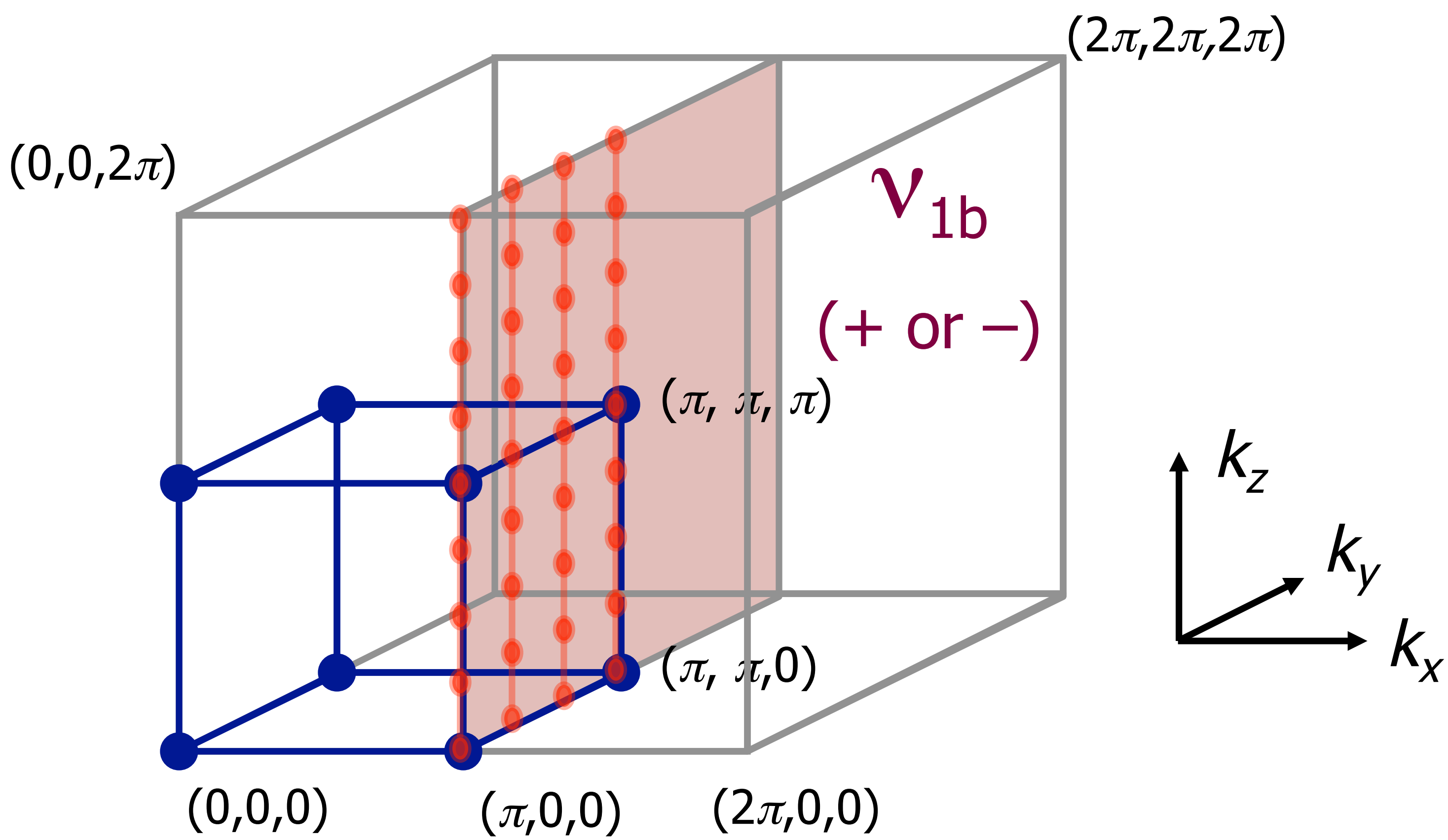
3D Brillouin zone of TR-invariant ins.



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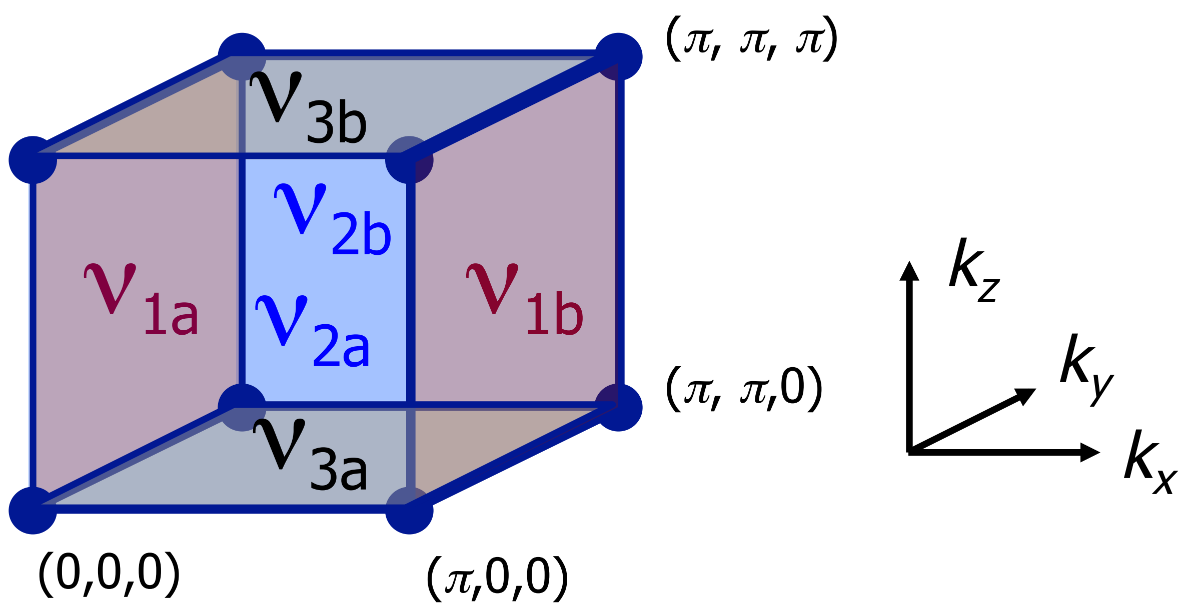
3D Brillouin zone of TR-invariant ins.



6 independent Z_2 indices? No, only 4…

(Moore and Balents , 2007)

3D TR-invariant insulators

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

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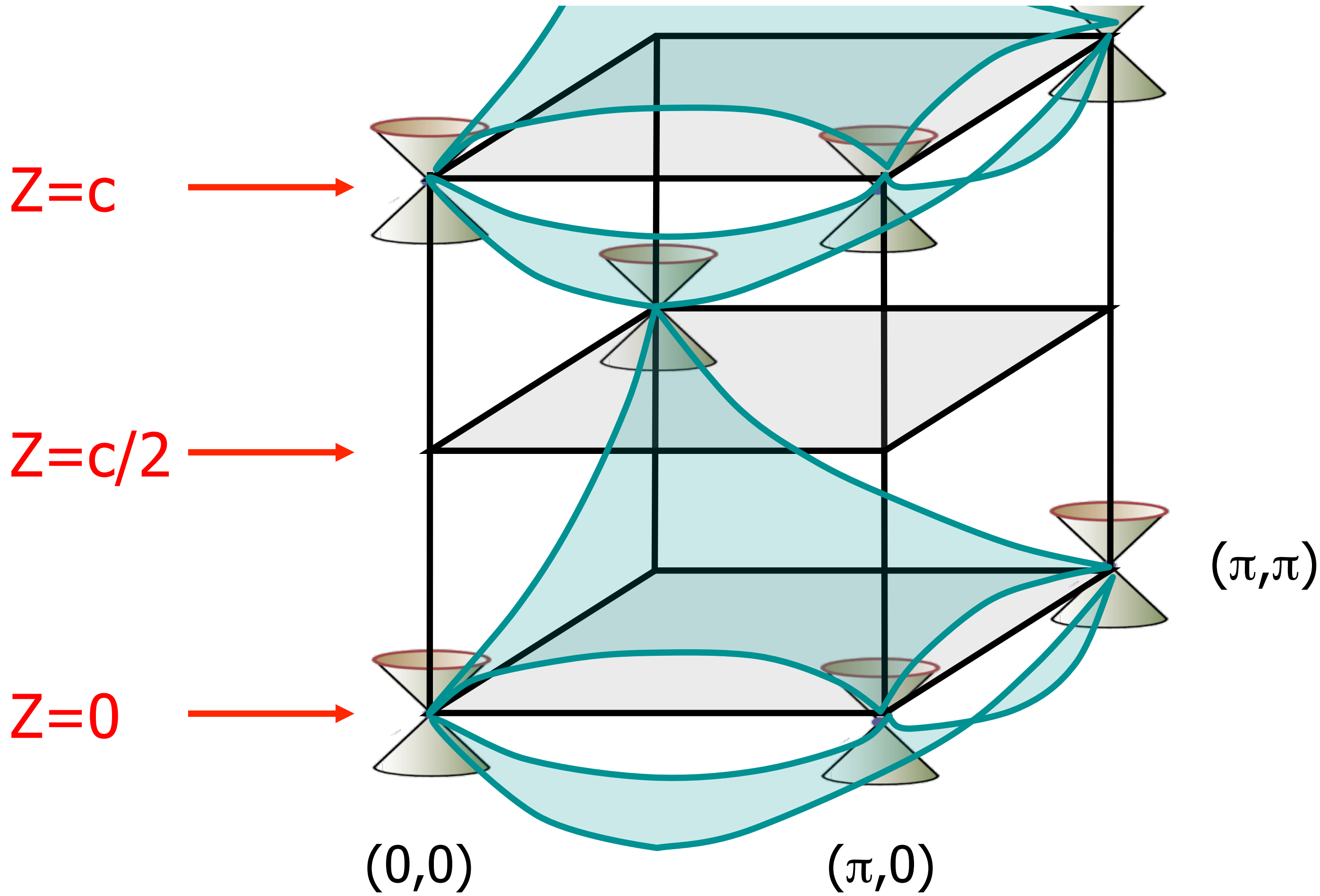
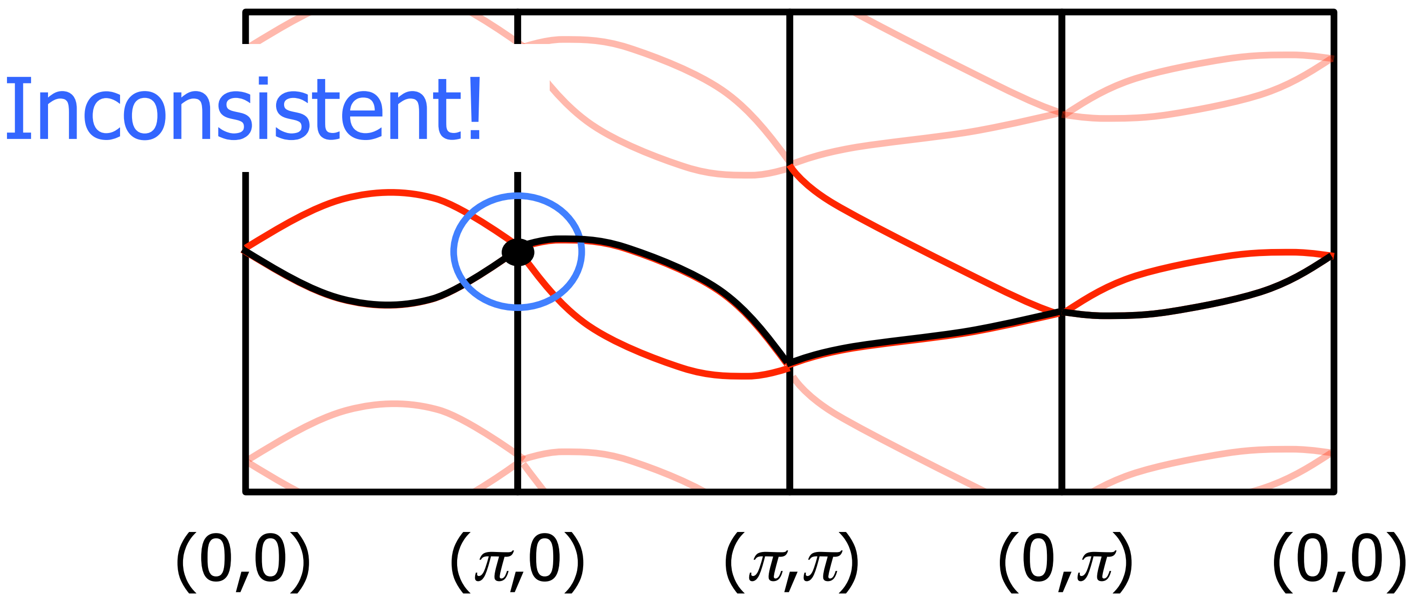
Sheet structure of Strong TI

