How to Visualize Topological Insulators

David Vanderbilt
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Collaborators

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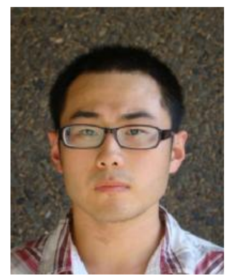
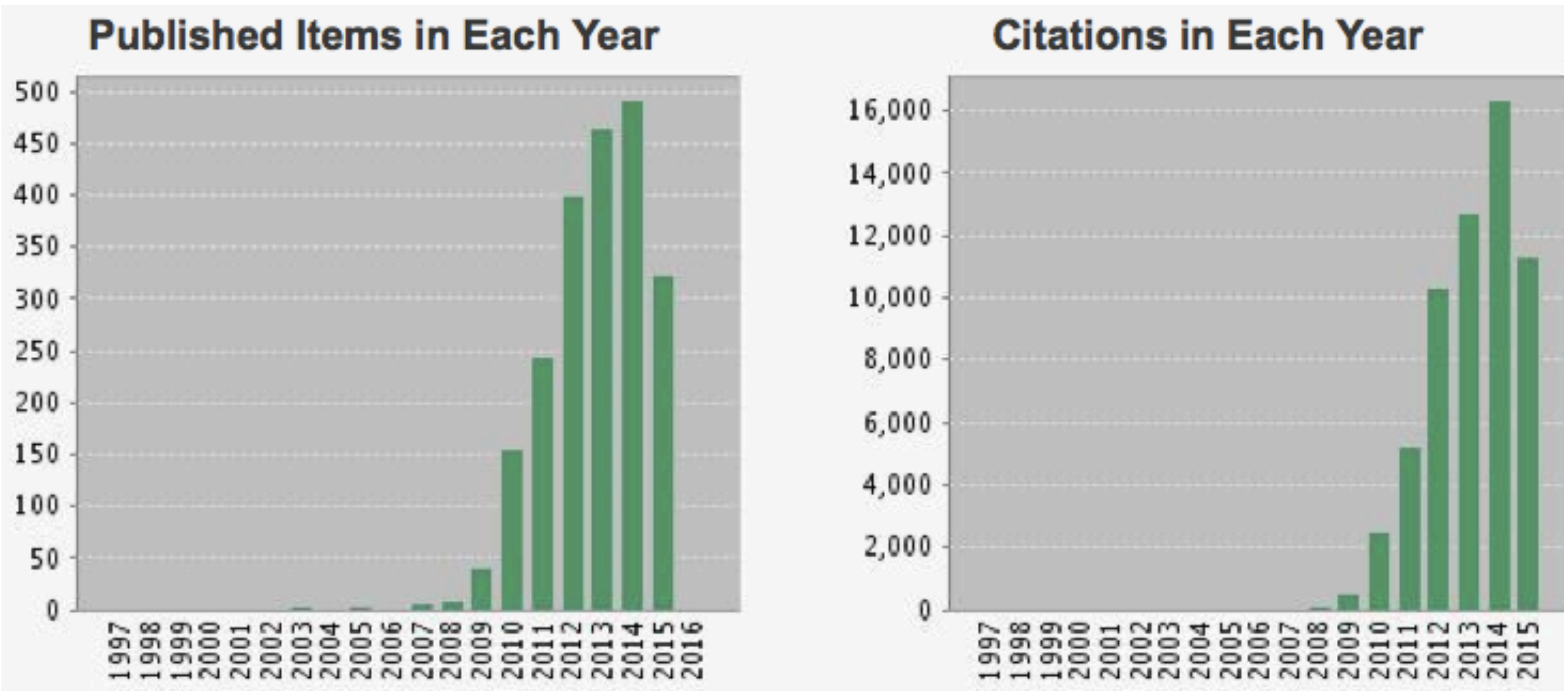


Jiangpeng
Liu

Kevin
Garrity

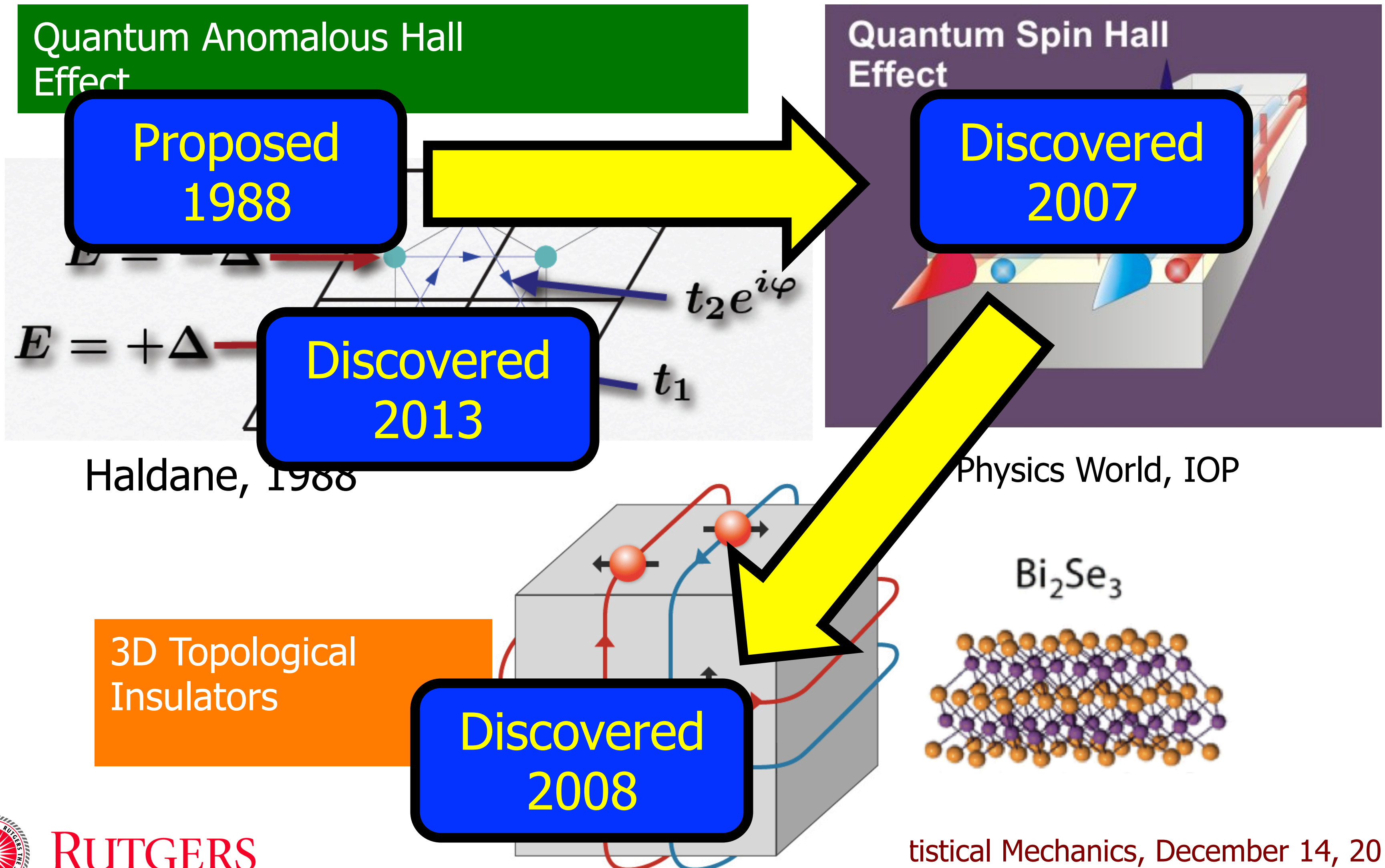
Topological insulators

A hot topic in condensed matter physics



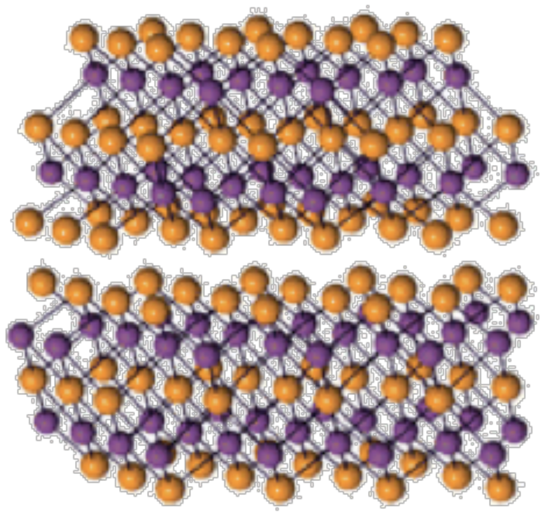
(Web of Science search on Title: "topological insulator")

Topological insulators (TIs)

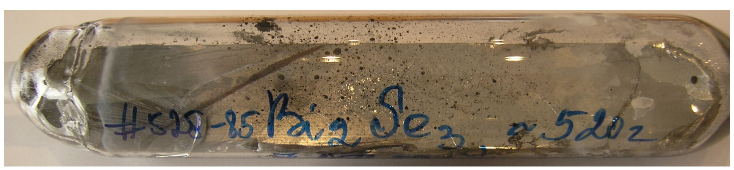


Topological insulators: Bi_2Se_3

Bi_2Se_3

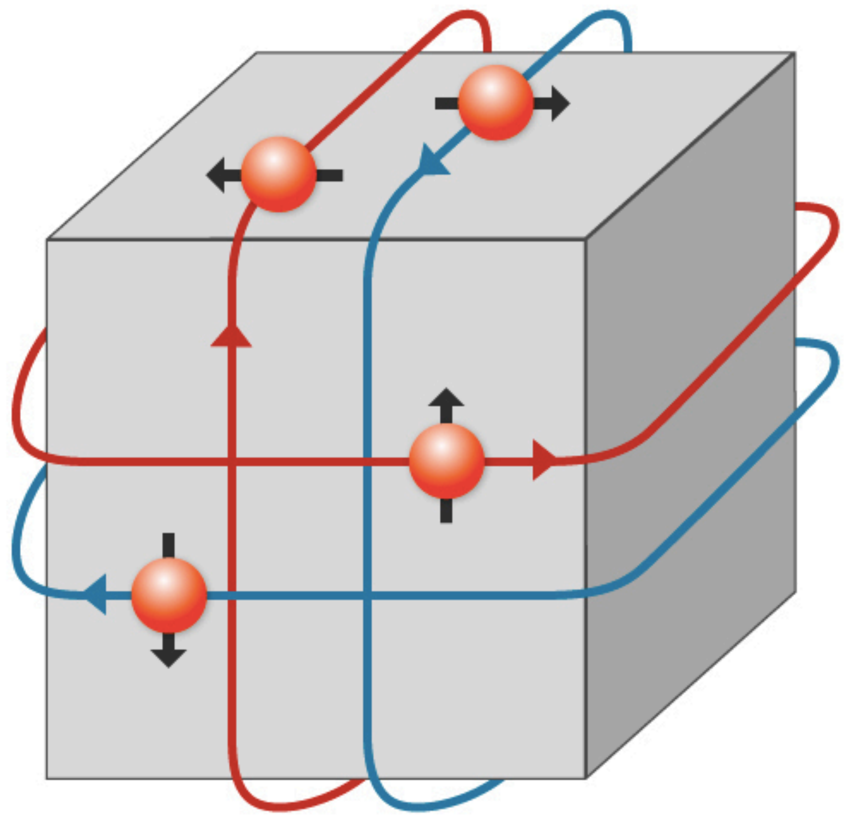


J. J. Cha,

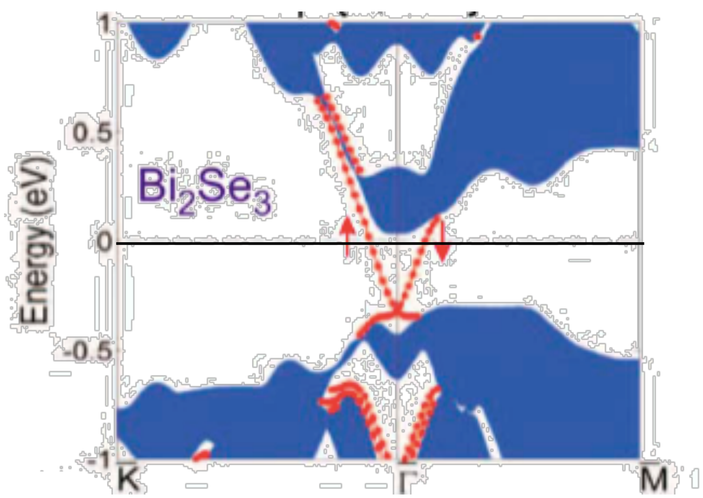


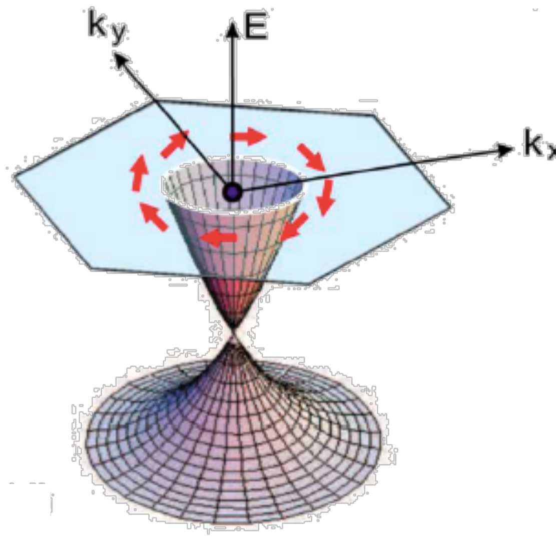
http://www.issp.ac.ru/lpcbc/DANDP/Bi-Ch.html

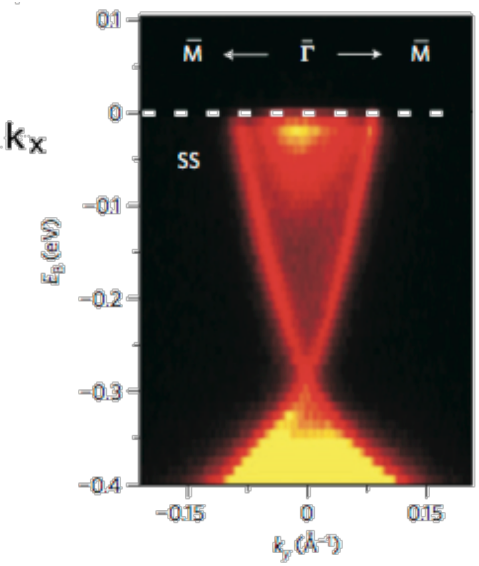
Bi_2Se_3 is topologically twisted!



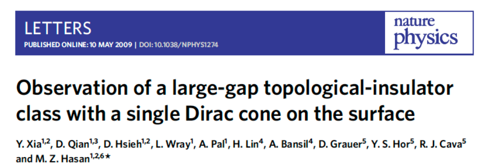
Surface of Bi_2Se_3







Figures 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)

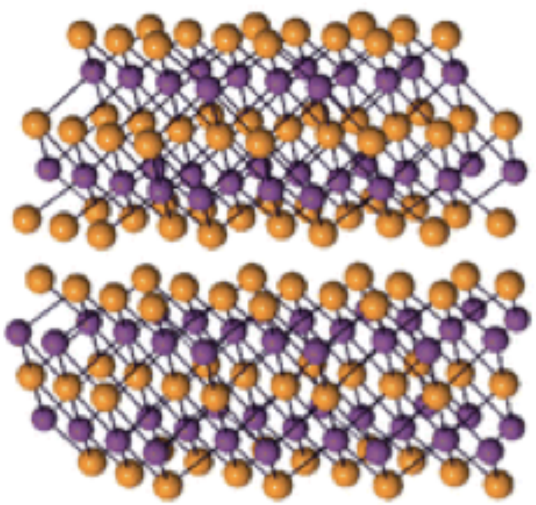

LETTERS
PUBLISHED ONLINE: 10 MAY 2009 | DOI: 10.1038/NPHYS1274
nature physics

Observation of a large-gap topological-insulator class with a single Dirac cone on the surface

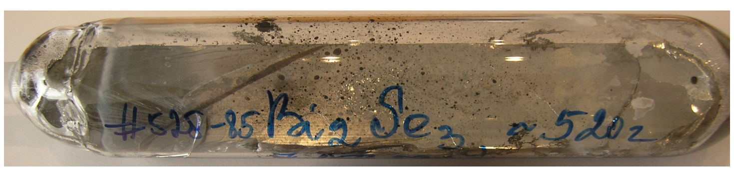
Y. Xia[1,2], D. Qian[1,3], D. Hsieh[1,2], L. Wray[1], A. Pal[1], H. Lin[4], A. Bansil[4], D. Grauer[5], Y. S. Hor[5], R. J. Cava[5] and M. Z. Hasan[1,2,6]★

Topological insulators: Bi_2Se_3

Bi_2Se_3

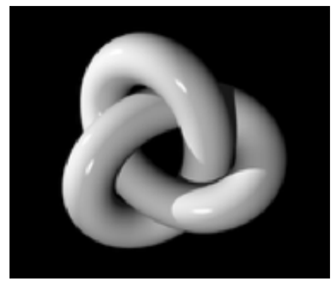


J. J. Cha,



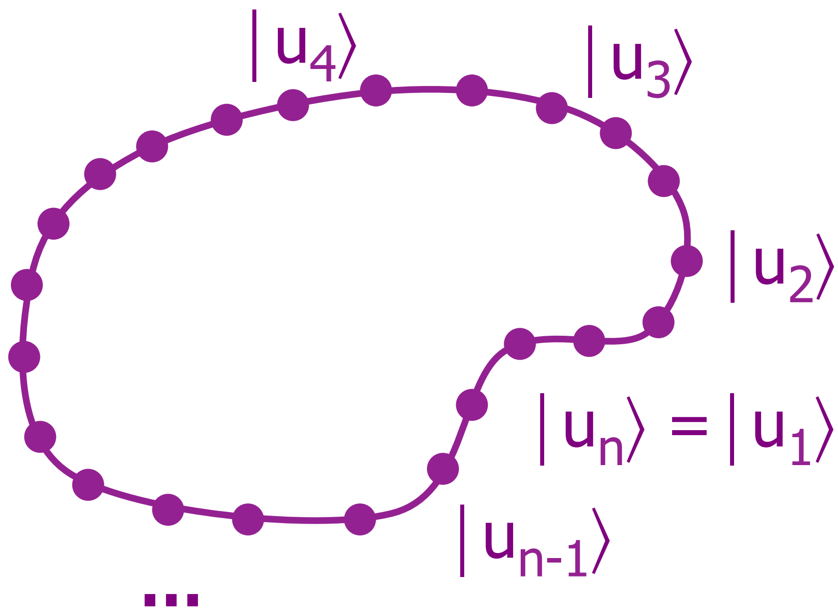
http://www.issp.ac.ru/lpcbc/DANDP/Bi-Ch.html

Bi_2Se_3 is topologically twisted!



But in precisely what sense?

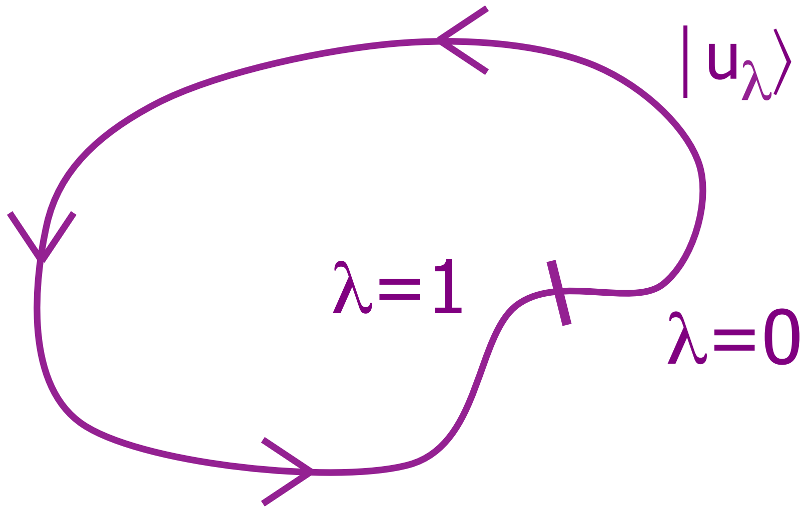
Berry phases



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



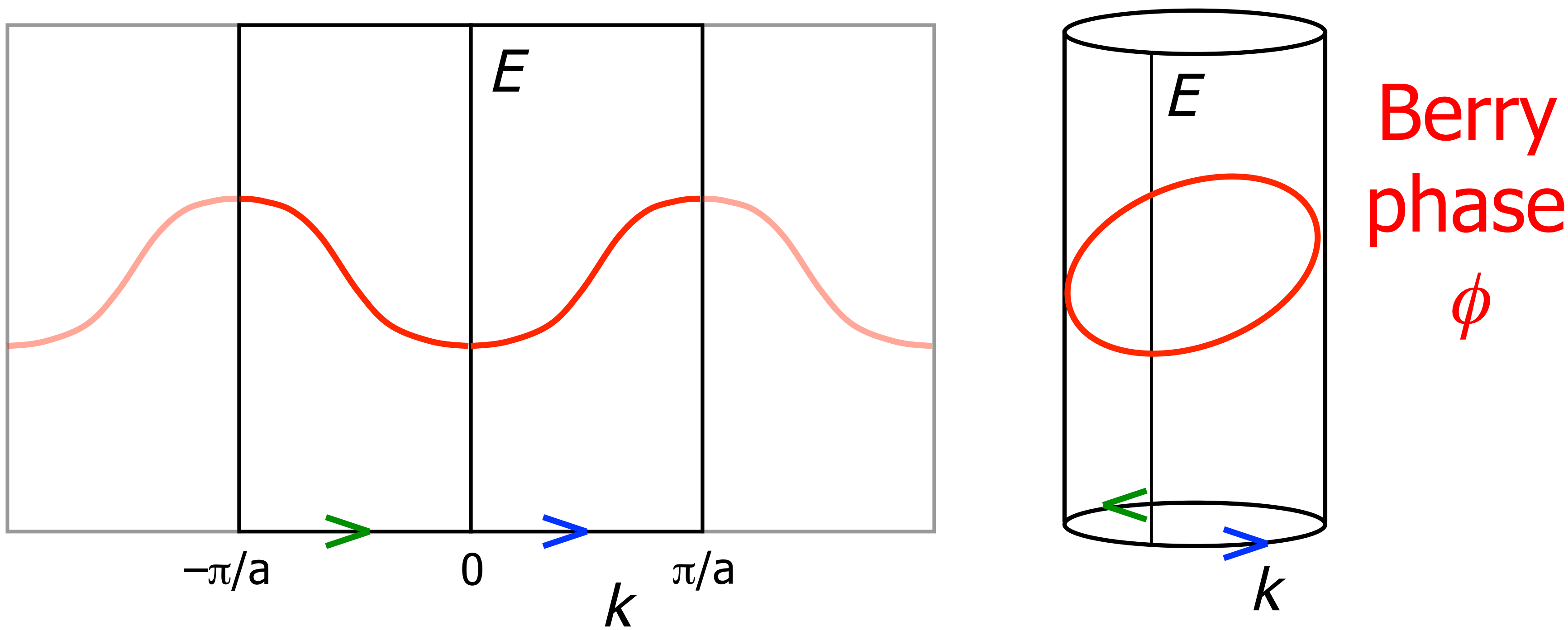
$$\phi = -\mathrm{Im} \oint d\lambda \, \langle u_\lambda | \tfrac{du_\lambda}{d\lambda} \rangle$$

ϕ is well-defined modulo 2π

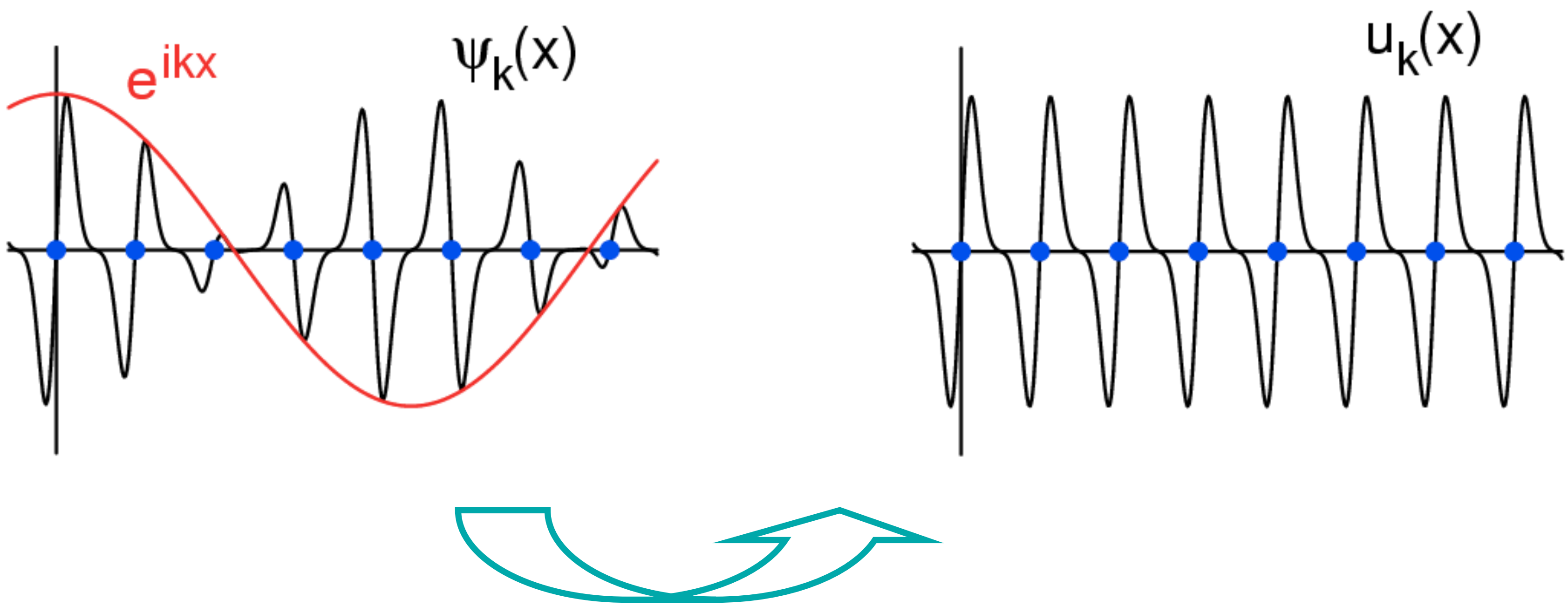
$\Rightarrow$ ϕ is a phase

Berry phase in 1D Brillouin zone

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



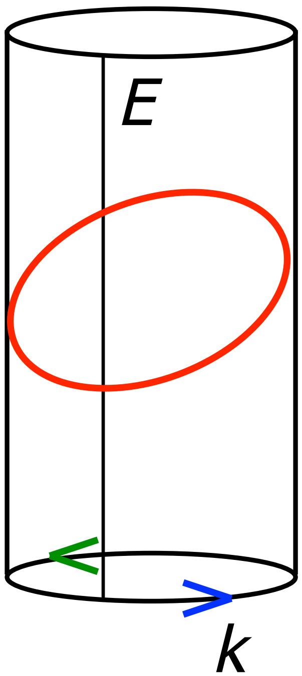
Berry phase in 1D Brillouin zone



Define the cell-periodic Bloch function $u_k(x)$:

$$u_k(x) = e^{-ikx}\psi_k(x)$$

Berry phase in 1D Brillouin zone



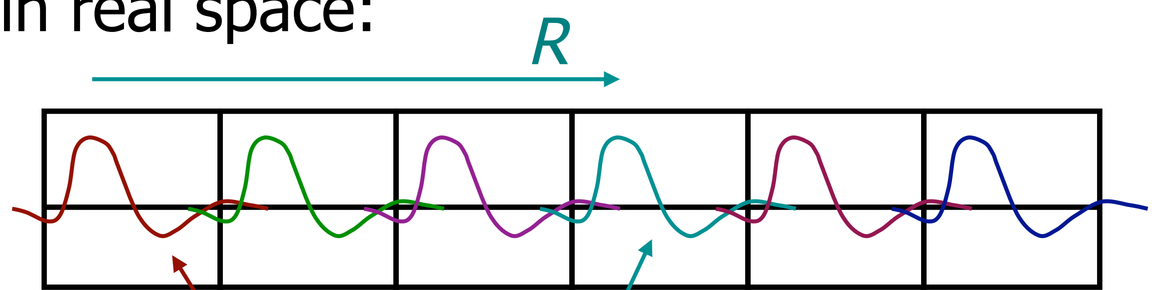
Berry phase ϕ

$$\phi_n = \int_0^{2\pi/a} \langle u_{nk} | \, i \frac{d}{dk} \, | u_{nk} \rangle \, dk$$

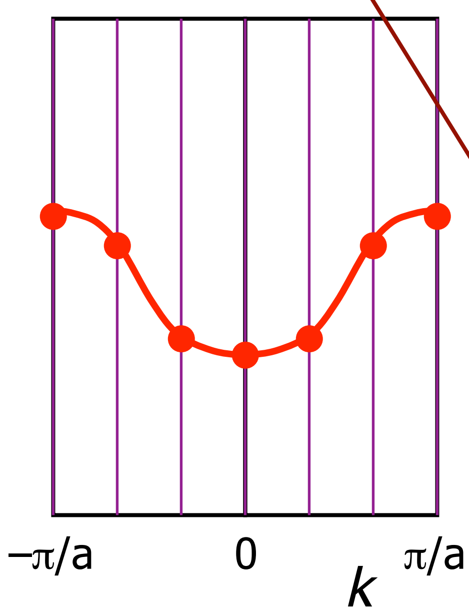
$$u_k(x) = e^{-ikx} \psi_k(x)$$

Wannier functions in 1D

Crystal in real space:



Brillouin zone in reciprocal space:



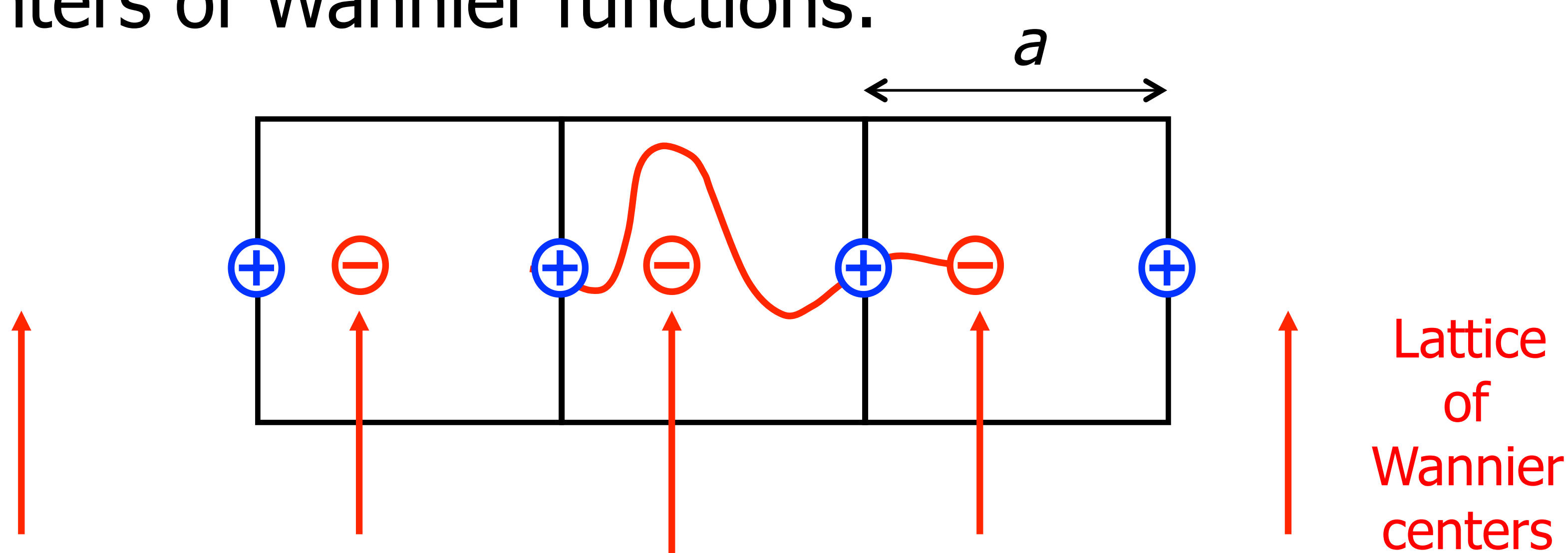
$$w_{\mathbf{R}}(\mathbf{r}) = \sum_{\mathbf{k}} \psi_{\mathbf{k}}(\mathbf{r})\, e^{-i\mathbf{k}\cdot\mathbf{R}}\, d\mathbf{k}$$