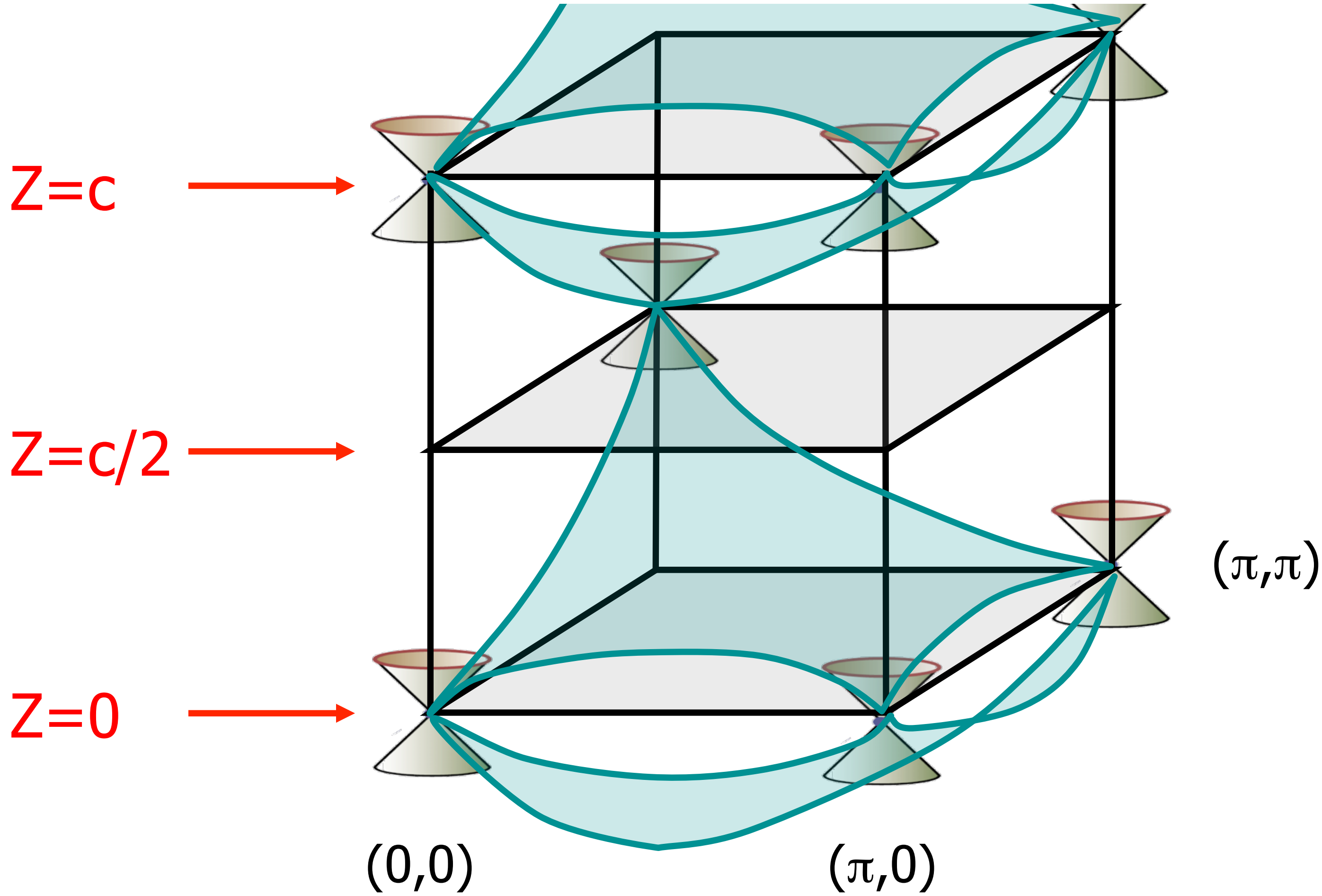


Moore-Balents rule



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

Sheet structure of Strong TI



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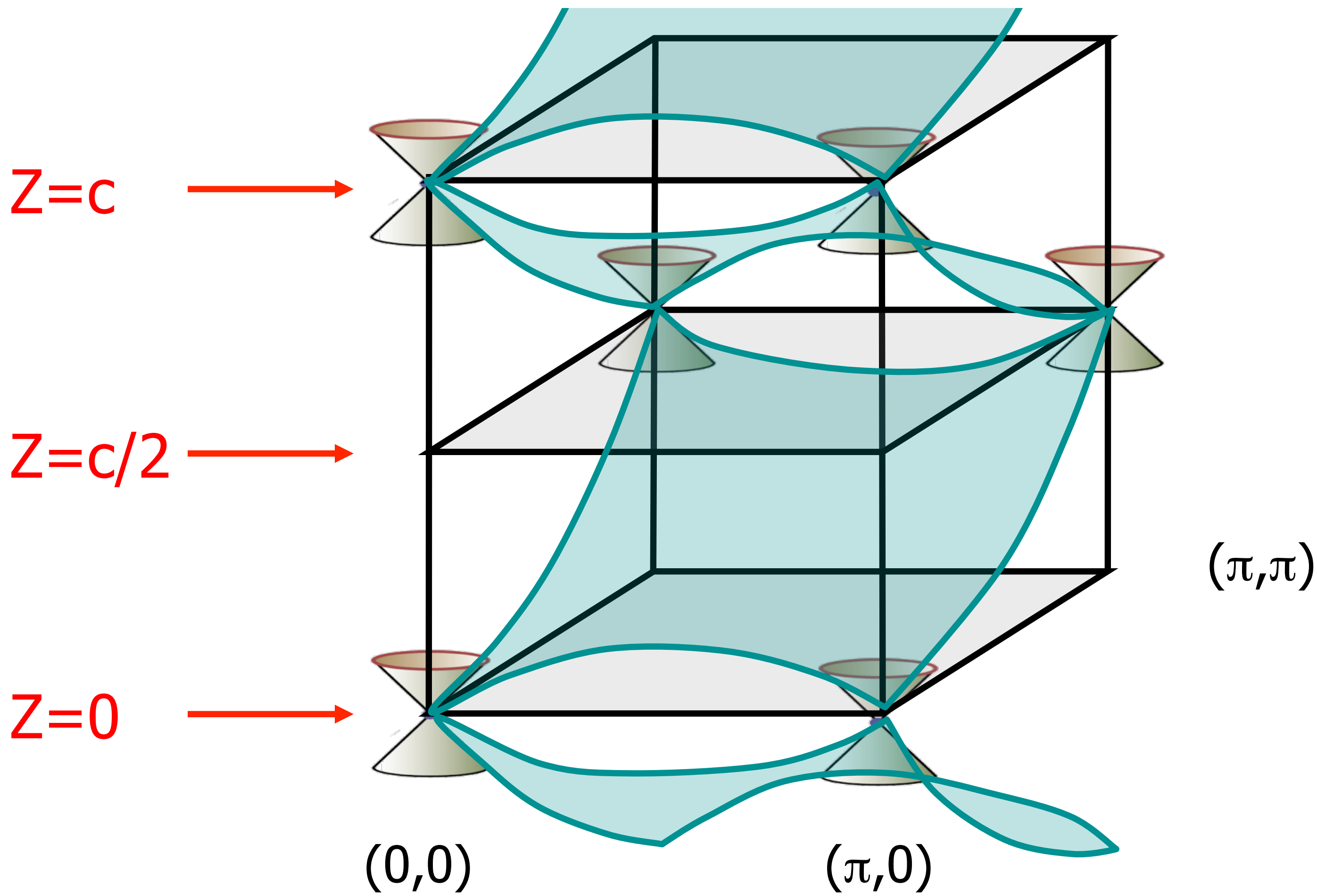
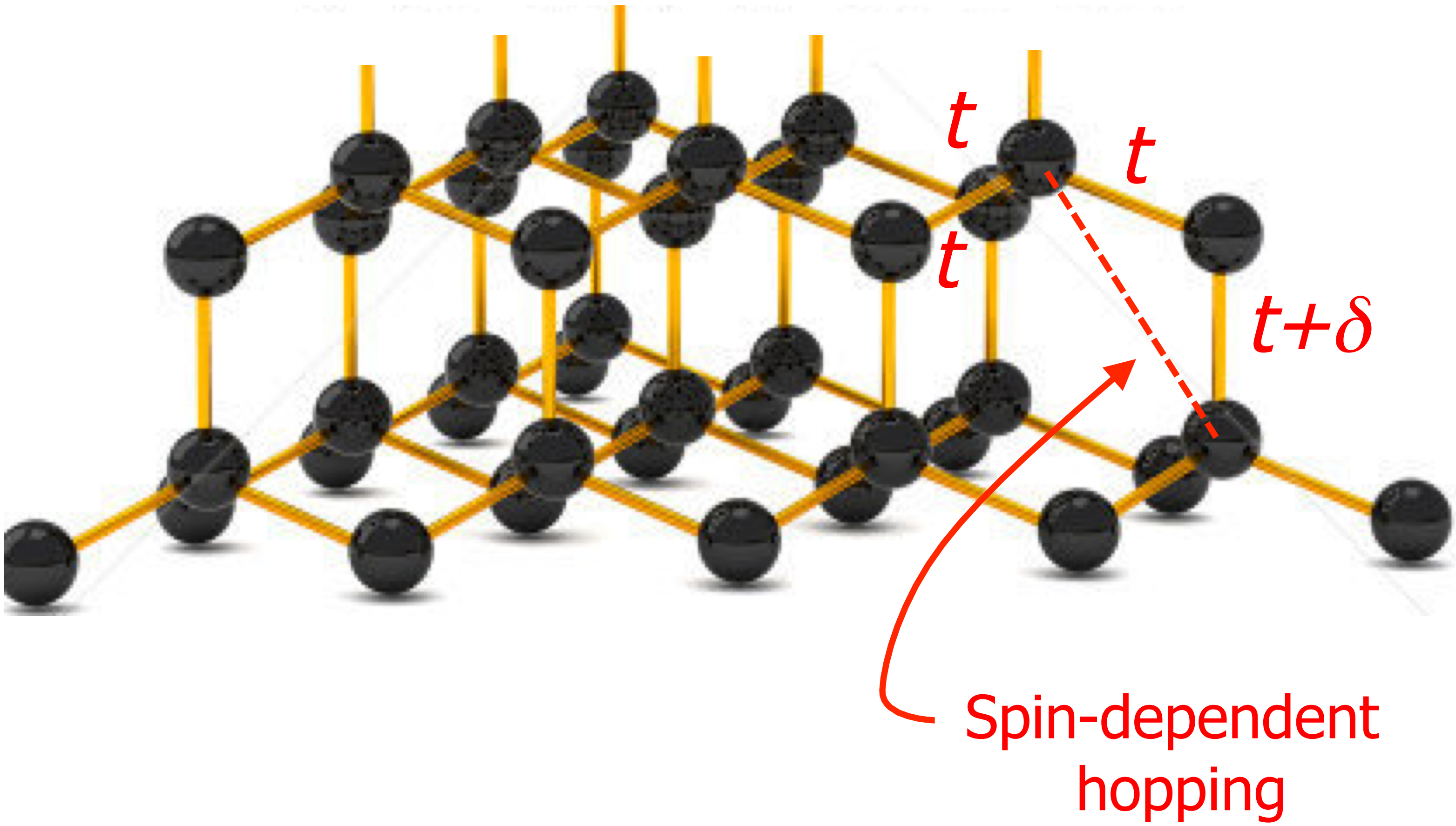
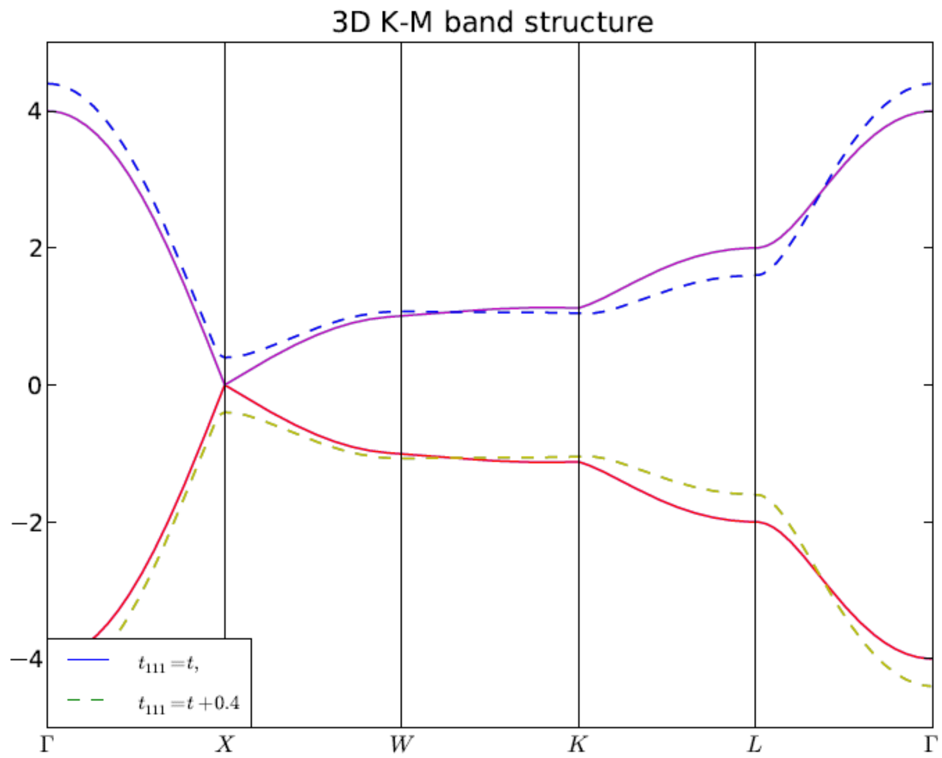
Sheet structure of Weak TI