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

Unitary transformation

Berry phases ↔ Wannier centers

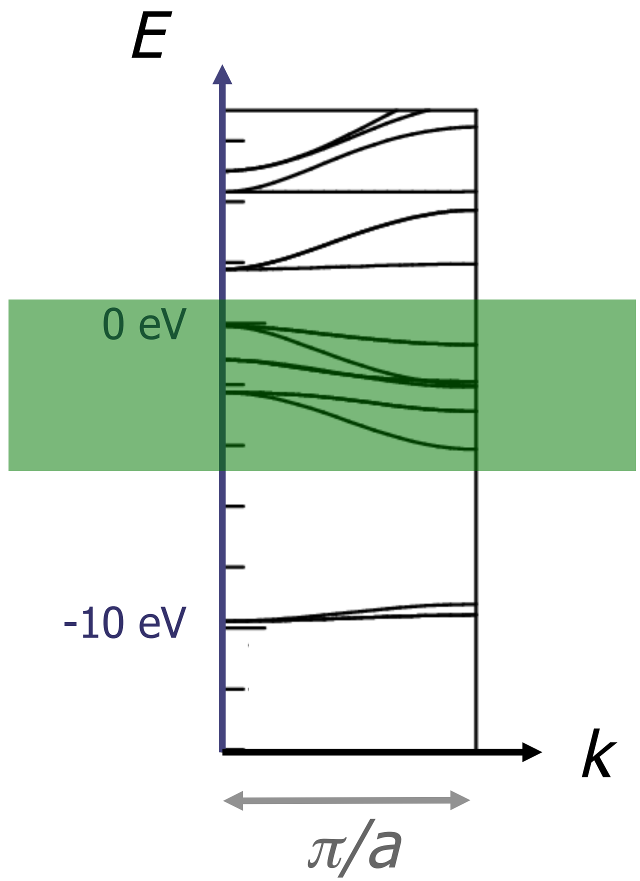
Centers of Wannier functions:



$$\langle w_n | x | w_n \rangle = \frac{a}{2\pi} \int_0^{2\pi/a} \langle u_{nk} | \, i \frac{d}{dk} \, | u_{nk} \rangle \, dk$$

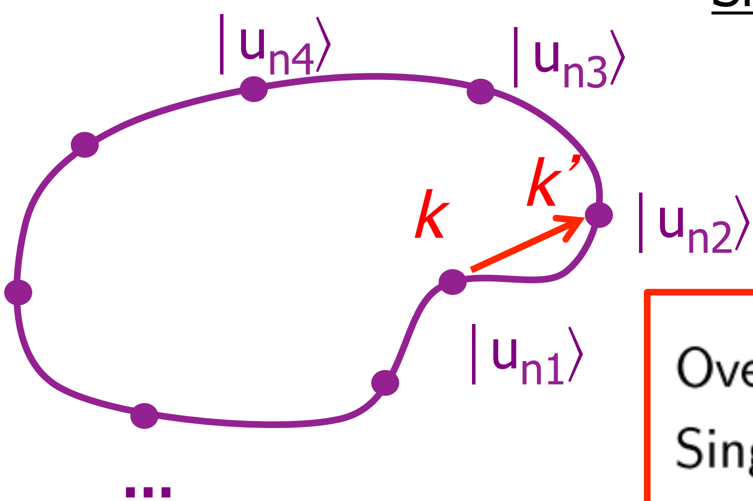
$$\langle w_n | x | w_n \rangle = \frac{a}{2\pi} \, \phi_n$$

Treat occupied bands as a group



- *N* bands *N* Wannier functions per cell
- Gauge freedom: Wannier centers are not unique
- "MaxLoc Wannier centers" are unique
- Same as generalized Berry phases = "Wilson loop eigenvalues"

Multi-band Wannier centers



Single band:

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

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

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

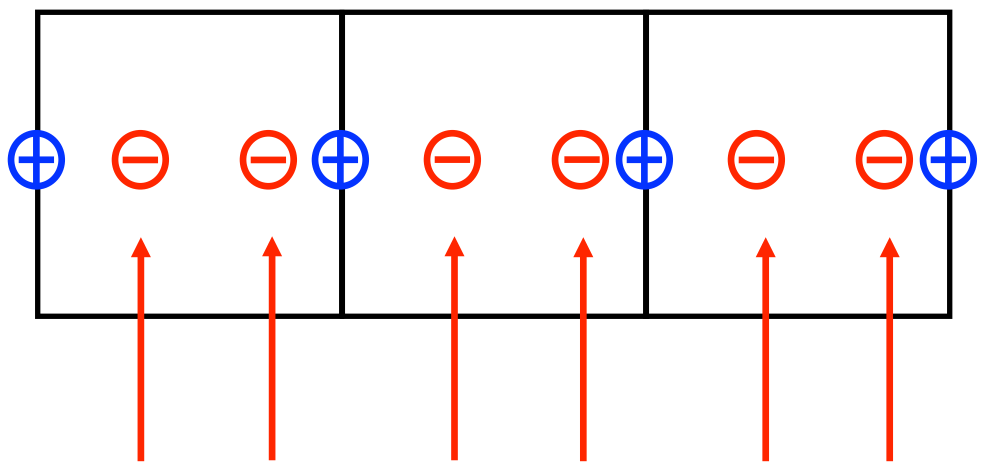
Unitary rotation: $W = UV^\dagger$

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

ϕ_j = Berry phases (“Wilson loop eigenvalues”)

Multi-band Wannier centers

1D insulator with two occupied bands:



Lattice of Wannier centers

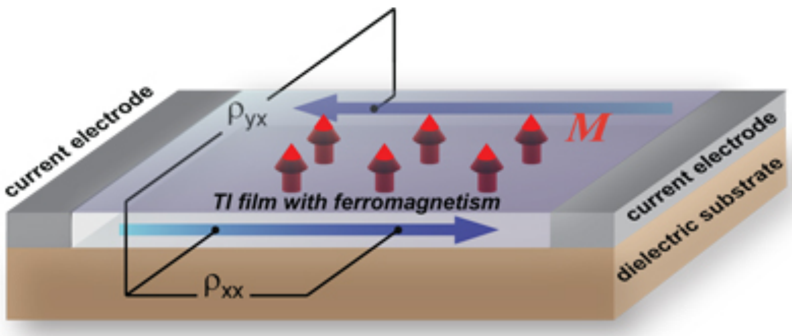
Tool: Visualize topological band structures

- For 2D crystal
  - Choose one direction to Wannierize (say, y)
  - Plot 1D WCC's along y as a function of k_x
- For 3D crystal
  - Choose one direction to Wannierize (say, z)
  - Plot 1D WCC's as a function of (k_x, k_y)

WCC = "Wannier charge center"

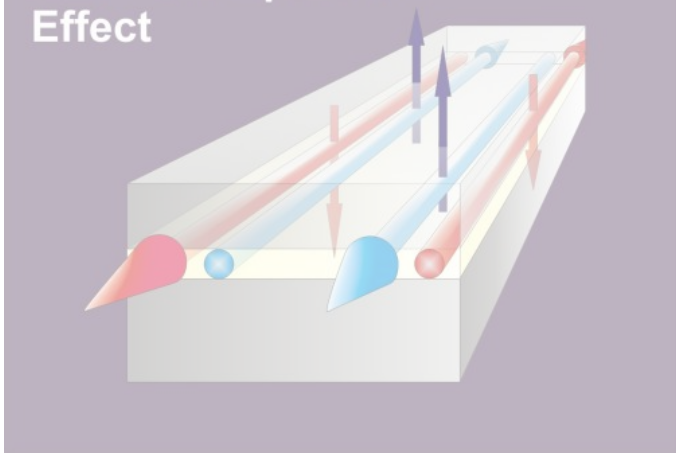
Plan of the talk

Quantum Anomalous Hall Effect

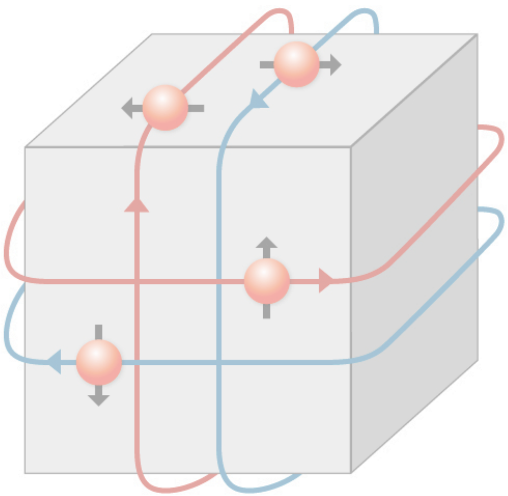


Qikun Xue, Tsinghua Univ.

Quantum Spin Hall Effect



Physics World, IOP



3D Topological Insulators

QAH proof of principle

VOLUME 61, NUMBER 18 PHYSICAL REVIEW LETTERS 31 OCTOBER 1988

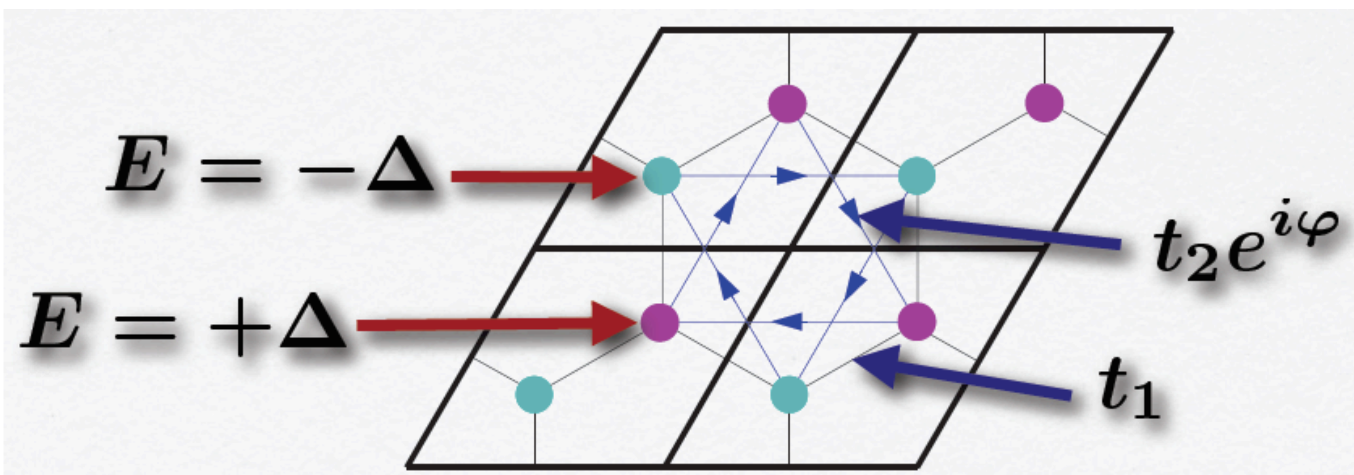
Model for a Quantum Hall Effect without Landau Levels: Condensed-Matter Realization of the "Parity Anomaly"

F. D. M. Haldane

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

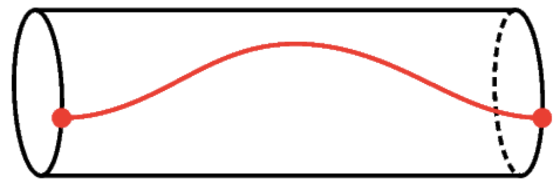
(Received 16 September 1987)

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.



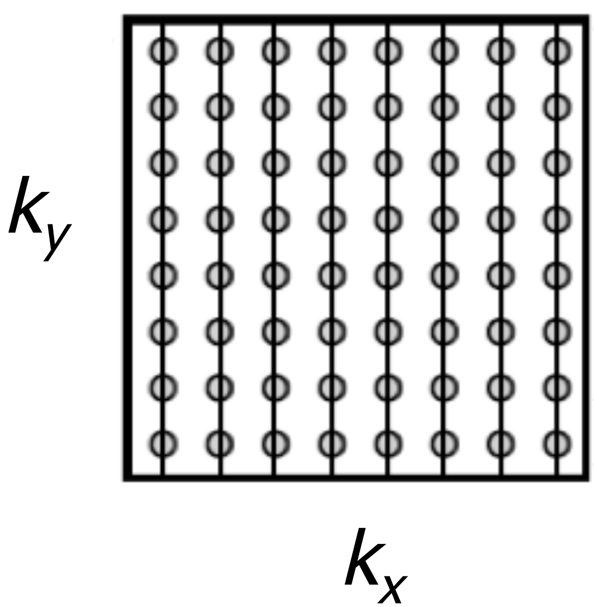
String Berry phases for normal band

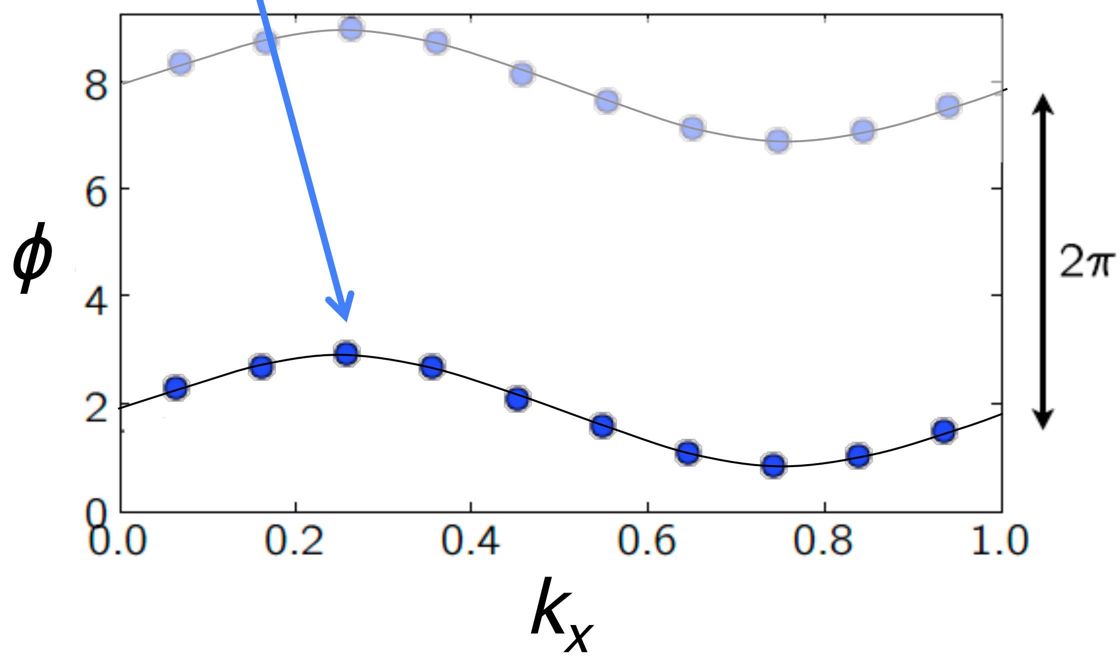
$$\phi\,(k_x) = -\mathrm{Im}\ \ln\left[\,\langle u_1|u_2\rangle\,\langle u_2|u_3\rangle \ldots \langle u_{n-1}|u_n\rangle\,\right]$$