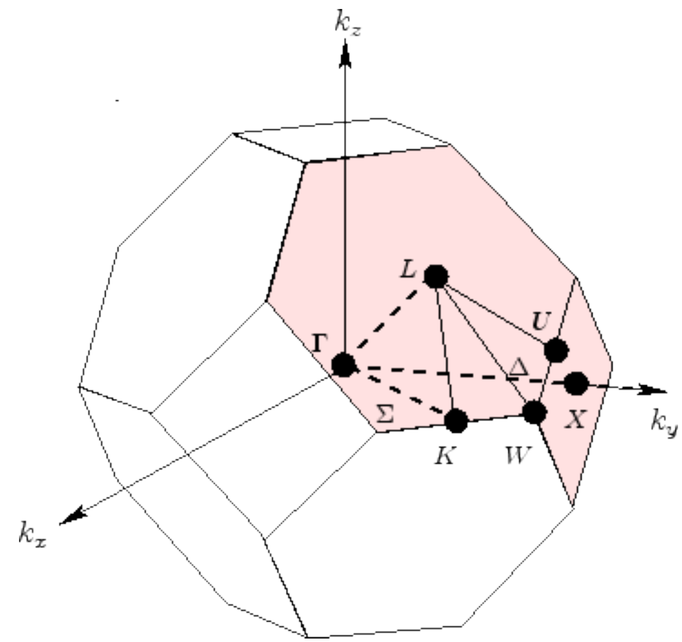


3D Kane-Mele model

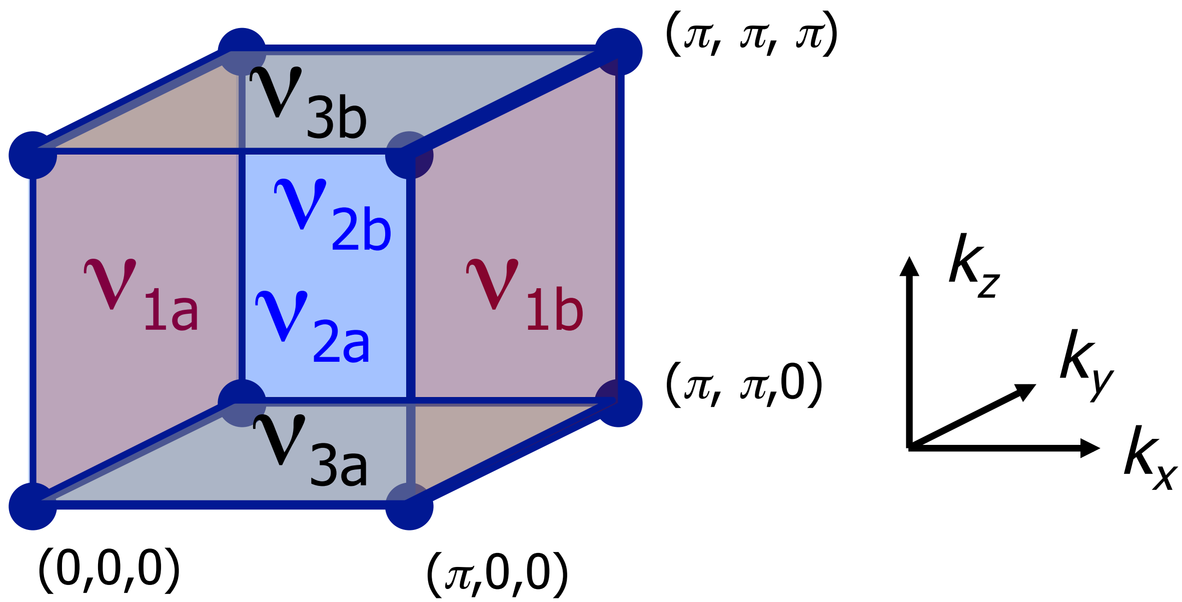


3D Kane-Mele model





3D Brillouin zone of TR-invariant ins.

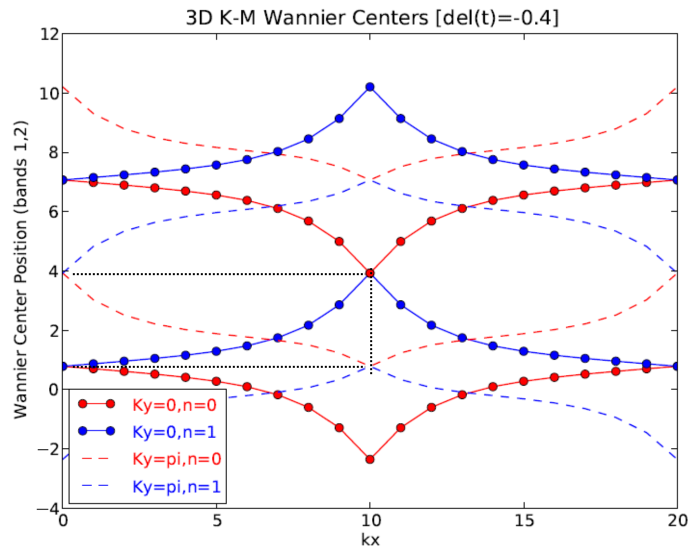


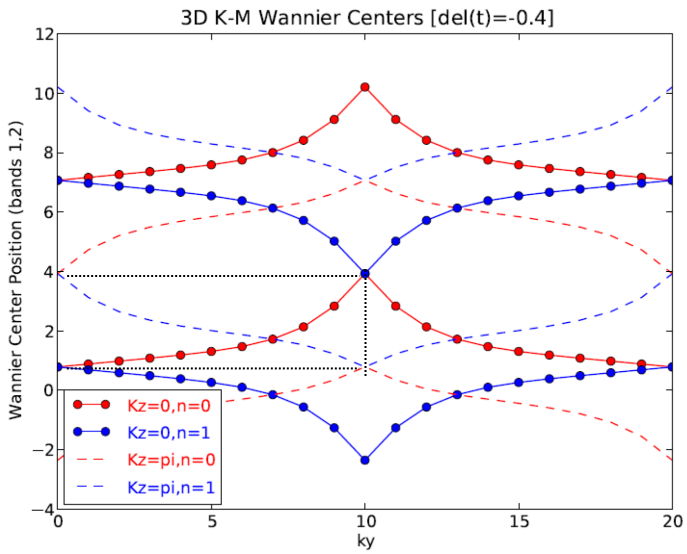
3D Kane-Mele model

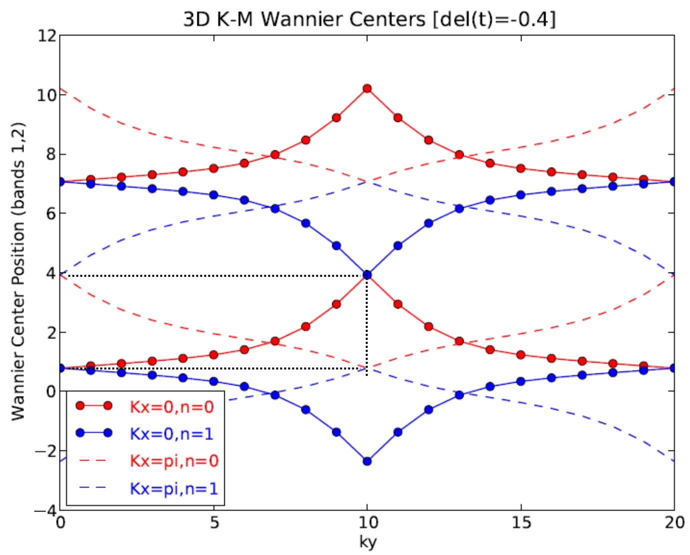
$\nu_0 = (+)$

$\nu_{1b} = \nu_{2b} = \nu_{3b} = (-)$

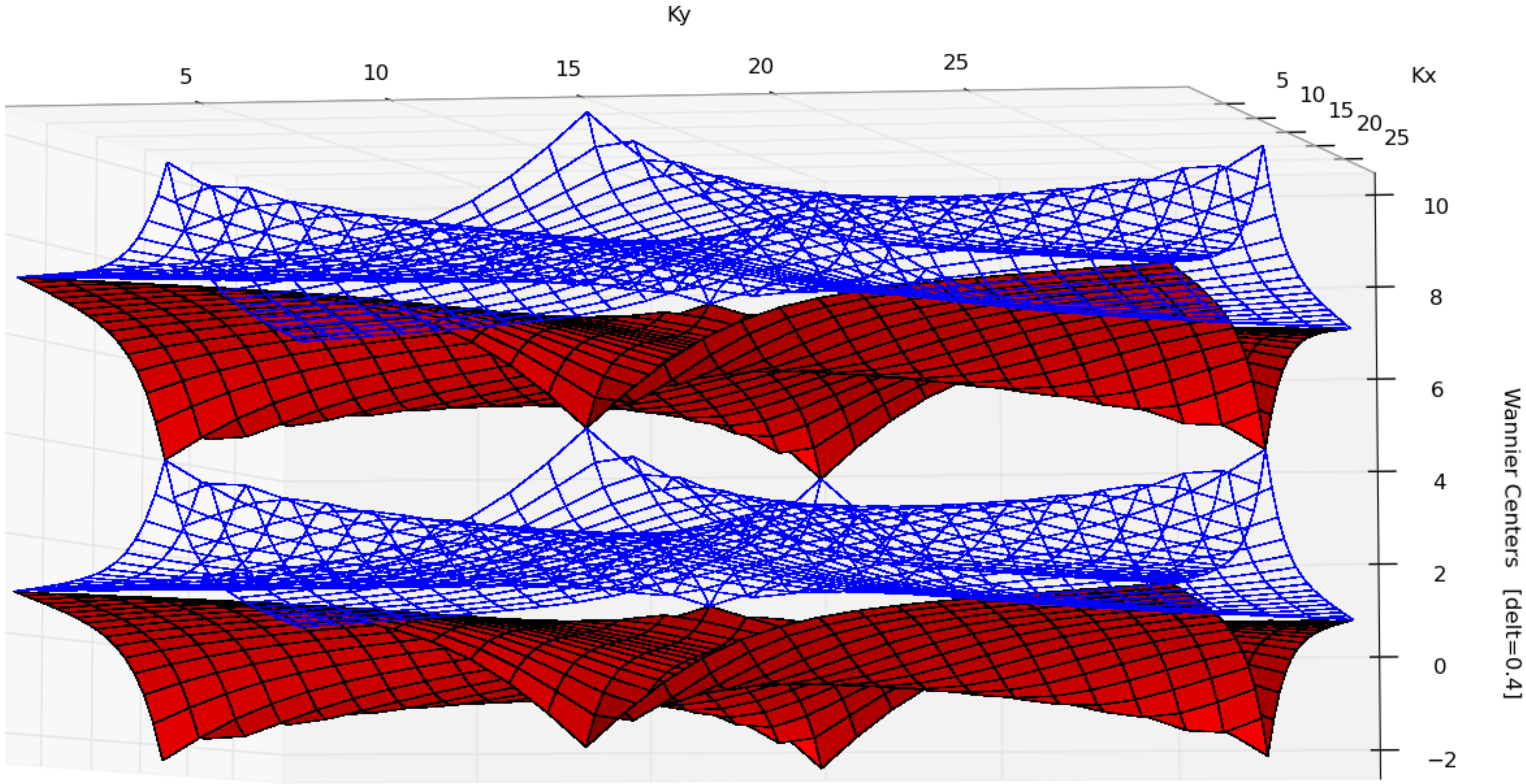
Weak topo ins!







3D Kane-Mele model

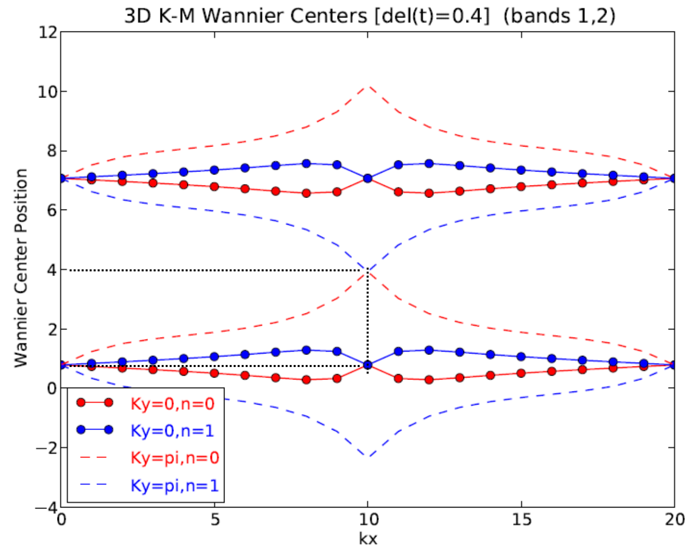


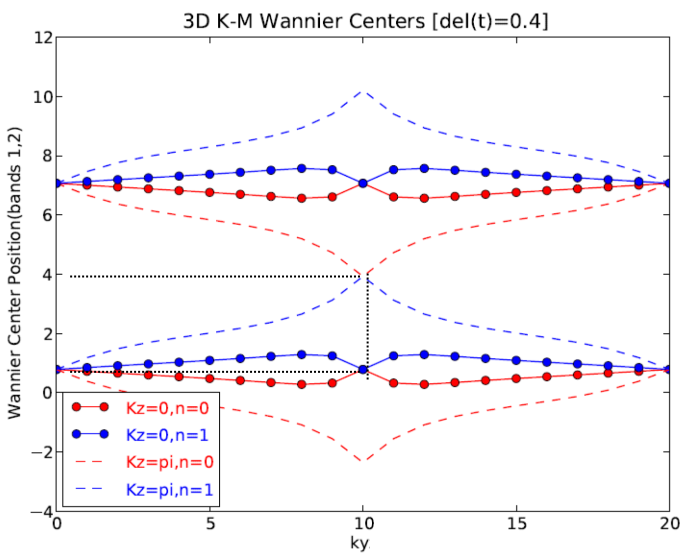
3D Kane-Mele model

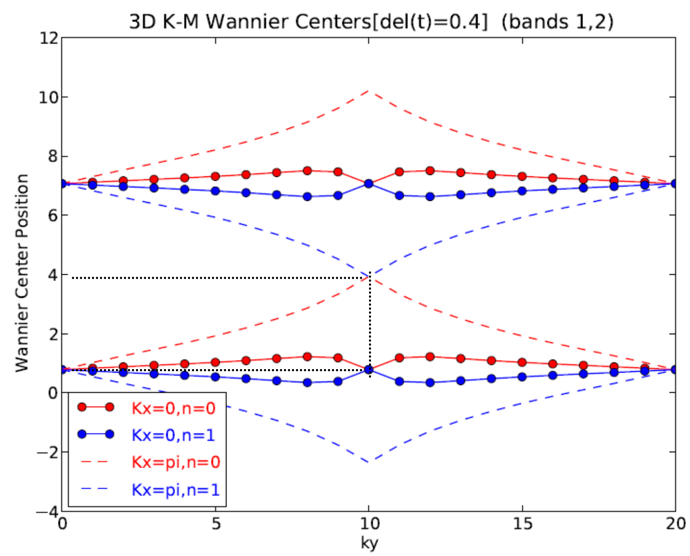
$\nu_0 = (-)$

$\nu_{1b} = \nu_{2b} = \nu_{3b} = (-)$

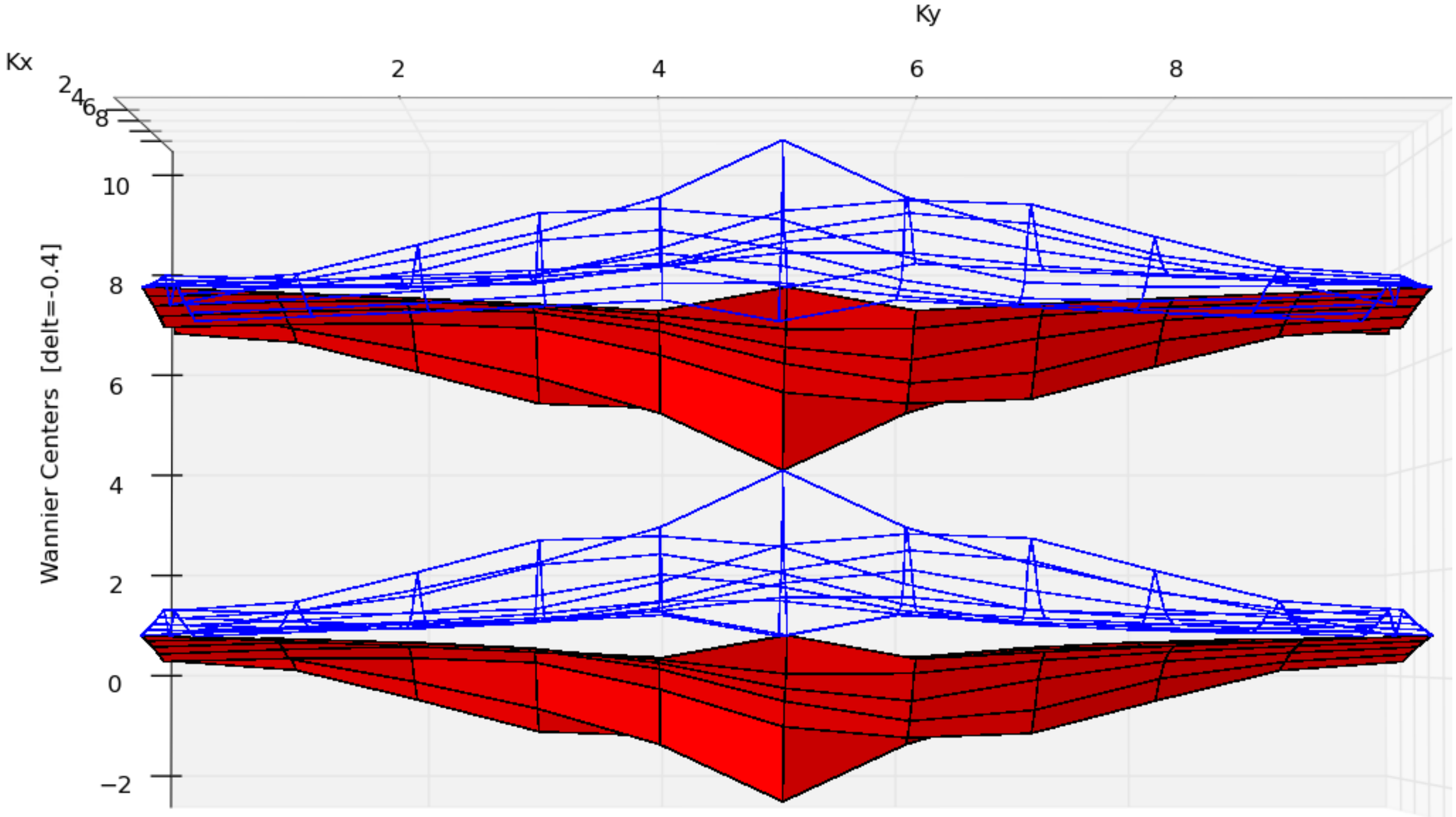
Strong topo ins!







3D Kane-Mele model



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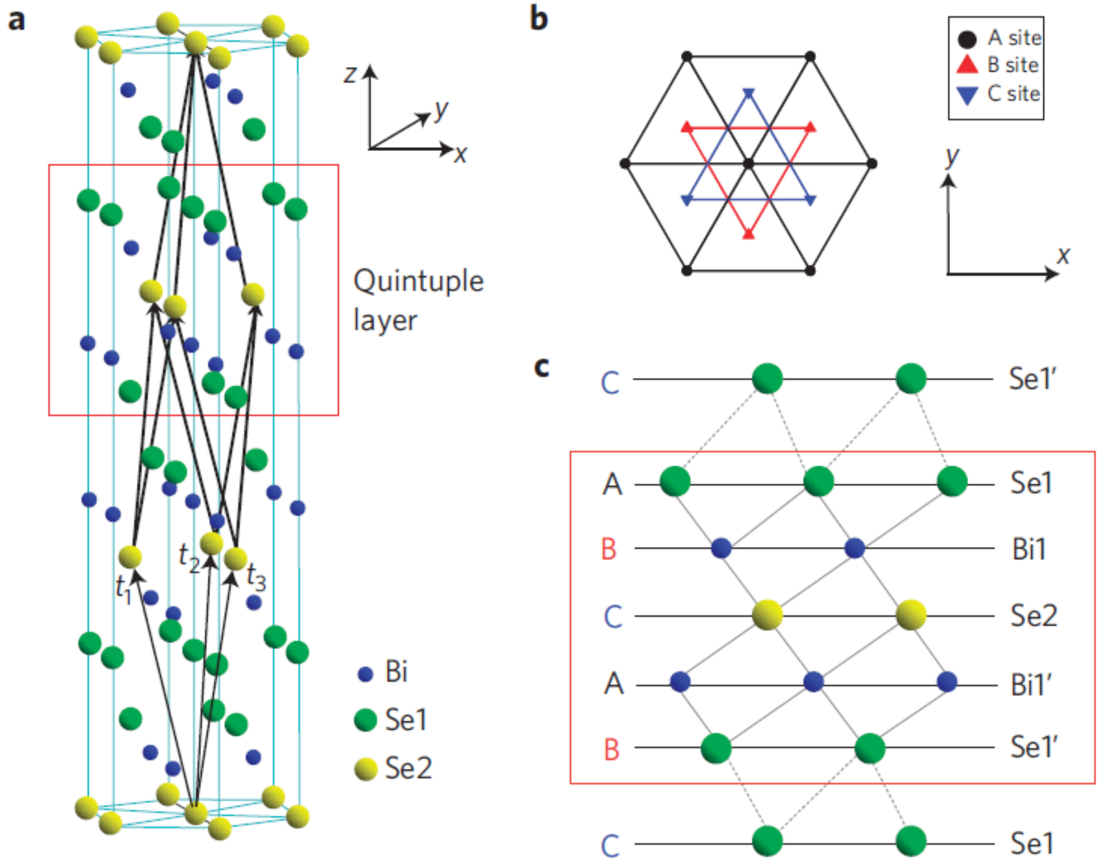
First-principles calculation: Bi_2Se_3



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

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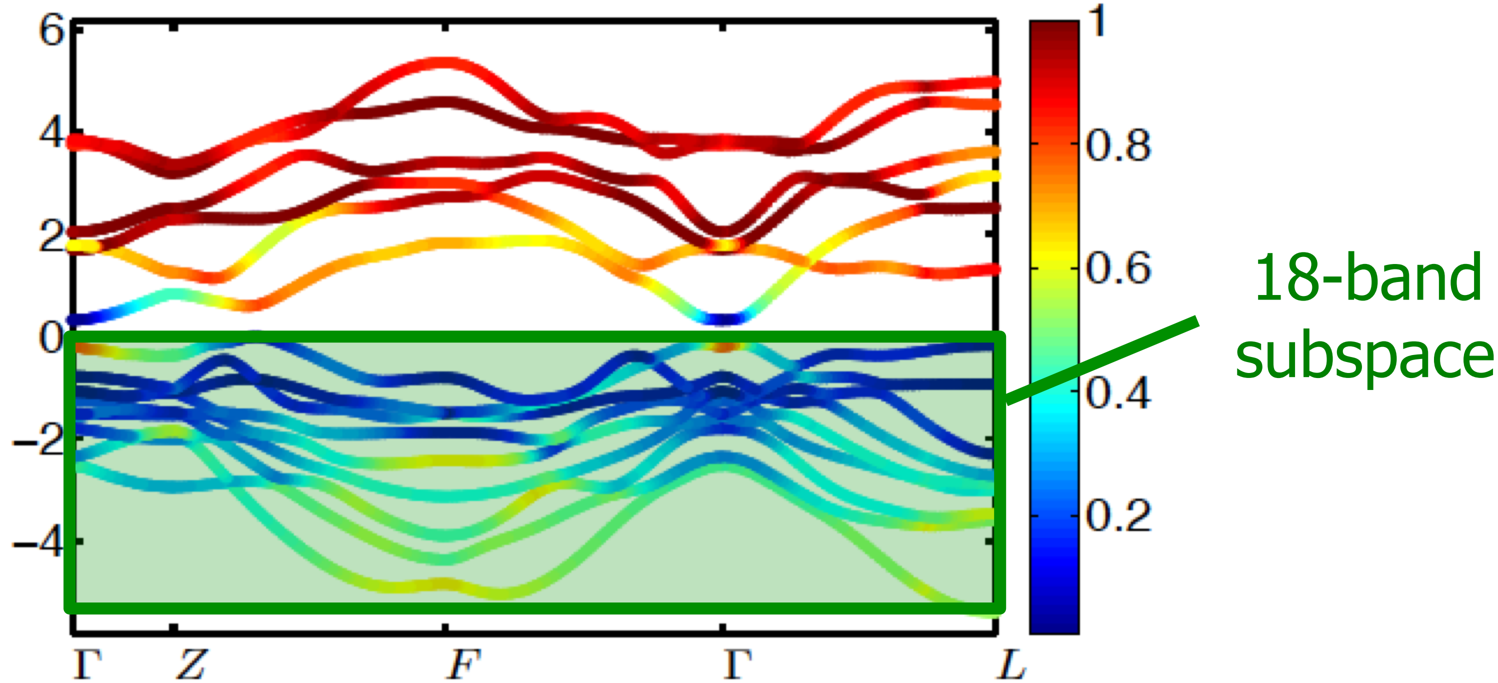
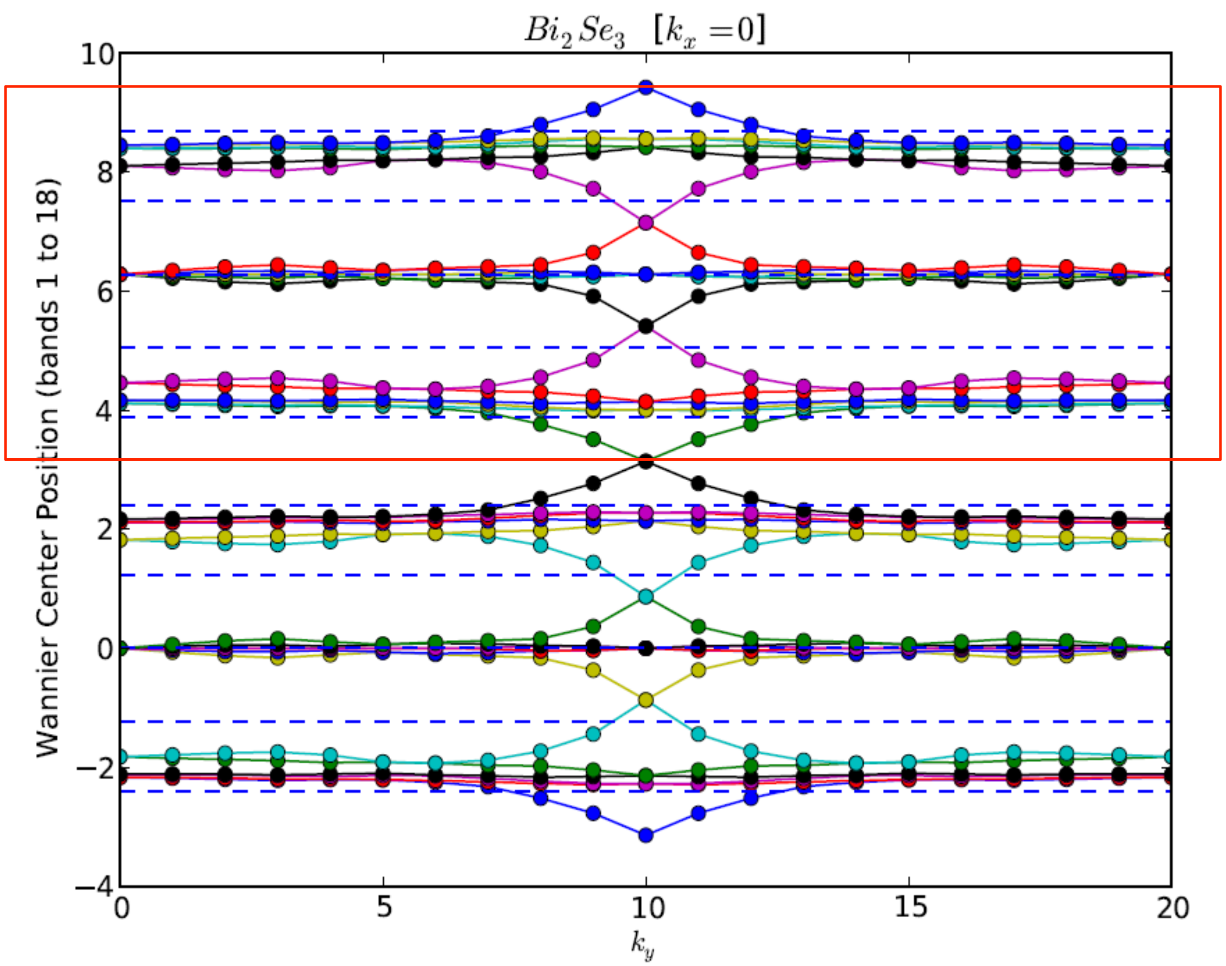
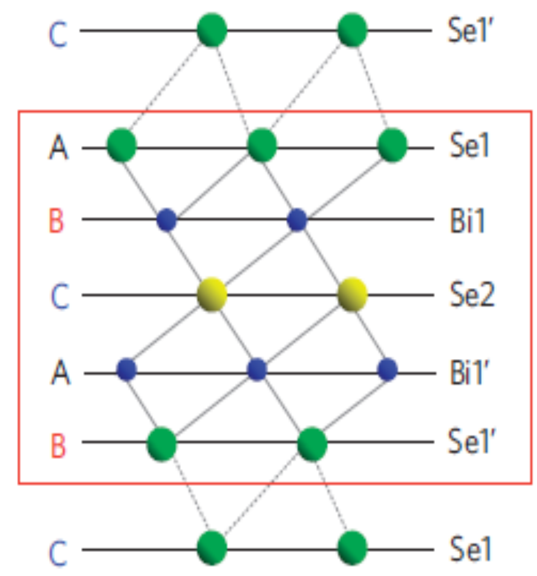
First-principles calculation: Bi_2Se_3