$$\boxed{\langle w_n|x|w_n\rangle \;=\; \frac{a}{2\pi}\,\phi_n}$$

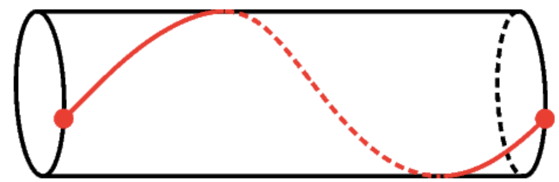
Equivalently, WCC's





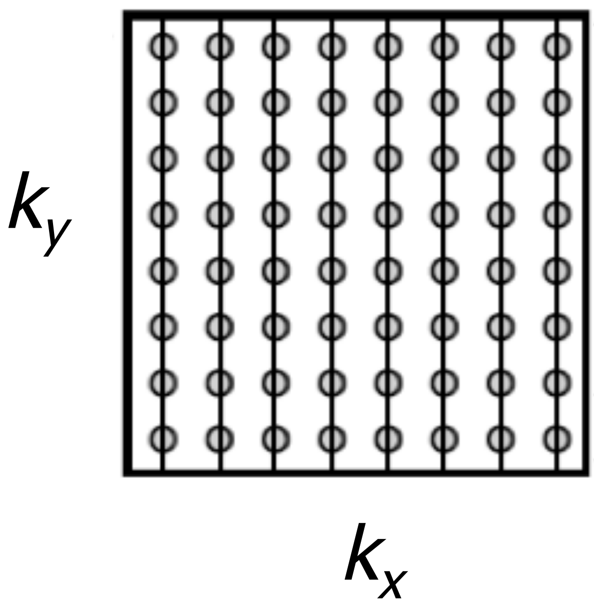
String Berry phases in QAH band

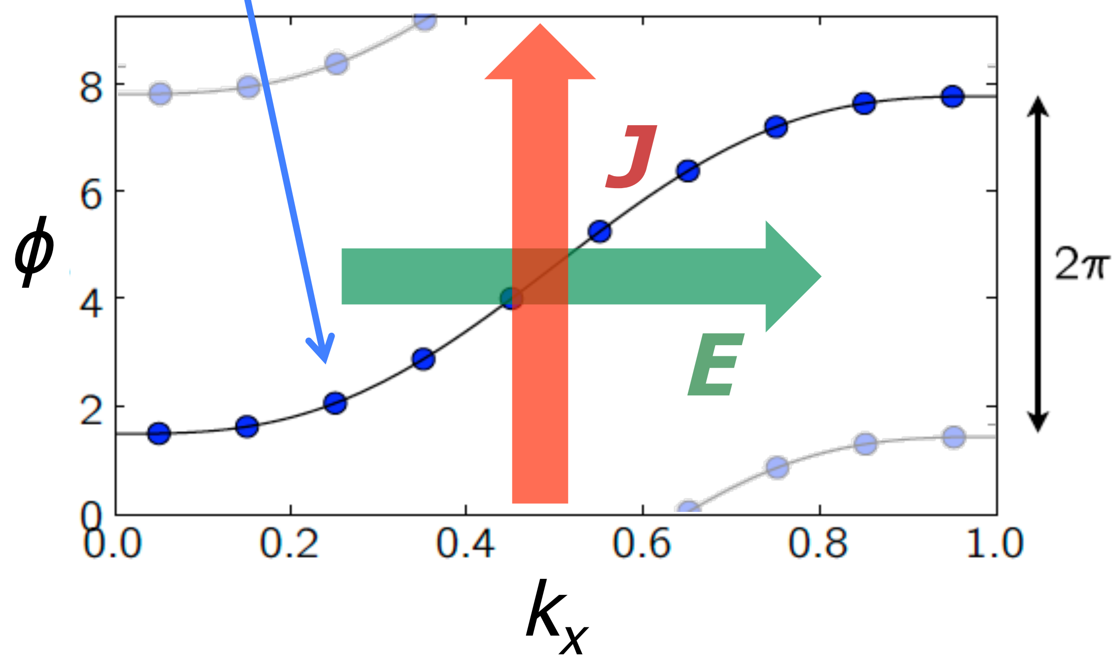
$$\phi\,(k_x) = -\mathrm{Im}\,\ln\,[\,\langle u_1|u_2\rangle\,\langle u_2|u_3\rangle ... \langle u_{n-1}|u_n\rangle\,]$$



$$\boxed{\langle w_n|x|w_n\rangle \;=\; \frac{a}{2\pi}\,\phi_n}$$

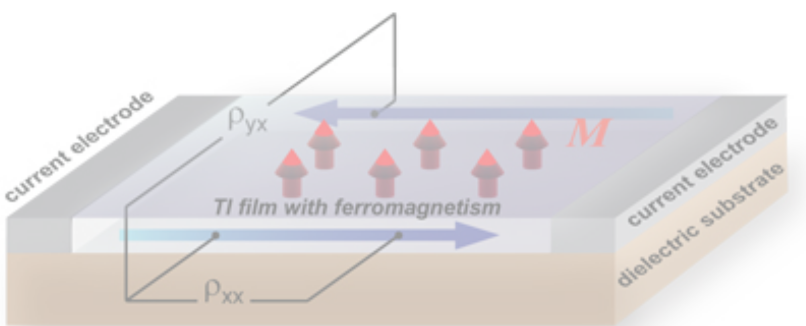
Equivalently, WCC's





Plan of the talk

Quantum Anomalous Hall Effect



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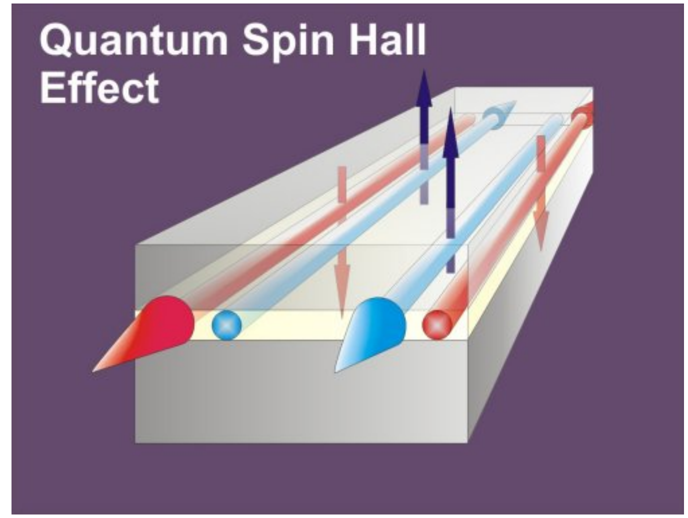
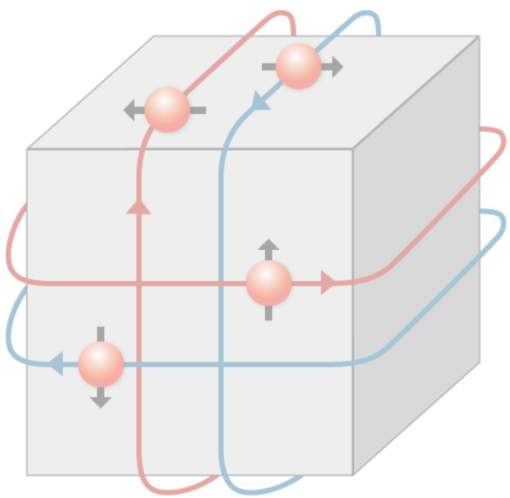
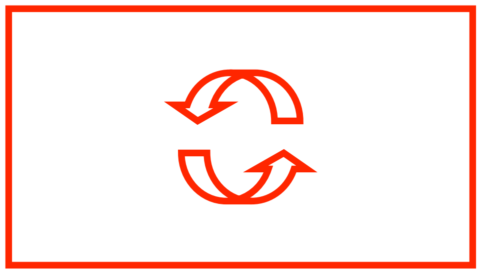


Physics World, IOP

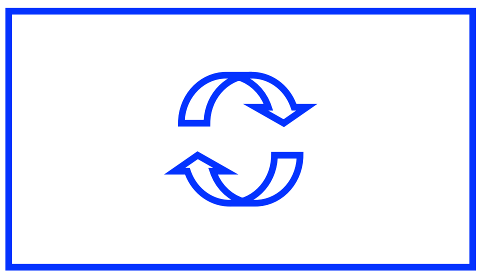


3D Topological Insulators

Z_2 Topological Insulator ("Quantum spin Hall")

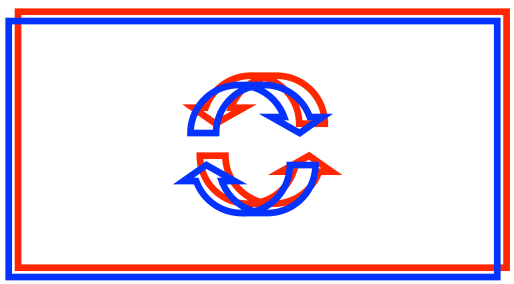


Spin up, $\sigma_{xy} = + e^2/h$



Spin down, $\sigma_{xy} = - e^2/h$

Z_2 Topological Insulator ("Quantum spin Hall")



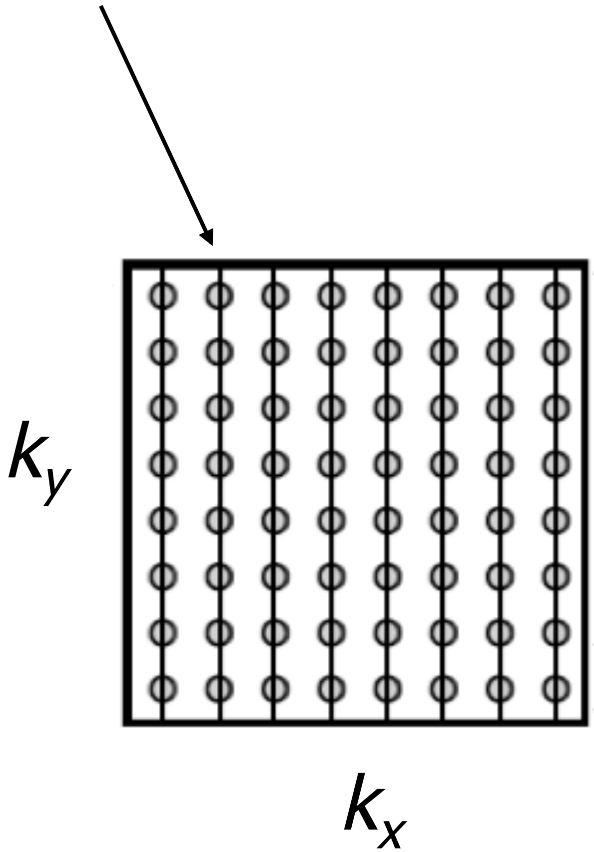
Total $\sigma_{xy} = 0$

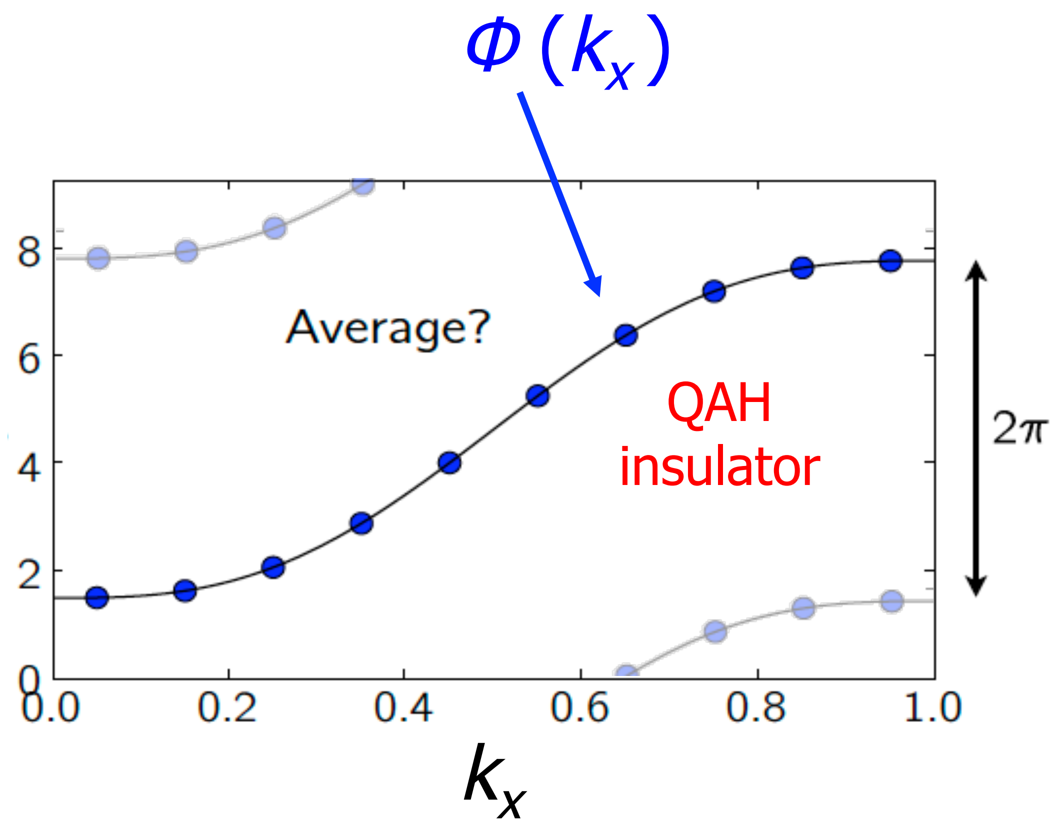
(And turn on spin-orbit coupling):

- Obeys T symmetry
- Charge Hall = 0
- Spin Hall instead ("Z2 invariant")

String Berry phases in QAH insulator

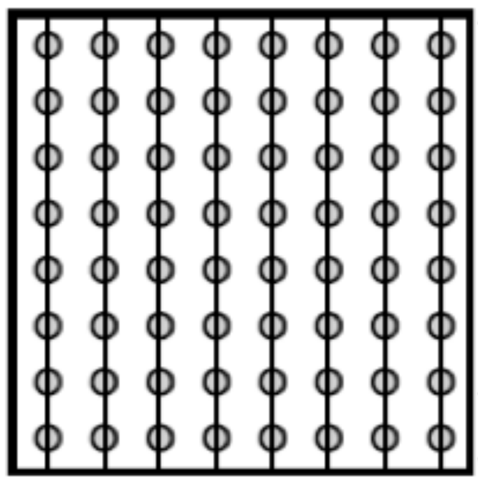
$$\phi\,(k_x) = -\mathrm{Im}\,\ln\left[\,\langle u_1|u_2\rangle\,\langle u_2|u_3\rangle ...\langle u_{n-1}|u_n\rangle\,\right]$$





String Berry phases in Z_2-odd insulator

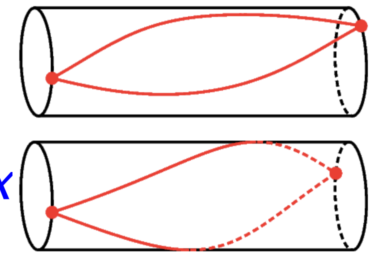
k_y

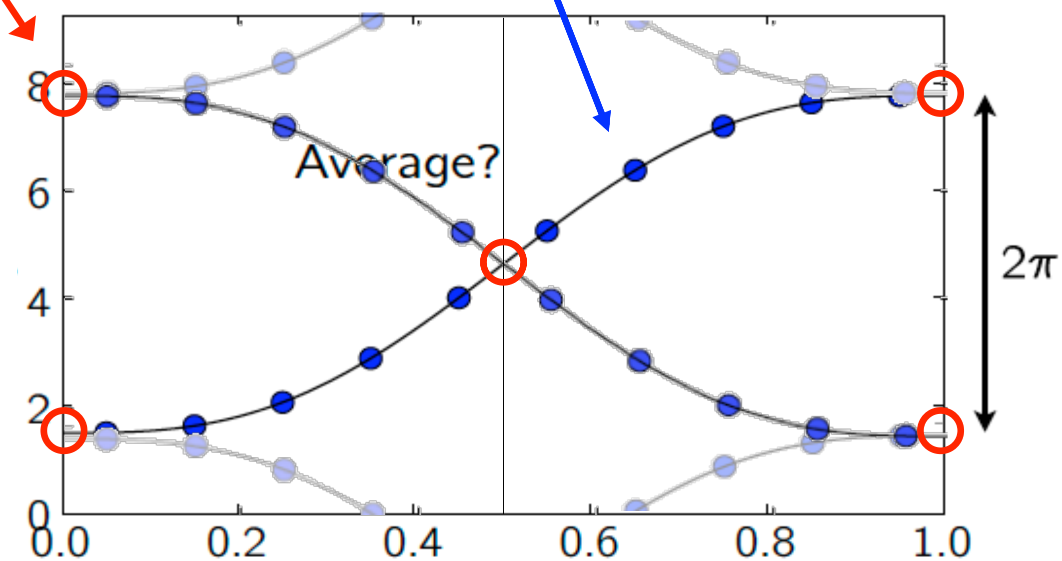


k_x

Kramers degeneracy
at $k_x = 0$ and π

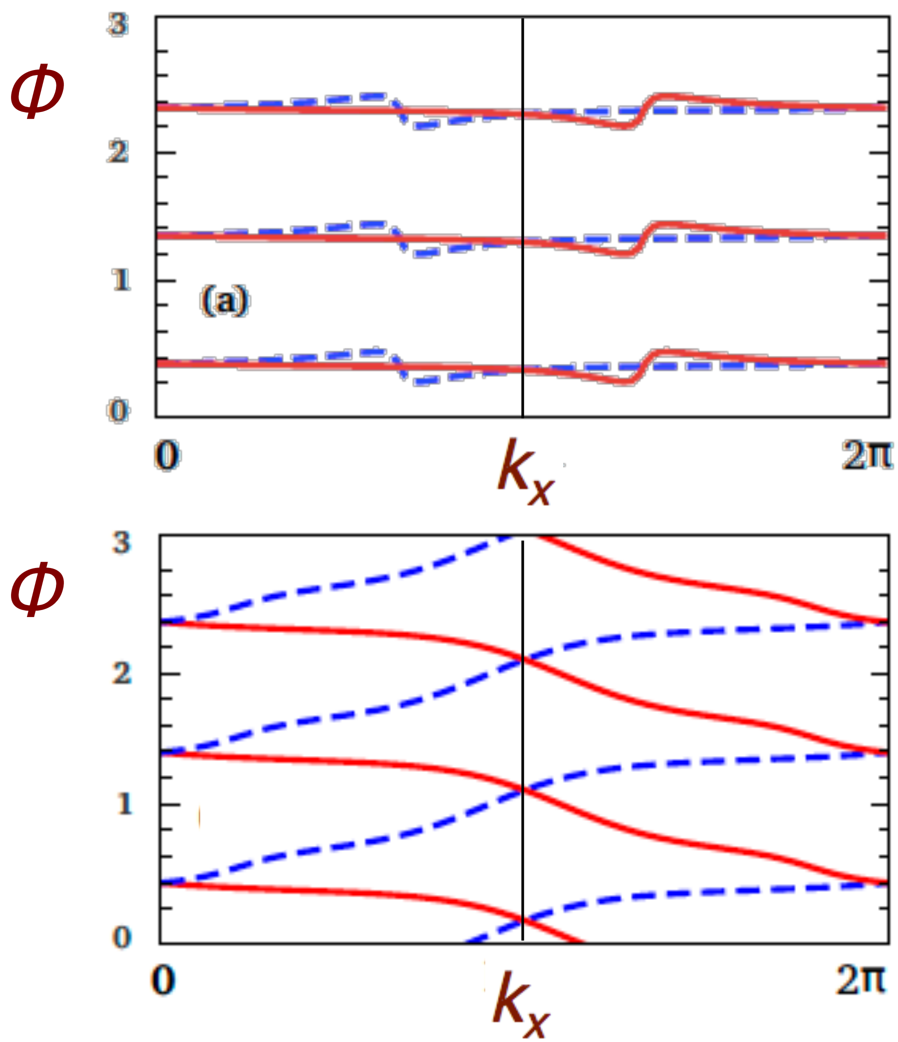
$\Phi\,(k_x$





k_x

String Berry phases in Z_2 even *vs.* odd



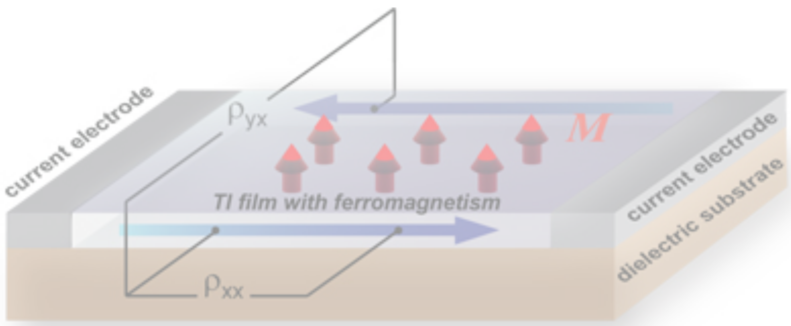
Normal

Kane-Mele tight-binding model

Z_2-odd

Plan of the talk

Quantum Anomalous Hall Effect



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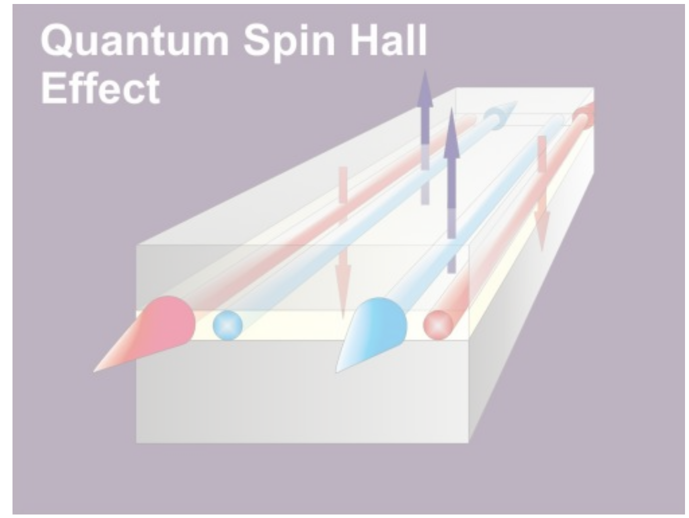
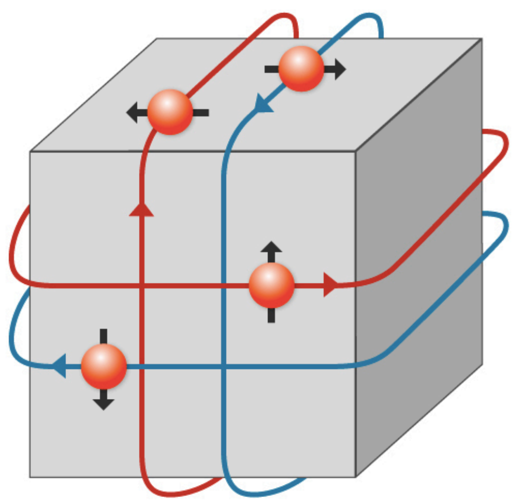
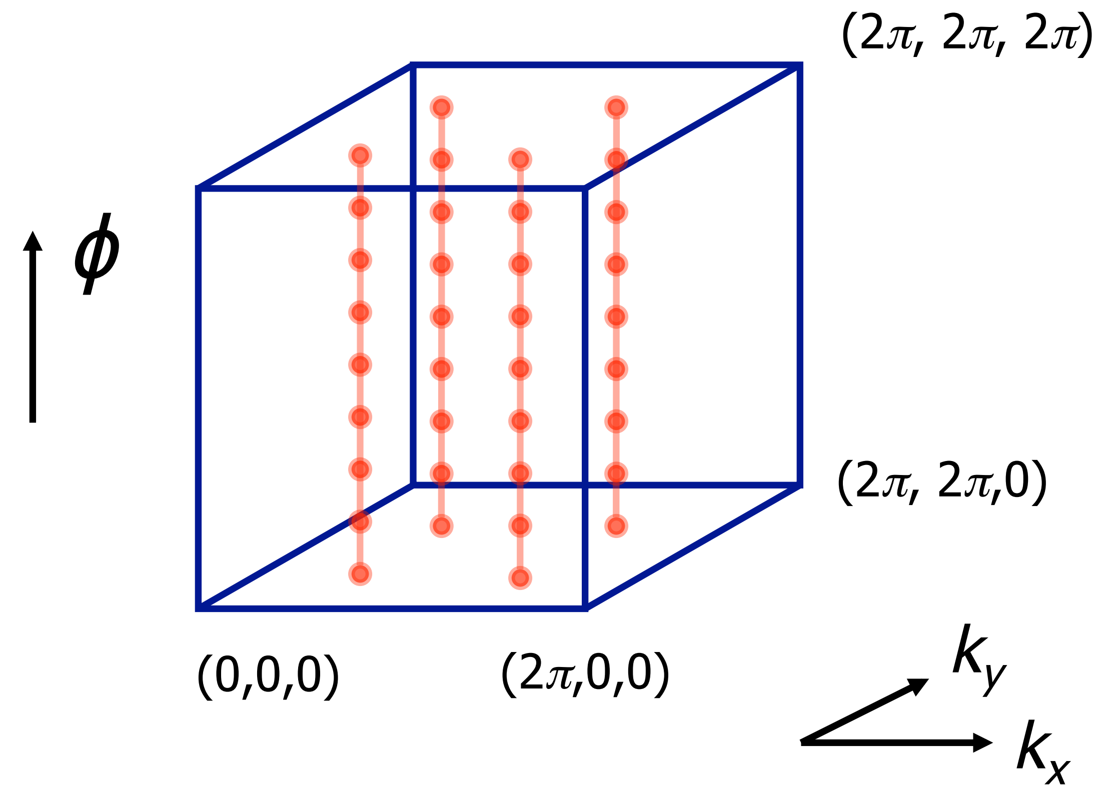


Physics World, IOP

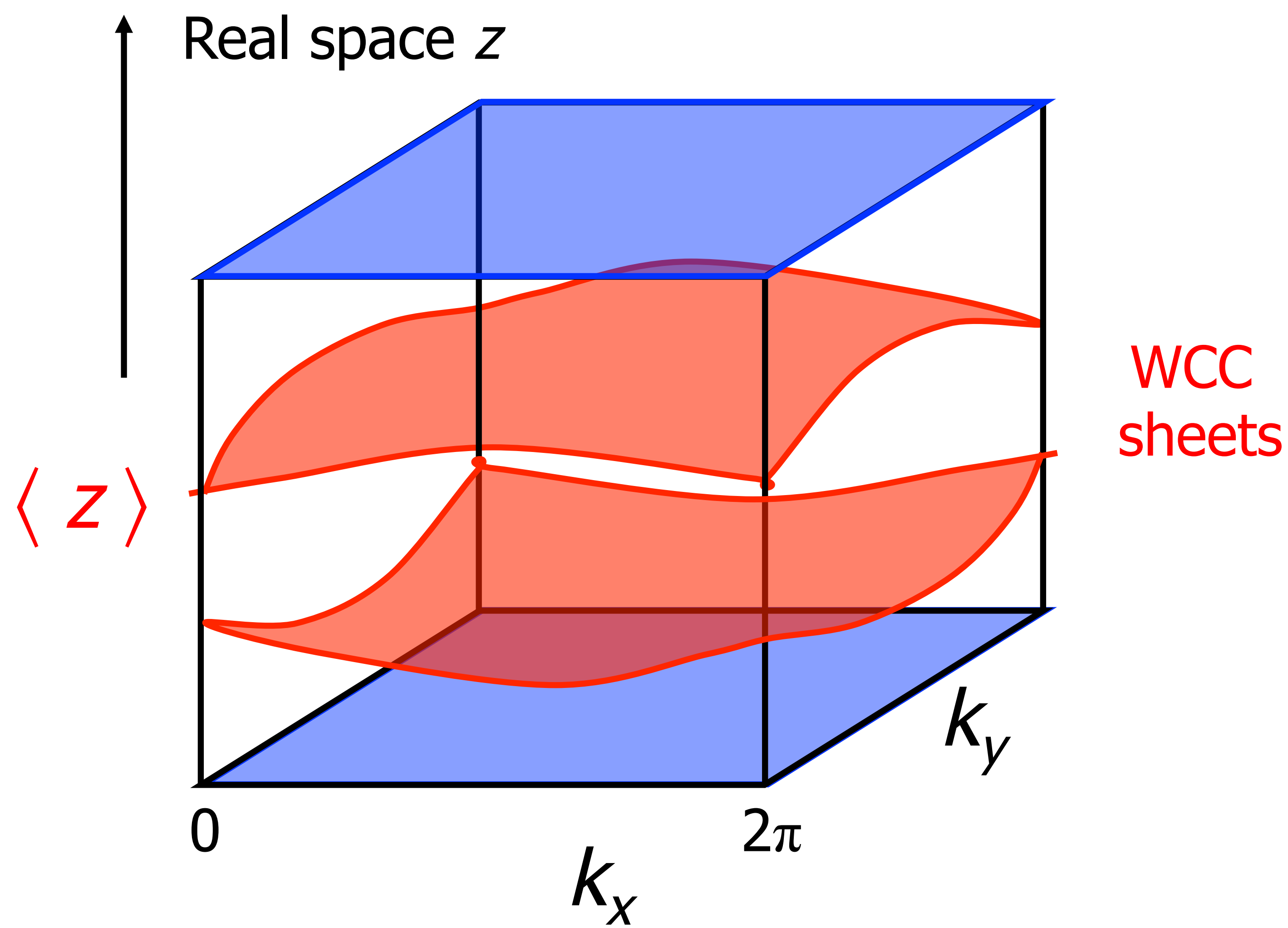


3D Topological Insulators

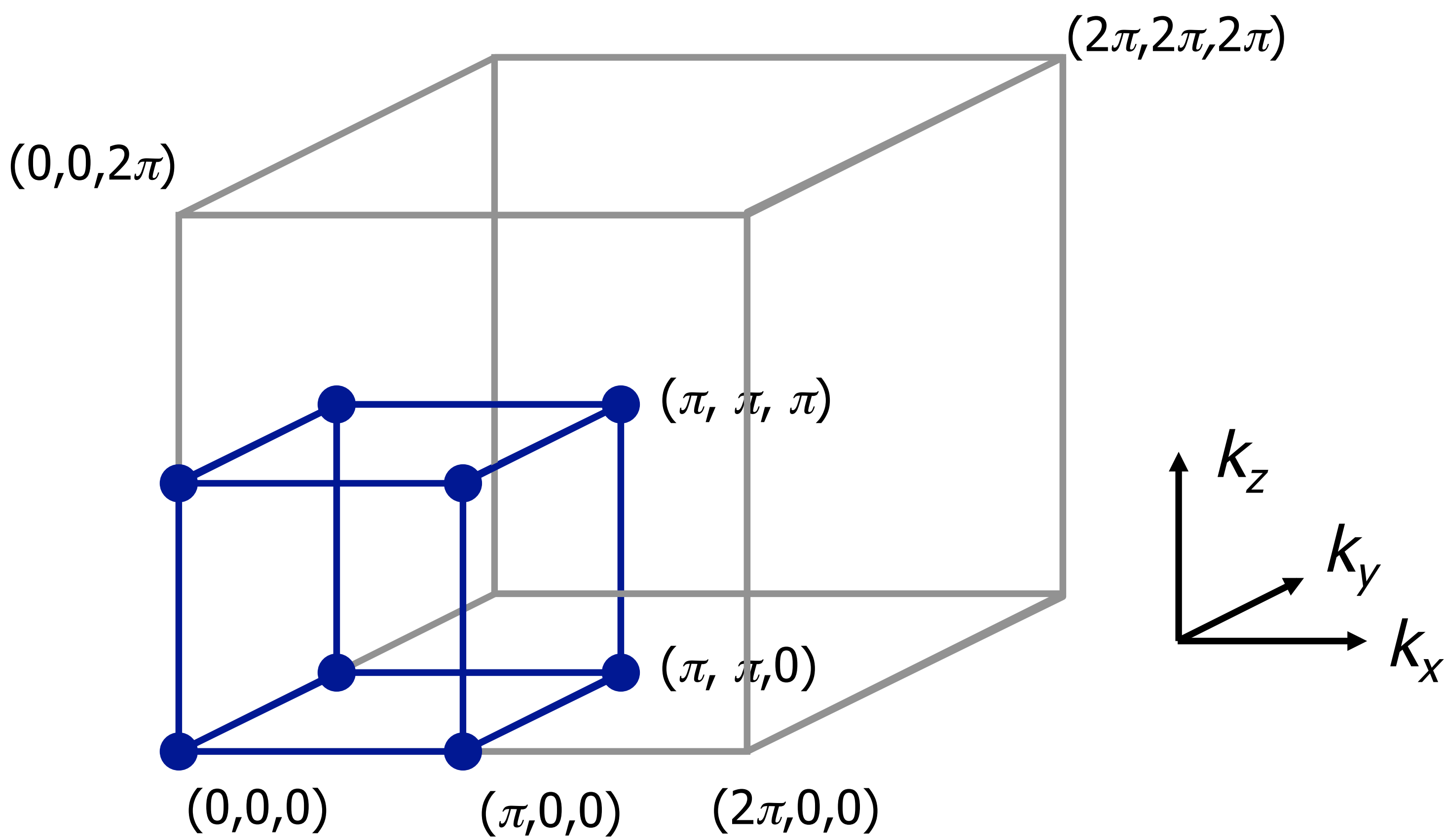
String berry phases (WCCs) vs. (k_x, k_y)