bulk bandstructure of Bi_2Se_3 projected onto Bi 6p orbitals

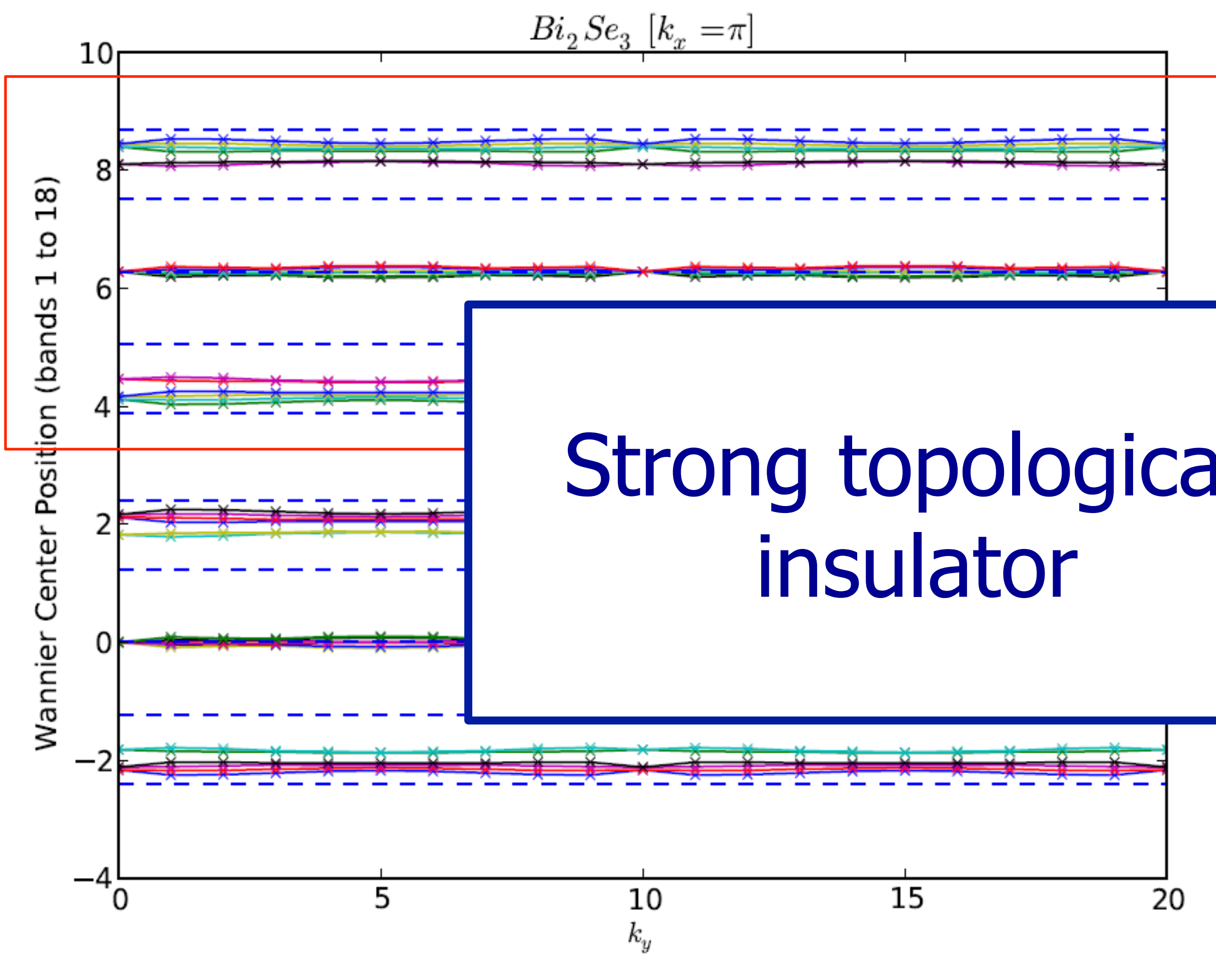
First-principles Bi_2Se_3 Wannier centers