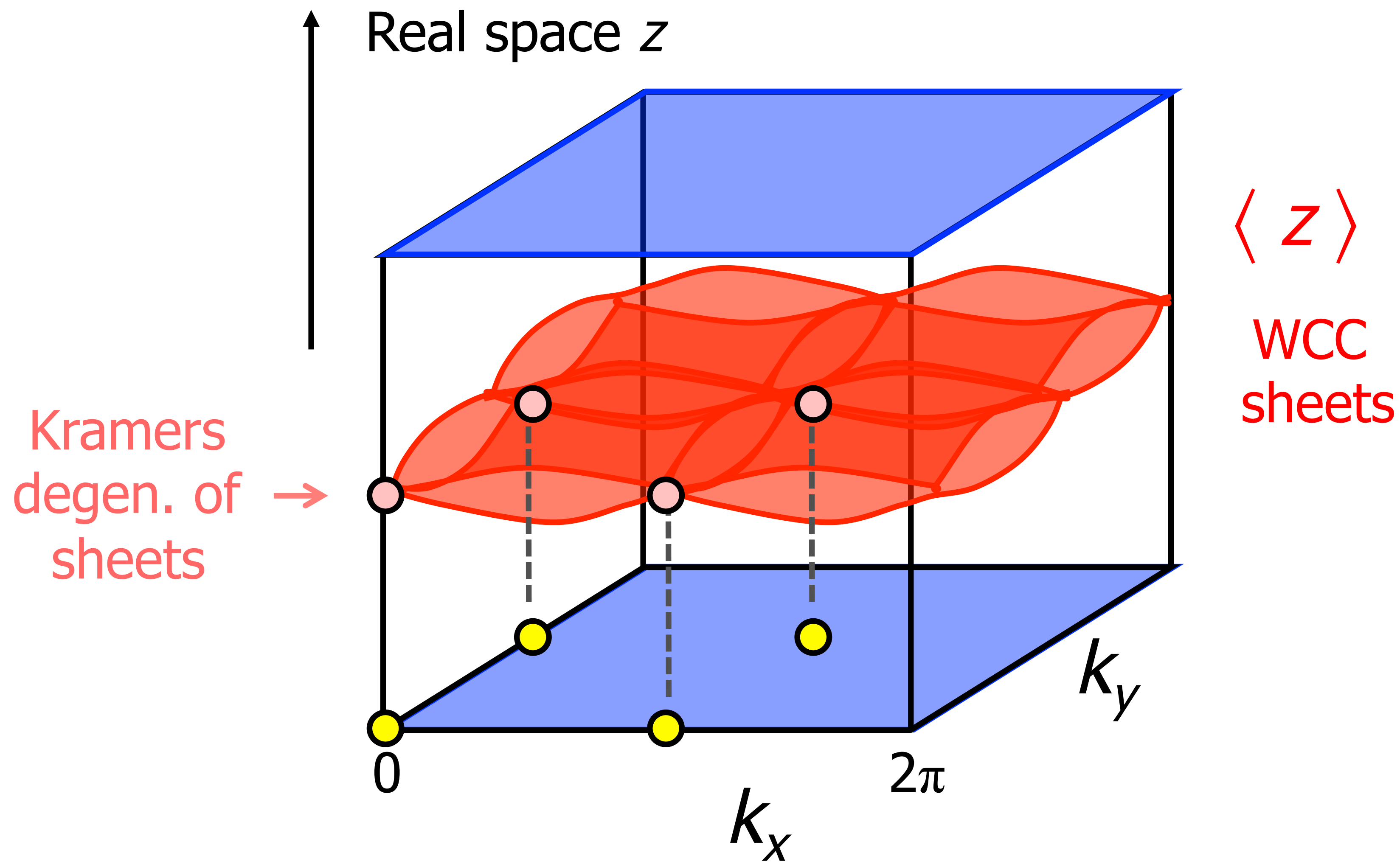
Normal, no TR symmetry



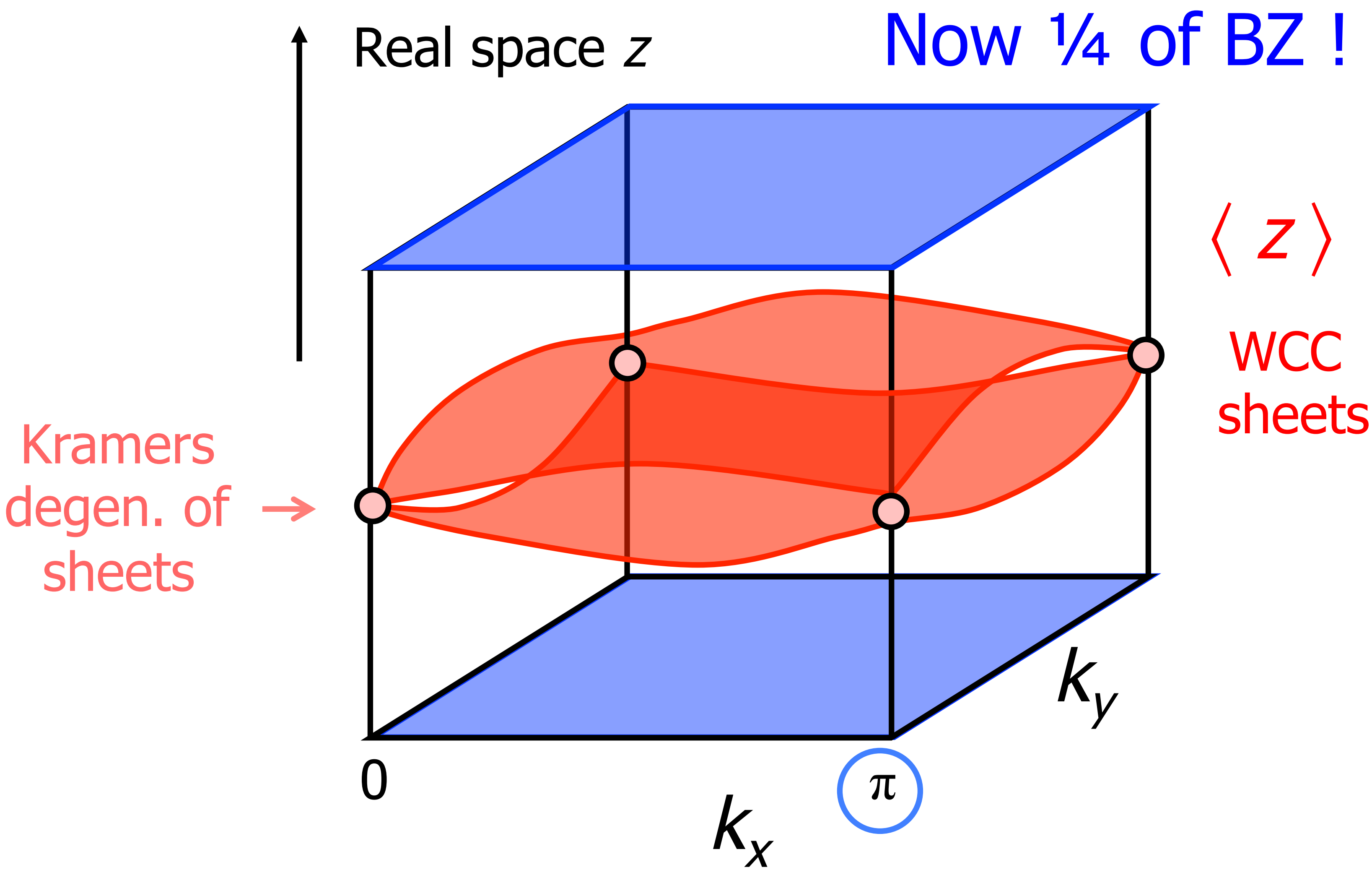
3D Brillouin zone of TR-invariant ins.



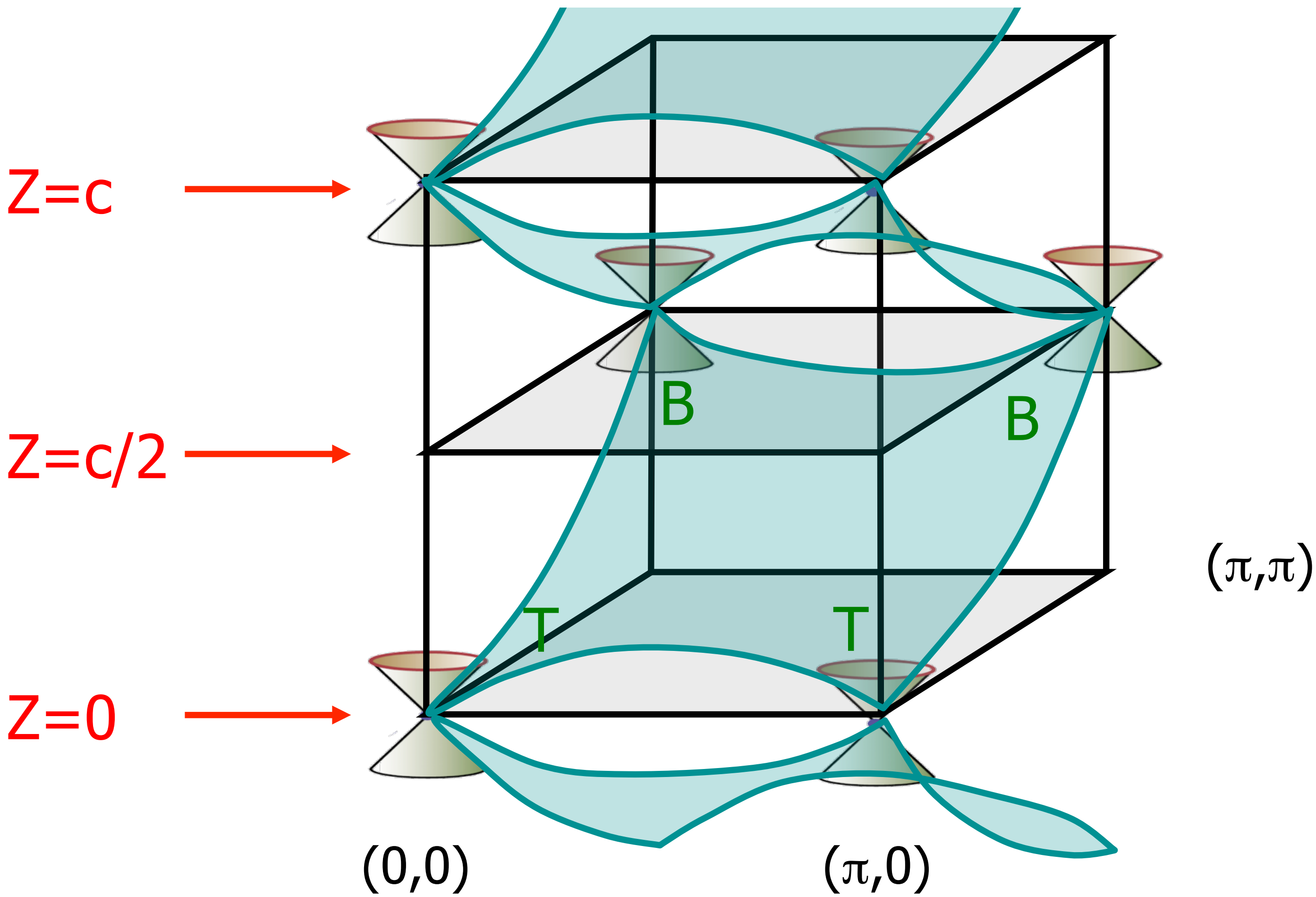
Normal, with TR symmetry



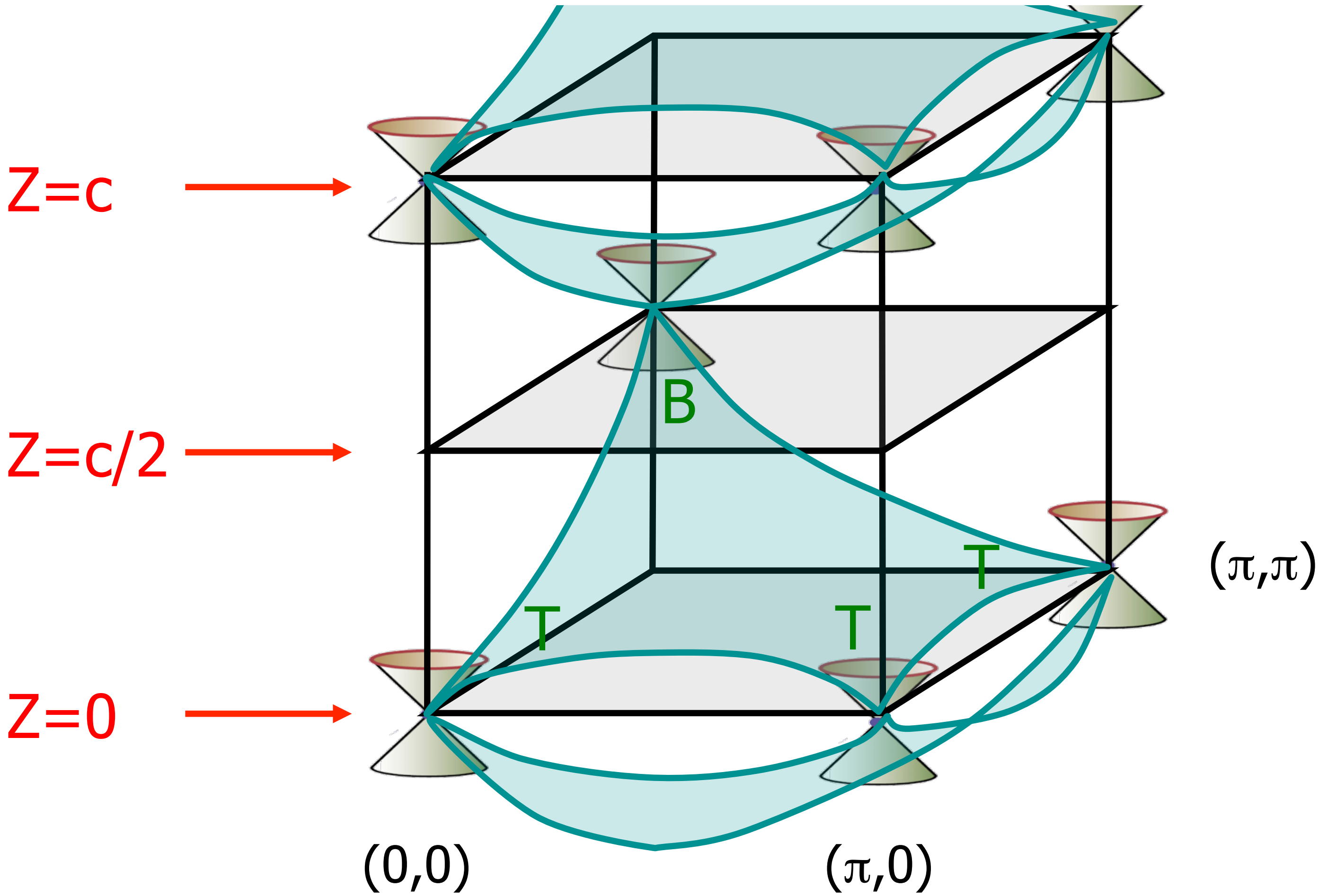
Normal, with TR symmetry



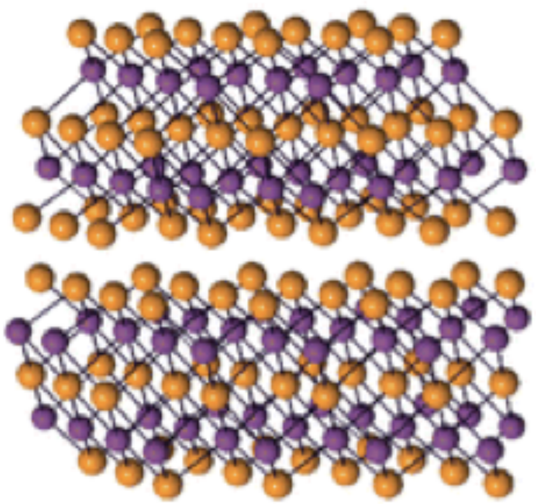
Weak TI



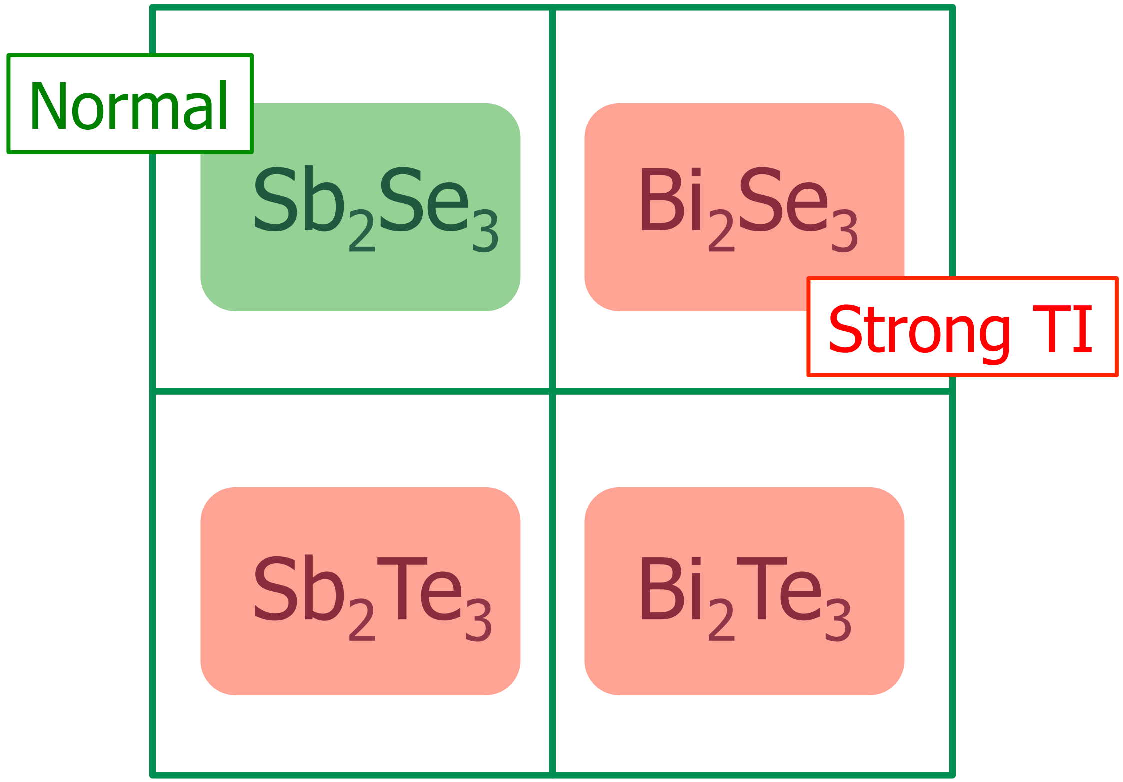
Strong TI



Chalcogenides of Bi_2Se_3 class

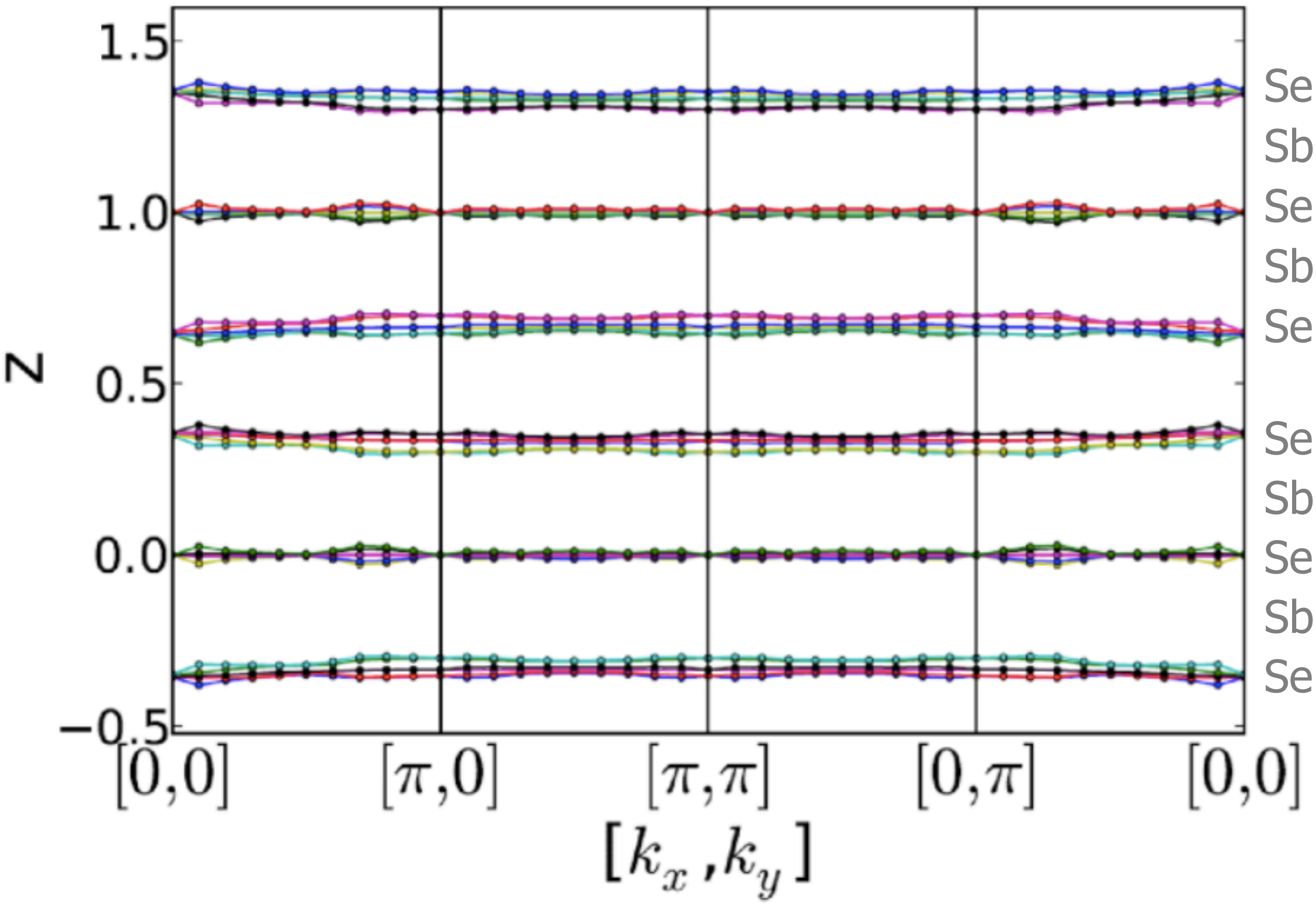


J. J. Cha,

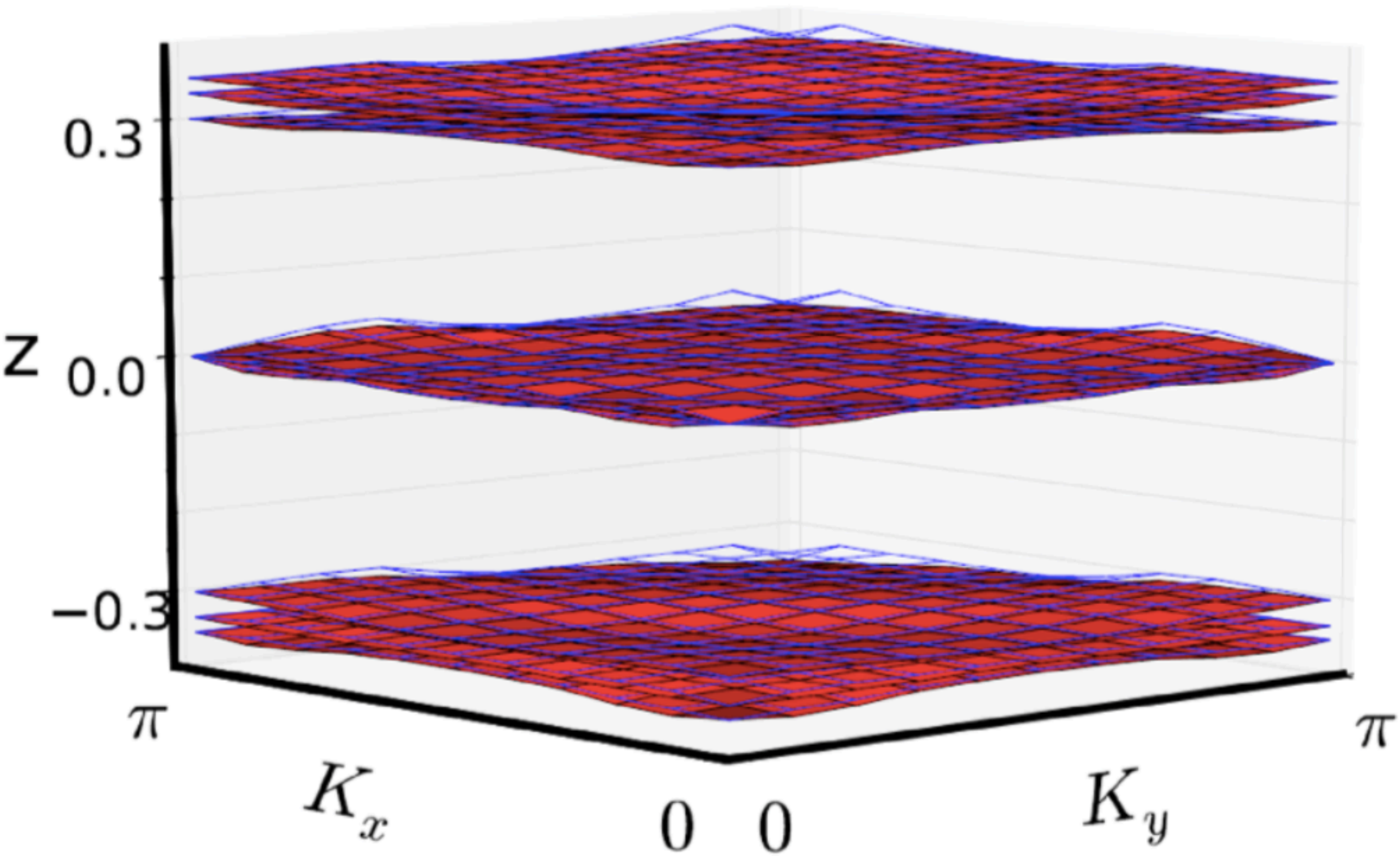


First-principles DFT calculations of "WCC bands" :