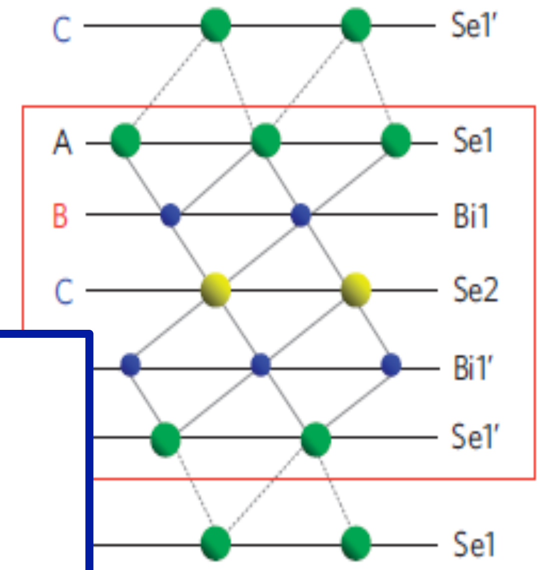




$$\nu_{1a} = \nu(k_x{=}0) = (-)$$

First-principles Bi_2Se_3 Wannier centers

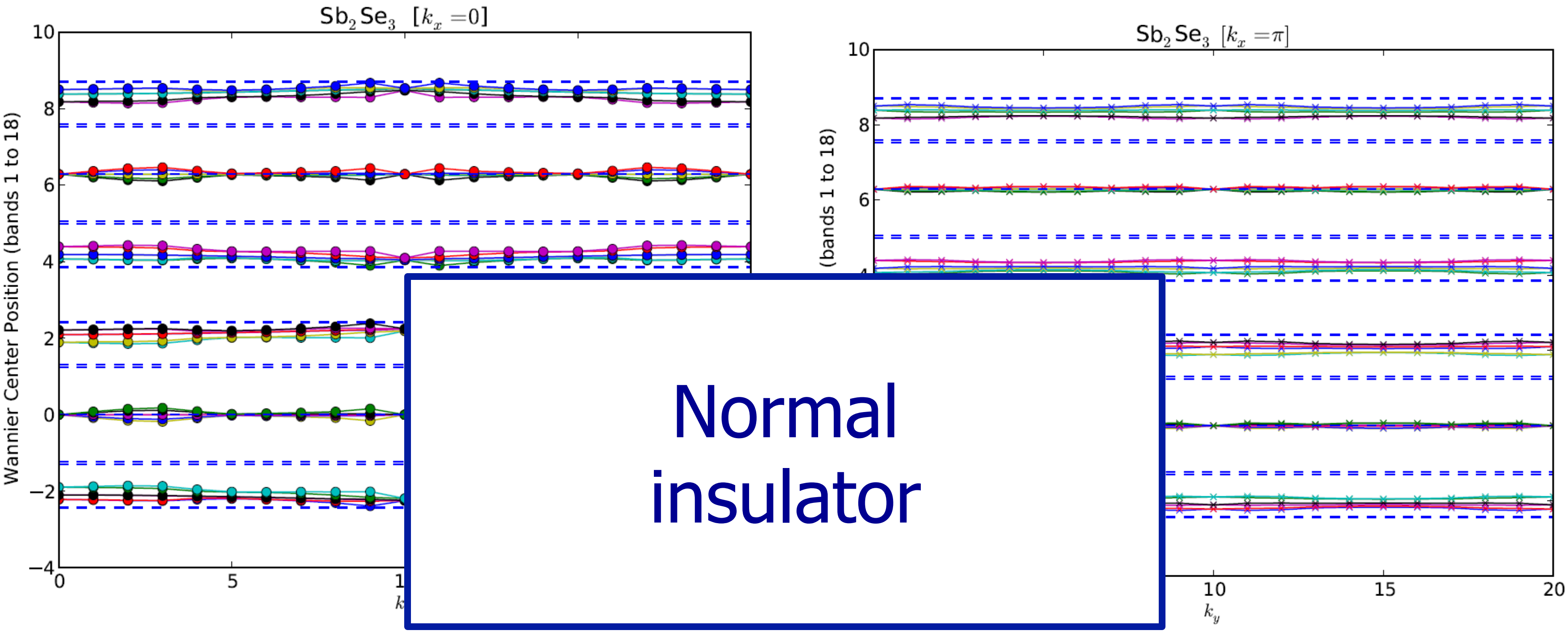




Strong topological insulator

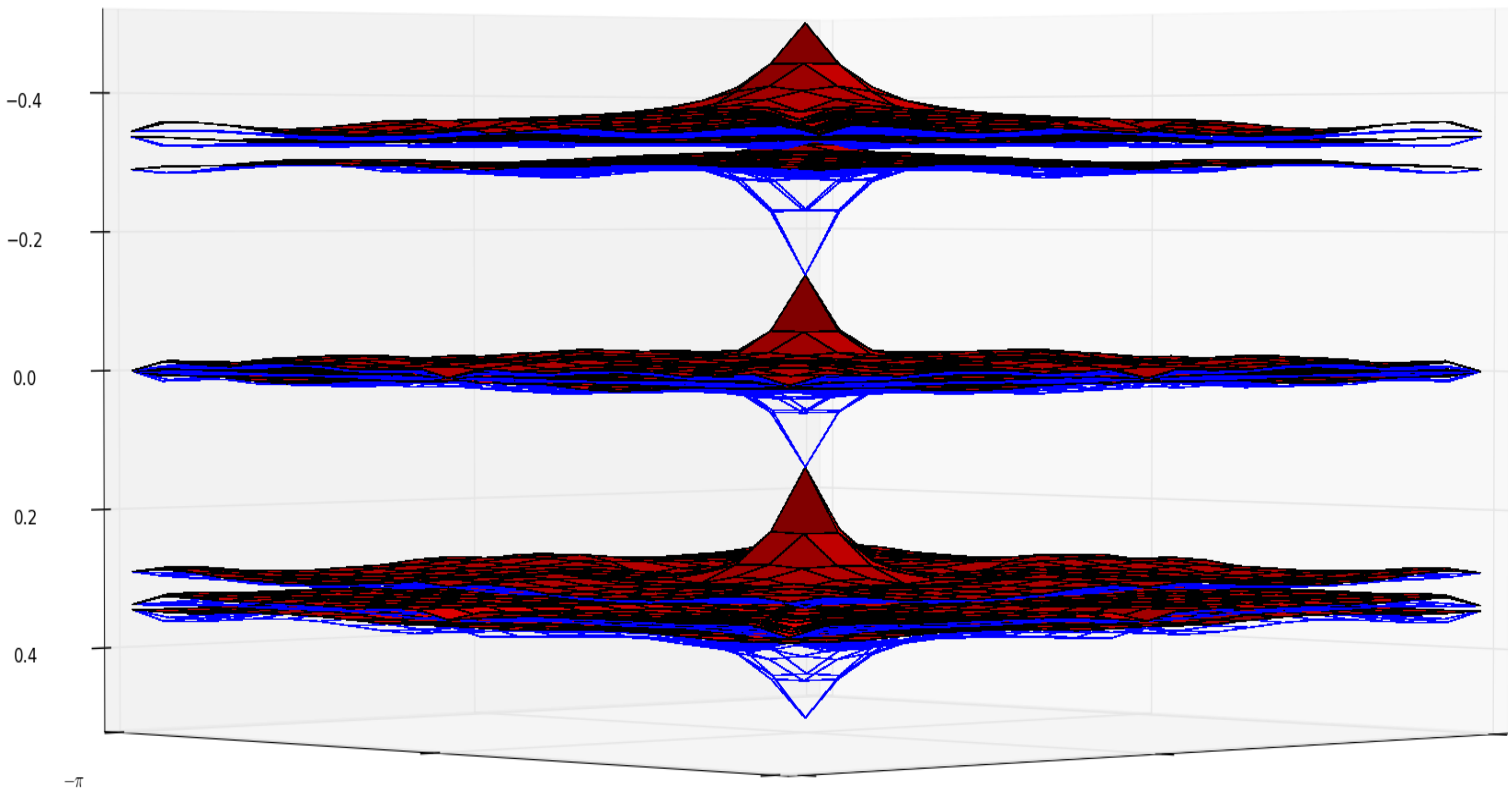
$$\nu_{1b} = \nu(k_x=\pi) = (+)$$

First-principles Sb_2Se_3 Wannier centers

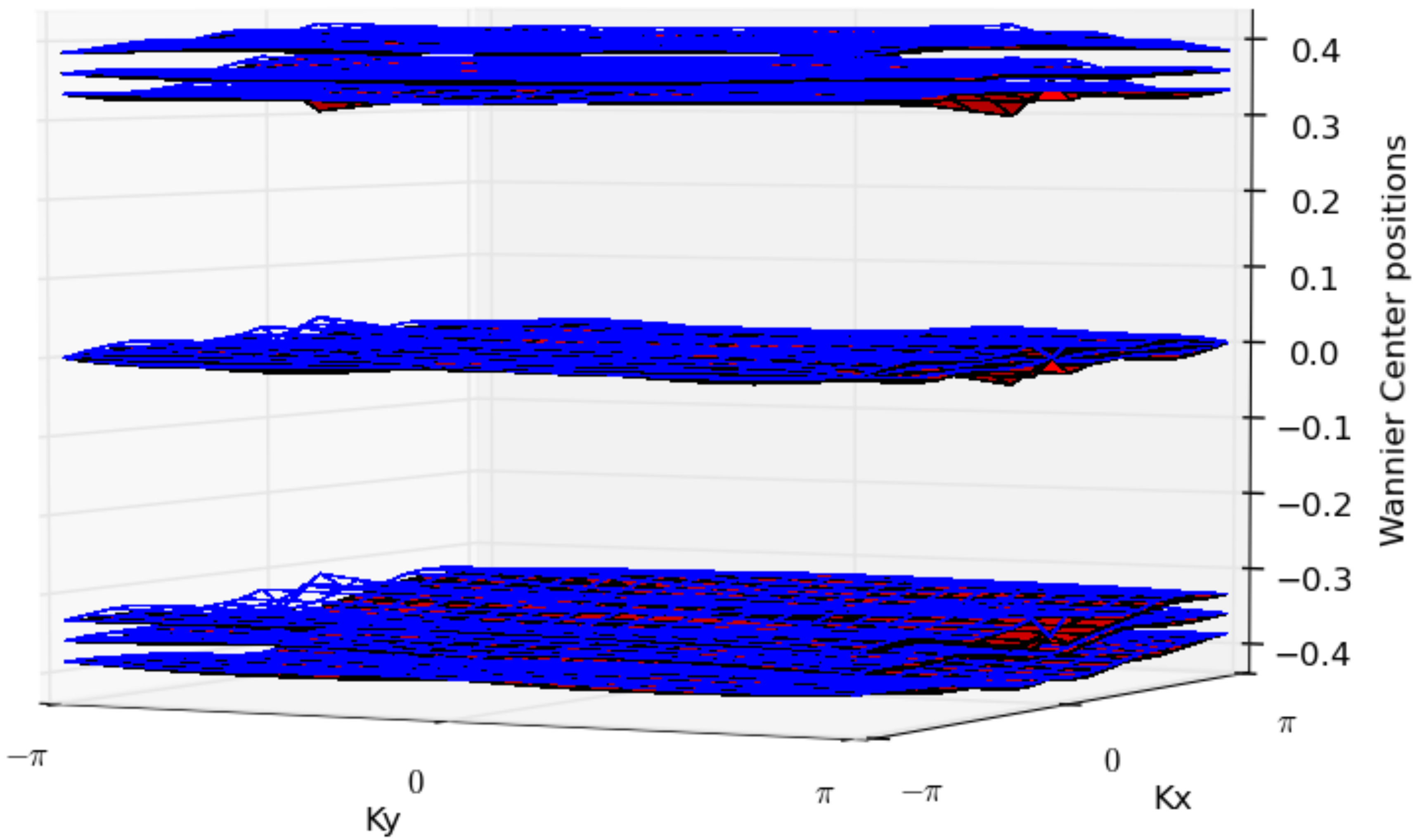


Normal insulator

First-principles Bi_2Se_3 Wannier centers



First-principles Sb_2Se_3 Wannier centers



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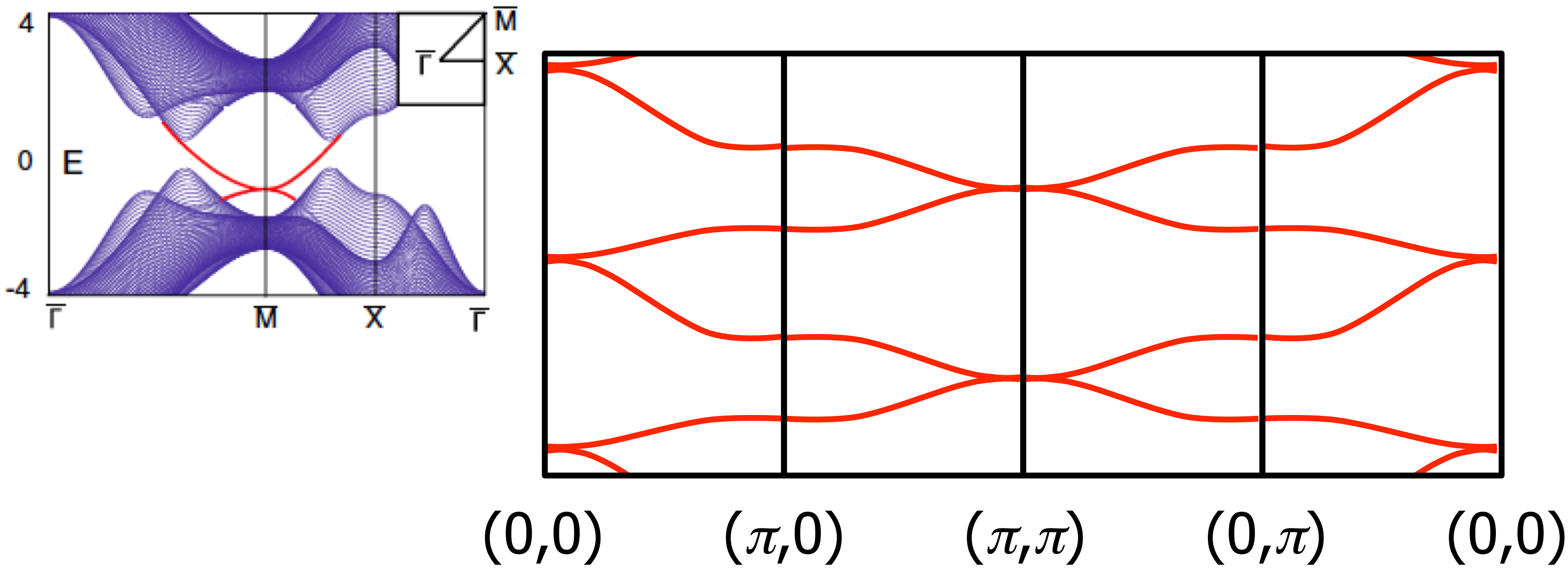
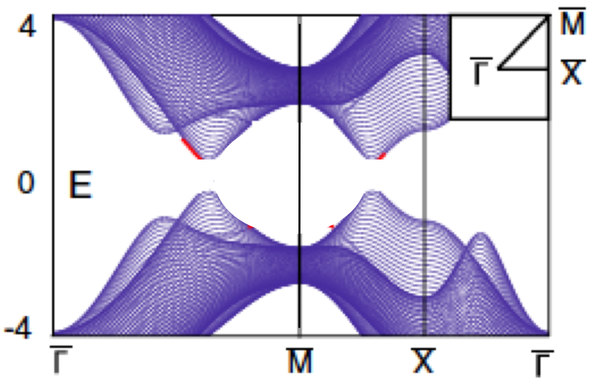
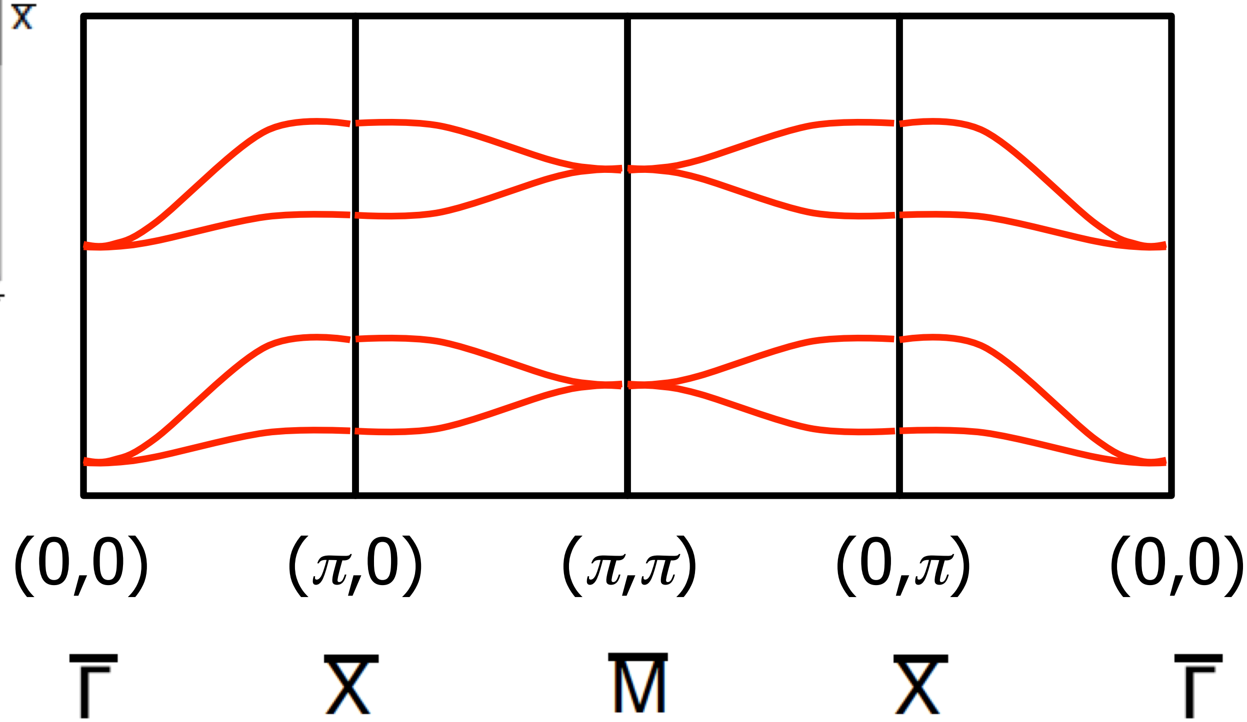
C_4 crystalline topological insulator?



C_4 normal insulator?





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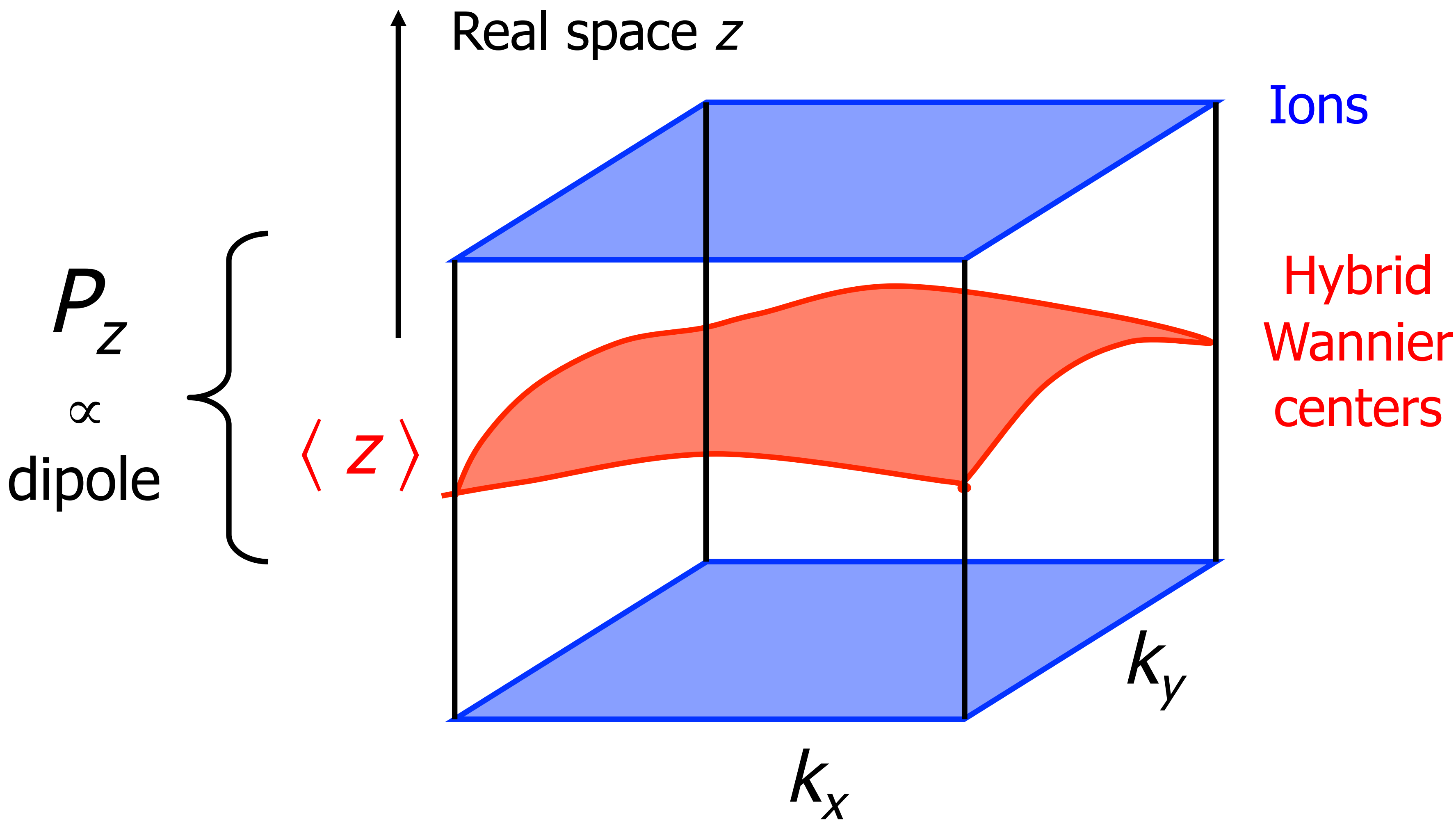
Polarization in 3D



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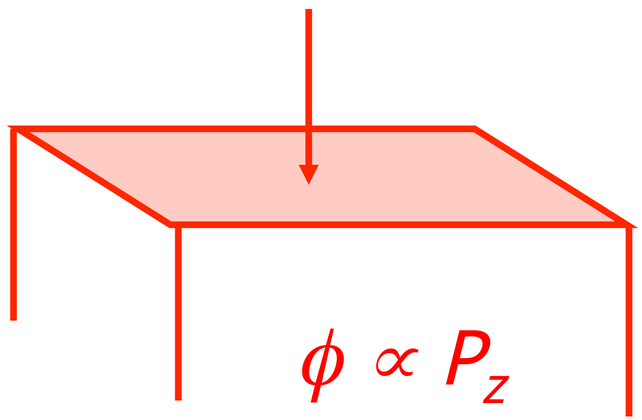
Insulating surface of bulk insulator