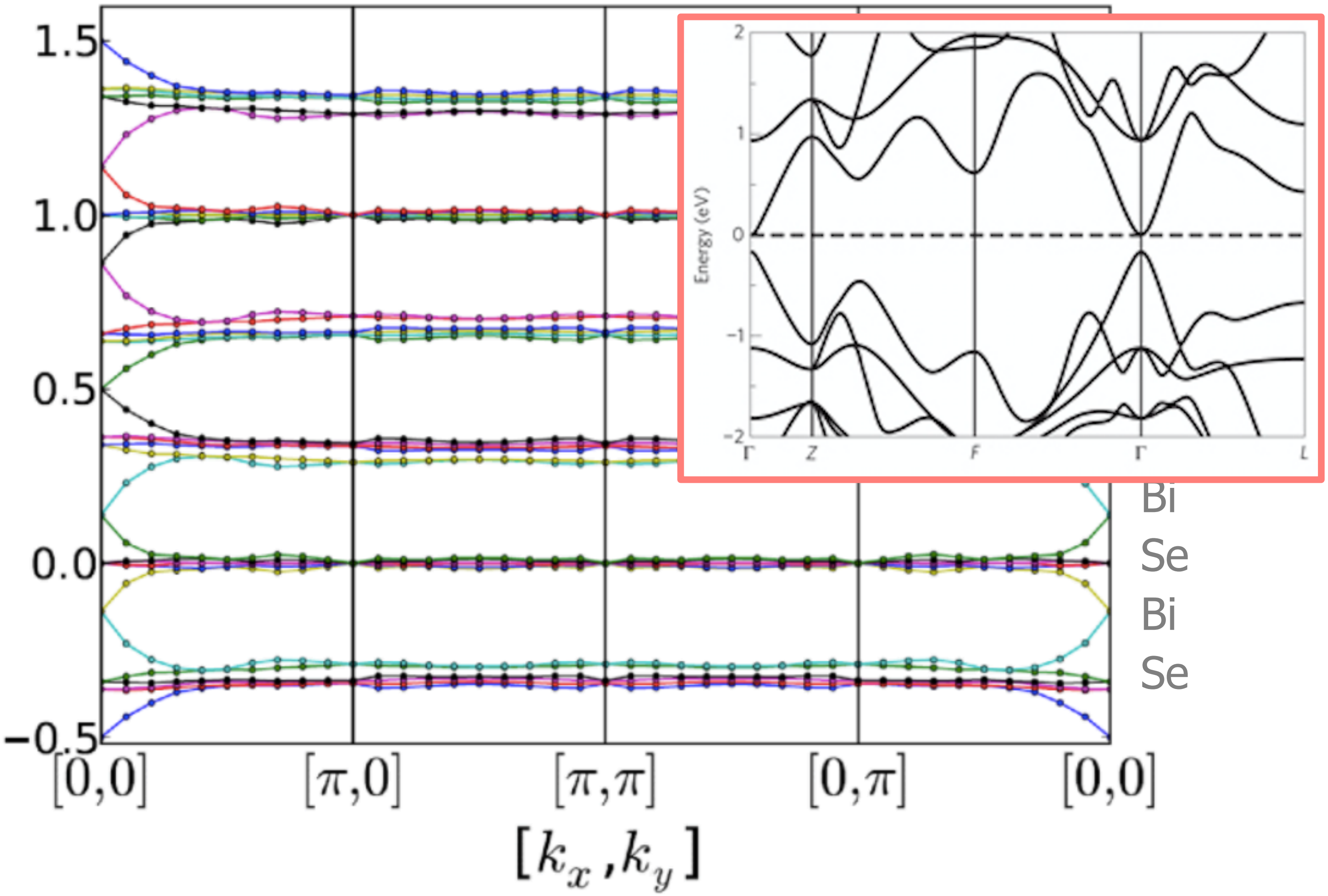
Normal insulator: Sb_2Se_3



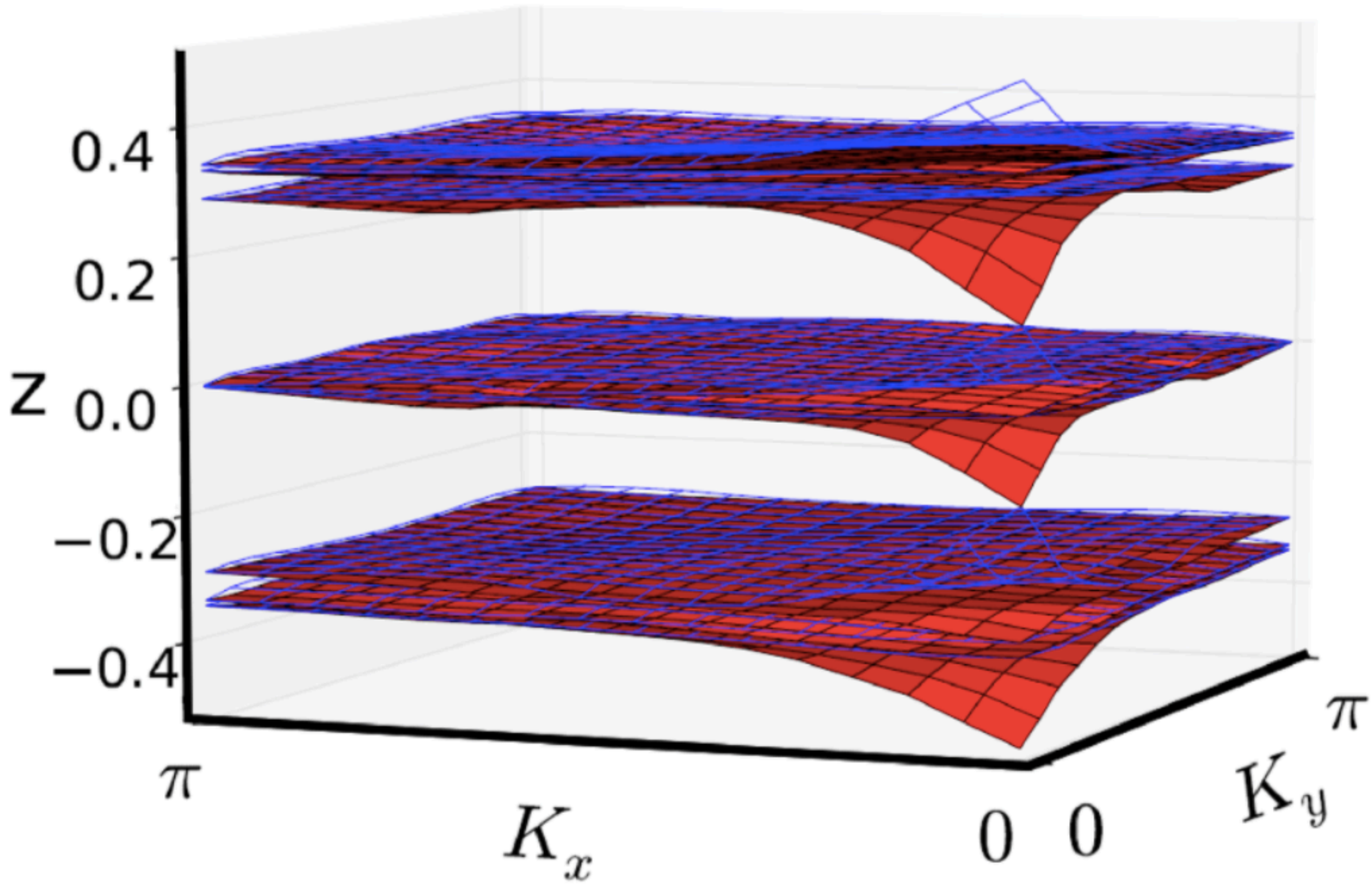
Normal insulator: Sb_2Se_3



Strong TI: Bi_2Se_3



Strong TI: Bi_2Se_3



More kinds of topological insulators

TR broken

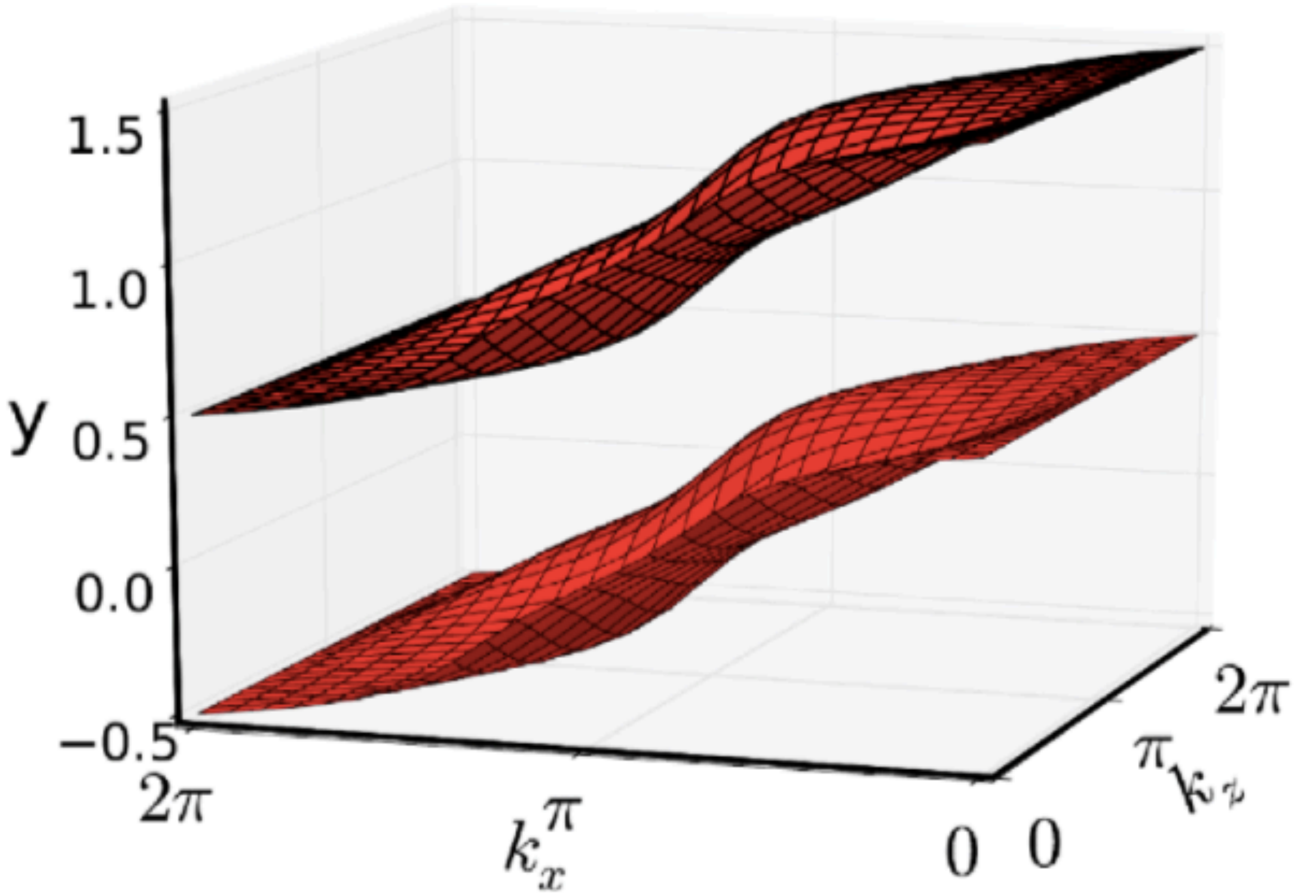
- 2D QAH
- 3D QAH
  - Stacks of QAH layers

TR invariant

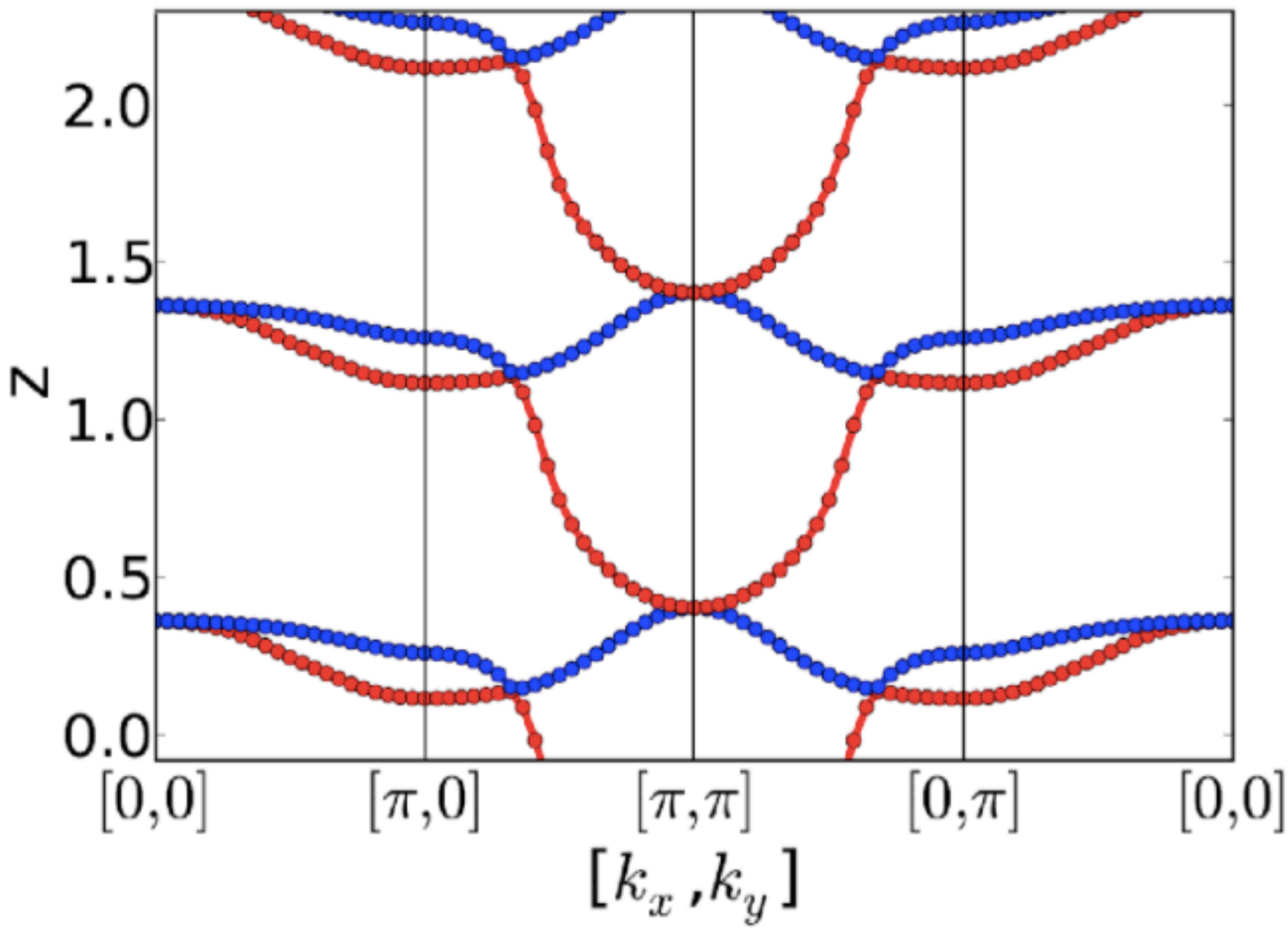
- 2D quantum spin Hall (QSH)
  - Like two +/- copies of QAH SOC added
- 3D weak TI
  - Stacks of QSH layers
- 3D strong TI
  - Like 3D weak TI, but with 3D entanglement
- “Crystalline TI”

Etc.

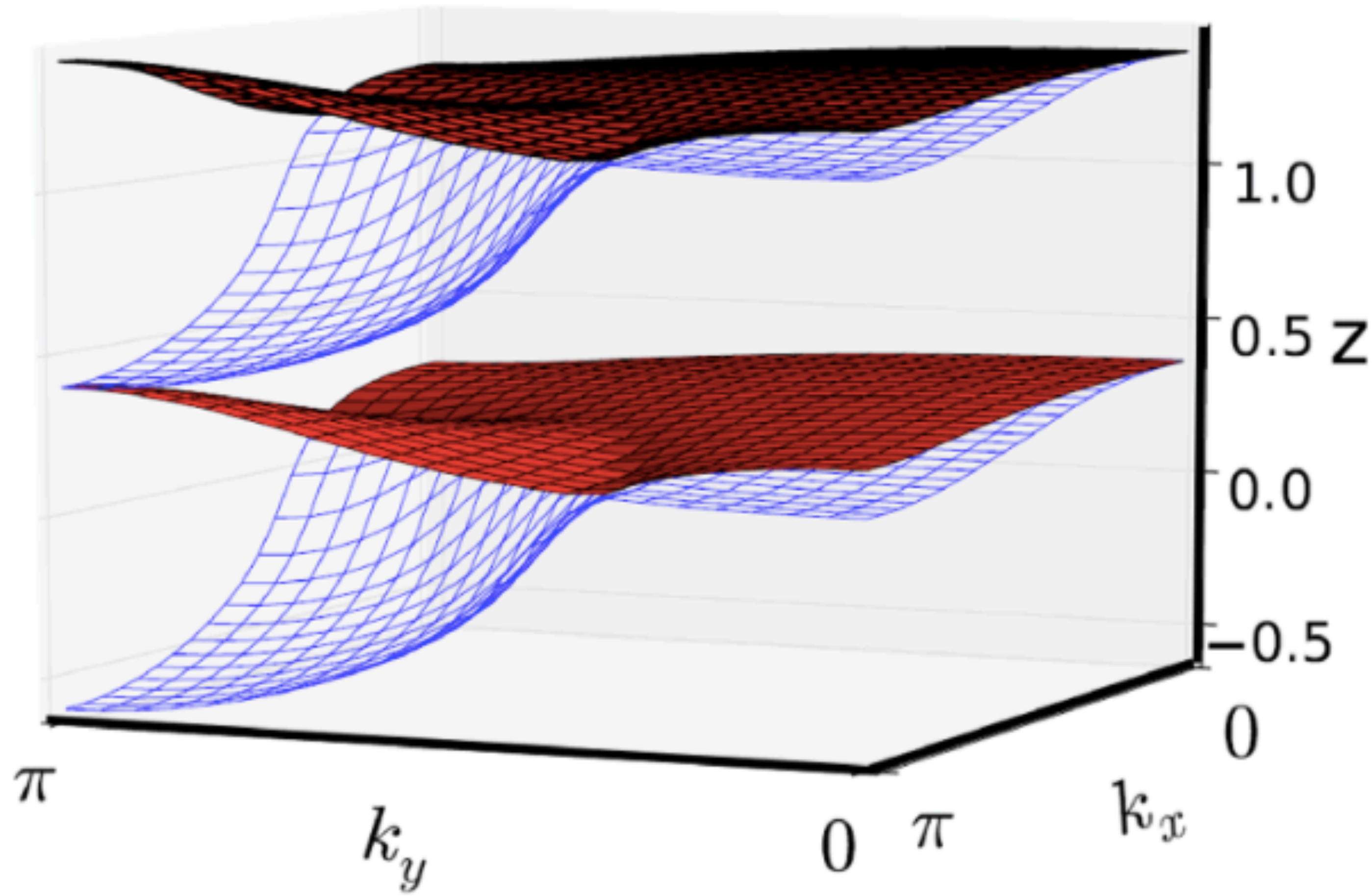
3D QAH (model Ham.)



Crystalline TI (Fu, PRL 106, 106802 (2011)



Crystalline TI (Fu, PRL 106, 106802 (2011))



Summary

- How are Bloch functions twisted in a TI
- We advocate use of tool:
  - 1D Wannier centers vs. other *k*-vector(s)
- Illustrated for
  - 2D Quantum Hall
  - 2D Quantum spin Hall
  - 3D topological insulators
- Not covered here
  - Weyl semimetals
  - Adiabatic pumping
  - Relation to surface states