Surface charge

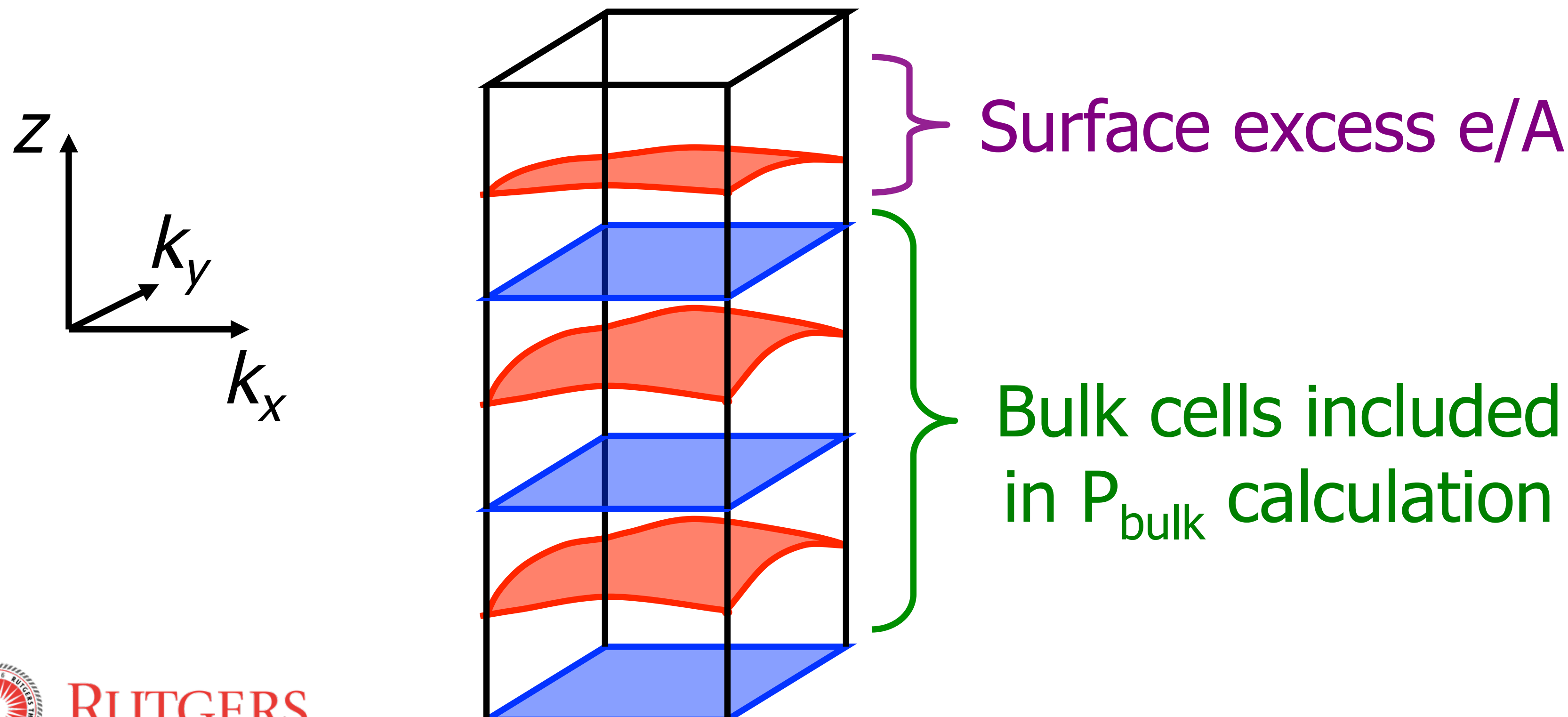
$$\boxed{\sigma = \frac{-e}{A}\left[\frac{\phi}{2\pi} + \text{integer}\right]}$$



ϕ is ill-defined
modulo 2π

Hybrid Wannier centers at surface

- Diagonalize $\mathcal{P} z \mathcal{P}$ at each (k_x,k_y)
- Plot these "sheets" at surface and into bulk



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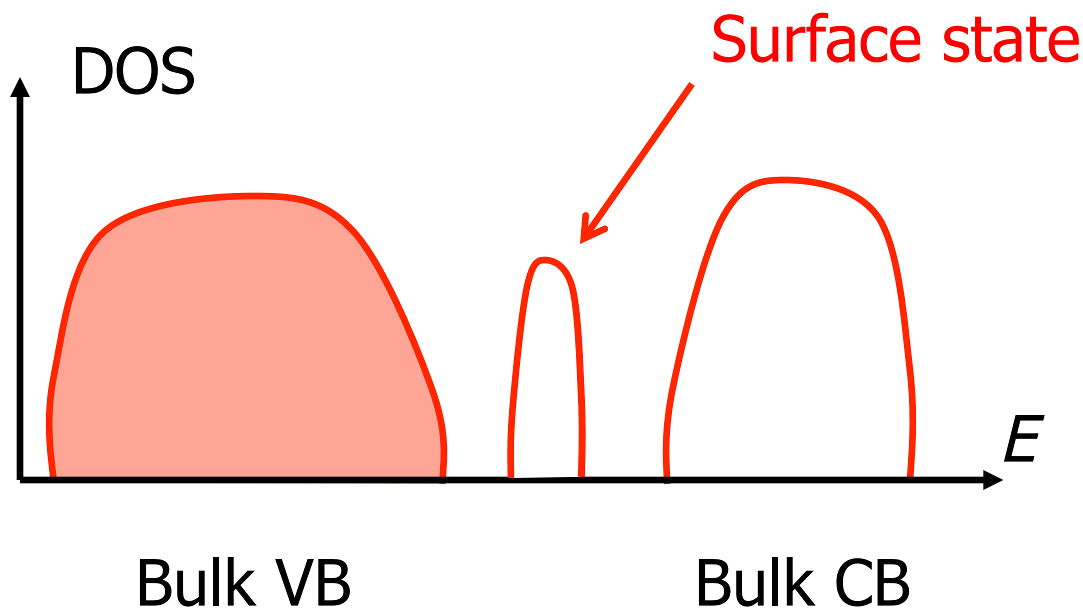

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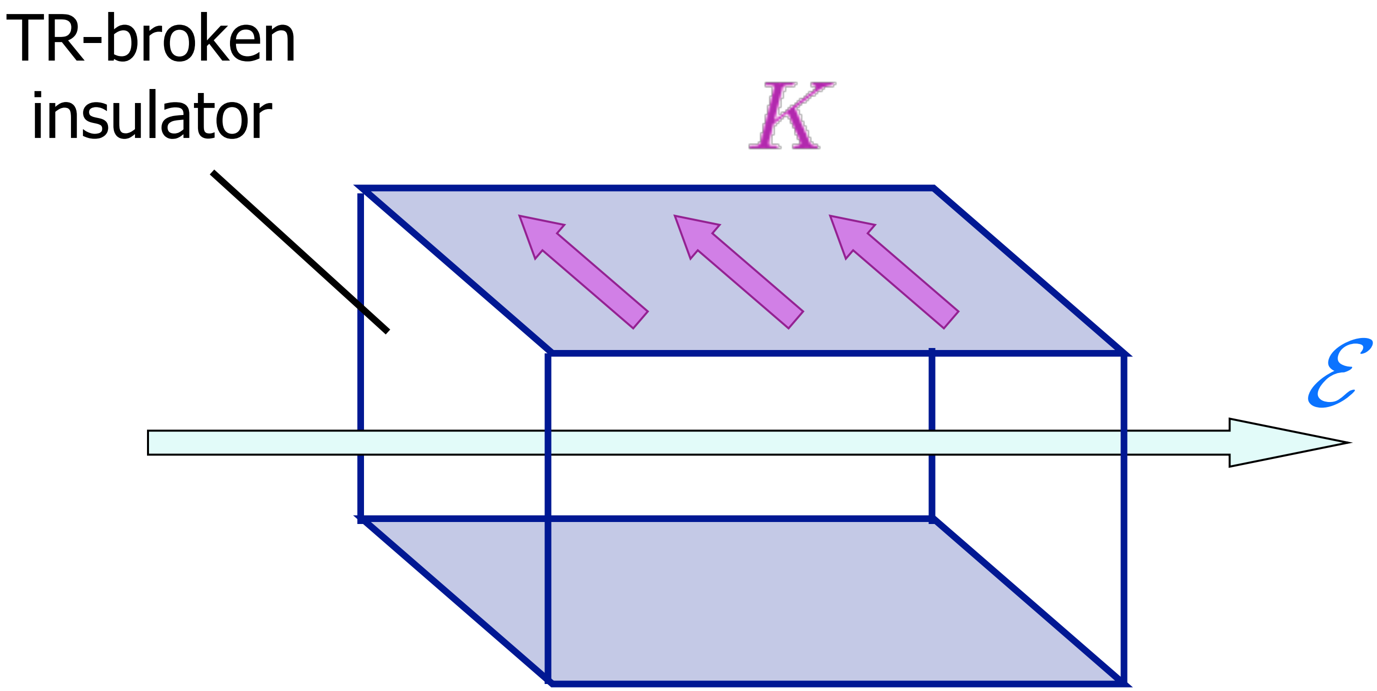
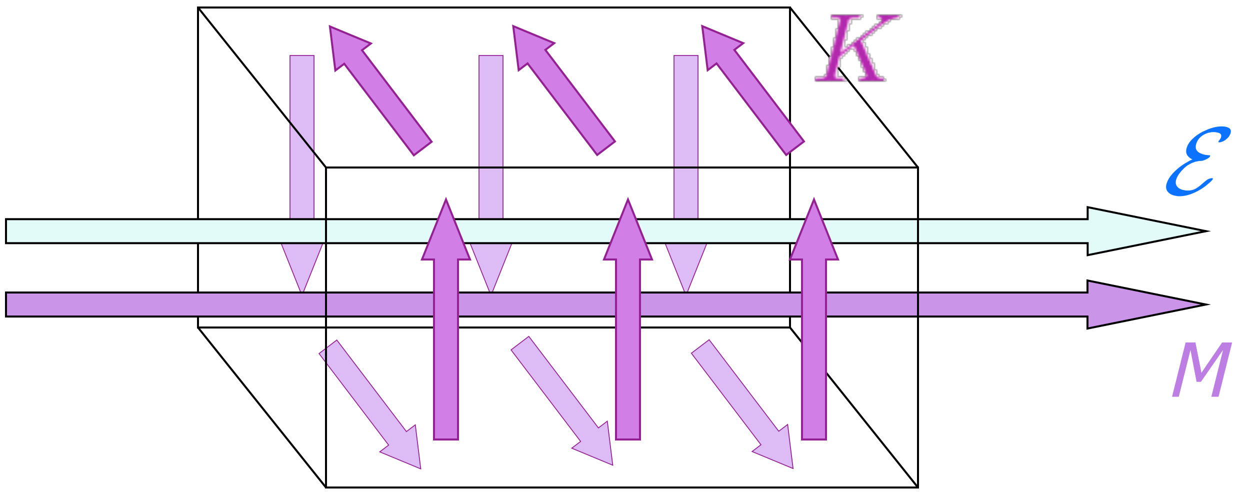
Surface AHC



... in absence of magnetic field

Orbital MEC ↔ Surface dissipationless σ_{xy}



Interpret magnetization $= M = K$

$$\mathbf{K} = \sigma_{\mathbf{xy}}\, \vec{\mathcal{E}} \times \hat{\mathbf{n}}$$

$$\boxed{\sigma_{xy}^{\mathrm{surf}} = \alpha^{\mathrm{CS}} = \frac{e^2}{h}\frac{\theta}{2\pi}}$$

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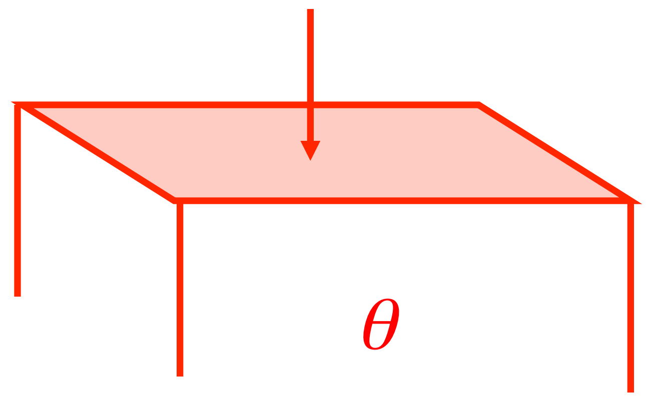
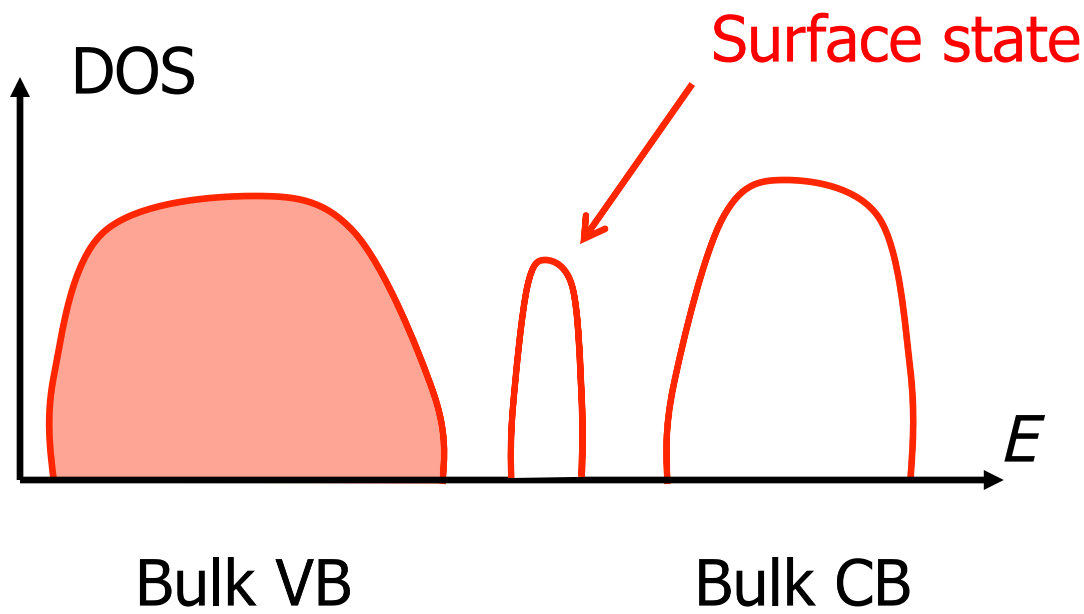
Insulating surface of bulk insulator

Surface anomalous Hall conductivity

$$\sigma^{\mathrm{AH}} = \frac{e^2}{h}\left[\frac{\theta}{2\pi} + \text{int}\right]$$

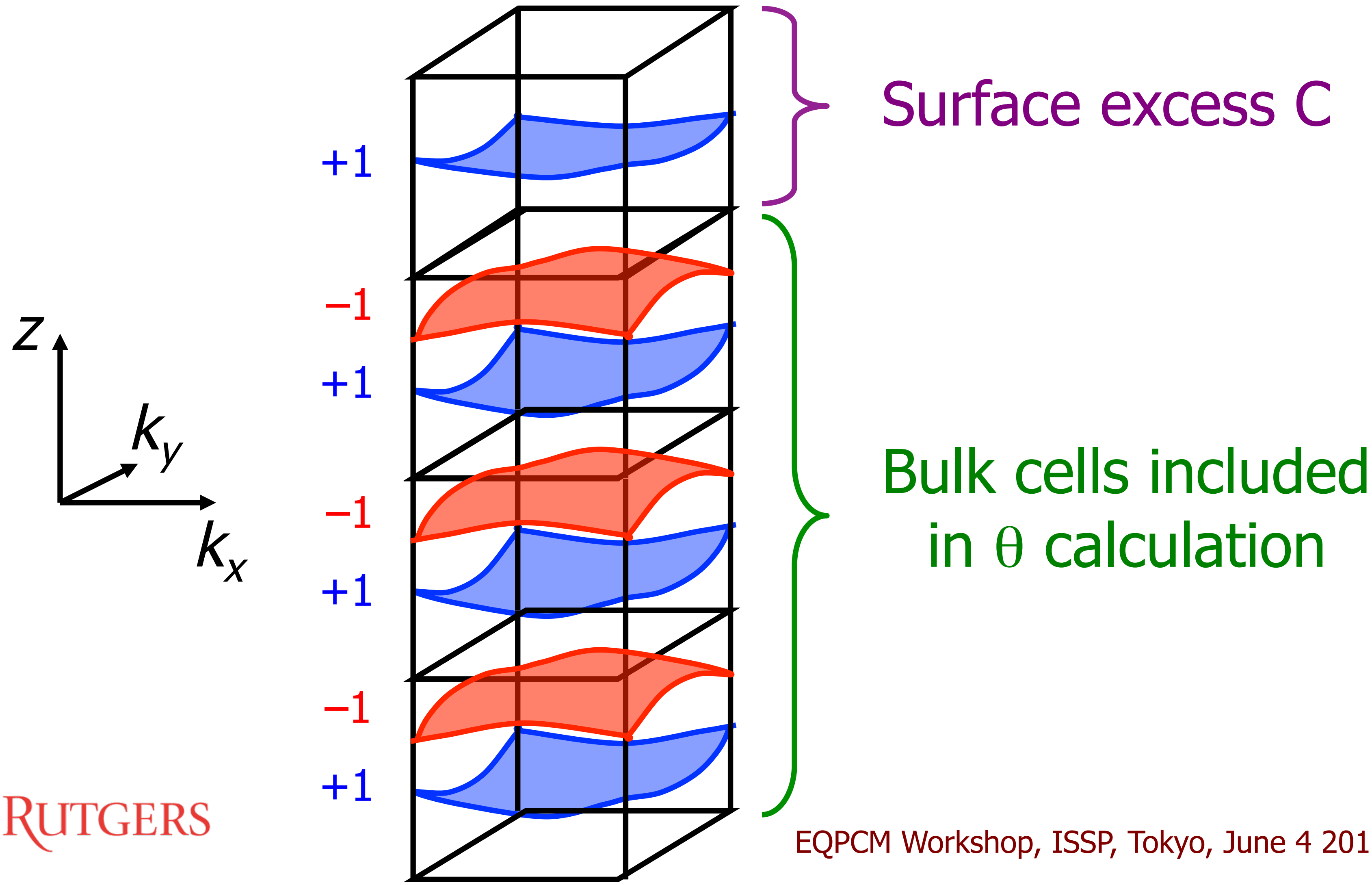


θ is ill-defined
modulo 2π


Surface state
DOS
E
Bulk VB
Bulk CB

Surface σ^{AH} (ins. surface of 3D bulk)

$$\sigma^{AH,surf} = (\theta/2\pi + C)\, e^2/h$$



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PythTB software package

Sinisa Coh

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PythTB

- About
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- Usage
- Resources

Quick search

Go

Enter search terms or a module, class or function name.

Python Tight Binding (PythTB)

PythTB is a software package providing a Python implementation of the tight-binding approximation. It can be used to construct and solve tight-binding models of the electronic structure of systems of arbitrary dimensionality (crystals, slabs, ribbons, clusters, etc.), and is rich with features for computing Berry phases and related properties.

- About
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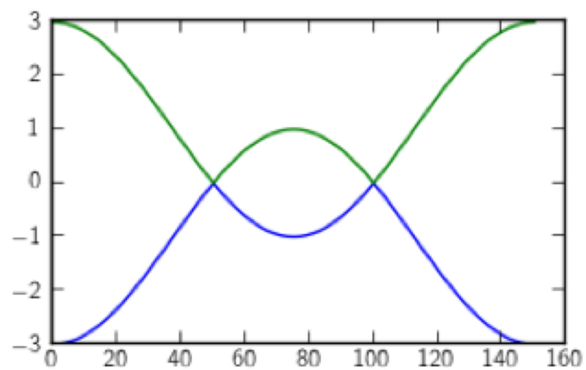
http://www.physics.rutgers.edu/pythtb

PythTB software package

Quick example

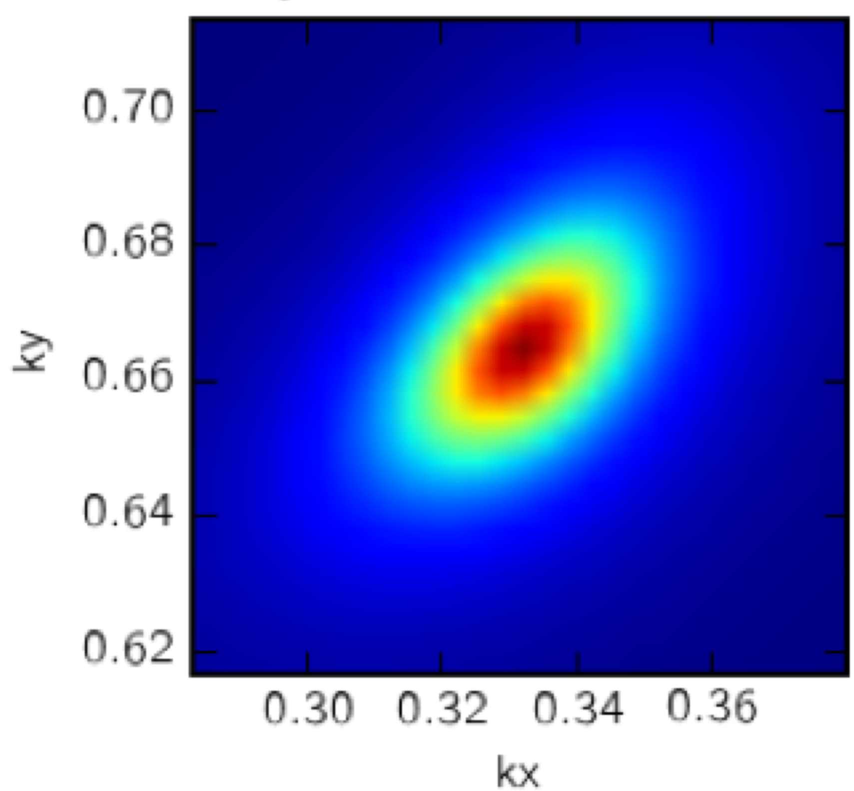
This is a simple example showing how to define graphene tight-binding model with first neighbour hopping only. Below is the source code and plot of the resulting band structure. Here you can find *more examples*.

```
from pythtb import *

# lattice vectors and orbital positions
lat=[[1.0, 0.0], [0.5, np.sqrt(3.0)/2.0]]
orb=[[1./3., 1./3.], [2./3., 2./3.]]
gra=tb_model(2, 2, lat, orb)

# define hopping between orbitals
gra.set_hop(-1.0, 0, 1, [ 0, 0])
gra.set_hop(-1.0, 1, 0, [ 1, 0])
gra.set_hop(-1.0, 1, 0, [ 0, 1])

# solve model on path in k-space
path=[[1.0, 0.0], [0.0, 1.0]]
kpts=k_path(path, 150)
evals=gra.solve_all(kpts)

# plot bandstructure
import matplotlib.pyplot as plt
plt.plot(evals[0, :])
plt.plot(evals[1, :])
plt.savefig("band.png")
```

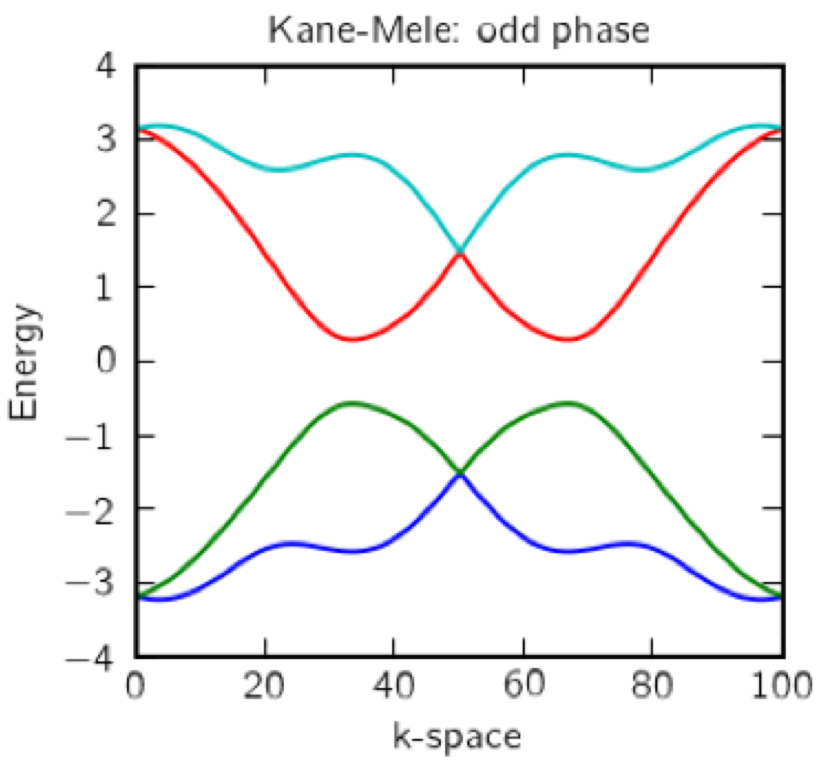


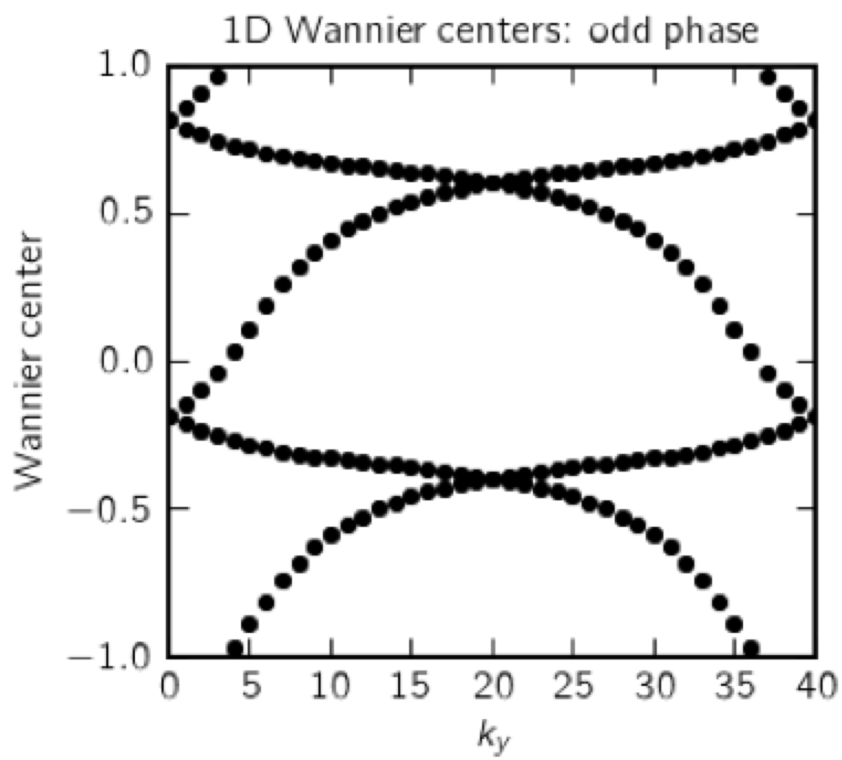
PythTB software package

Berry curvature near slightly opened Dirac cone
Graphene with on-site staggered potential



PythTB software package





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z2pack software package

Alexei Soluyanov

Z_2-package (z2pack)

Postprocessing tool for computing the Z_2 invariant using the output of first-principles packages.

The package is a Fortran/Python implementation of the method described in *Phys. Rev. B* **83**, *235401 (2011)* to compute the Z_2 topological indices of 2D and 3D time-reversal symmetric insulators. The output (spinor wavefunctions) of some first-principles codes is taken as an input for the calculation.

- version 0.1 (beta) (Jan 4, 2013)

  Supports: Abinit; norm-conserving pseudopotentials

- version 0.2 (under construction)

  Supports: Abinit and Quantum Espresso; norm-conserving and ultrasoft pseudopotentials

http://www.physics.rutgers.edu/z2pack

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