Adiabatic cycles, surface anomalous Hall conductivity, and Chern-Simons axion coupling

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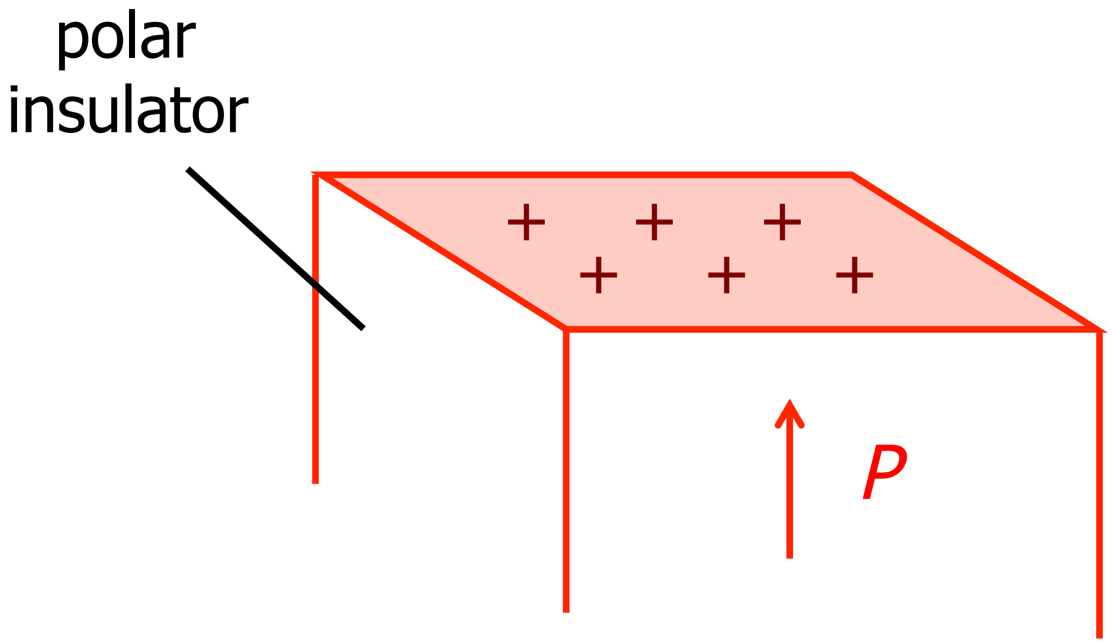
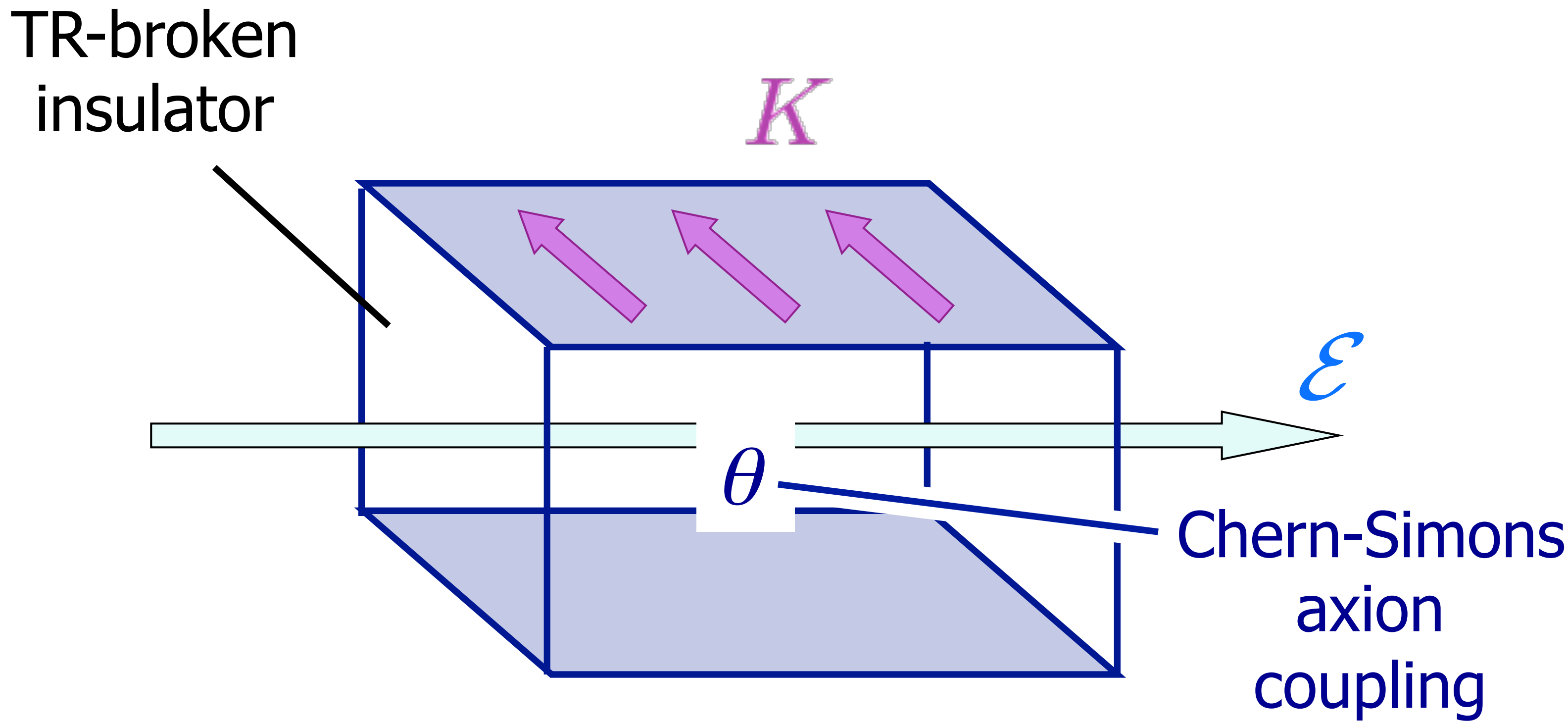
NSF DMR-1408838

Surface charge



Surface anomalous Hall conductivity

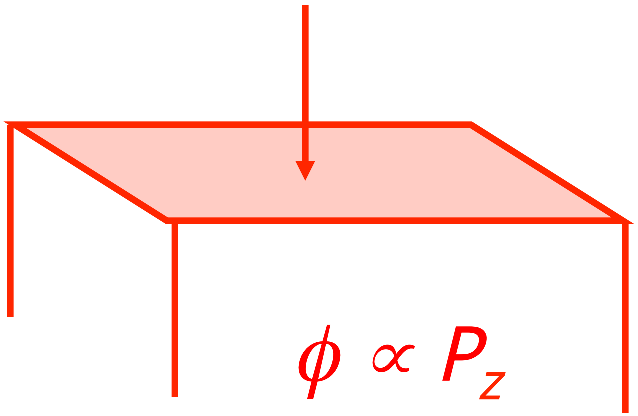


Anomalous Hall Conductivity = "AHC"

Insulating surface of bulk insulator

Surface charge

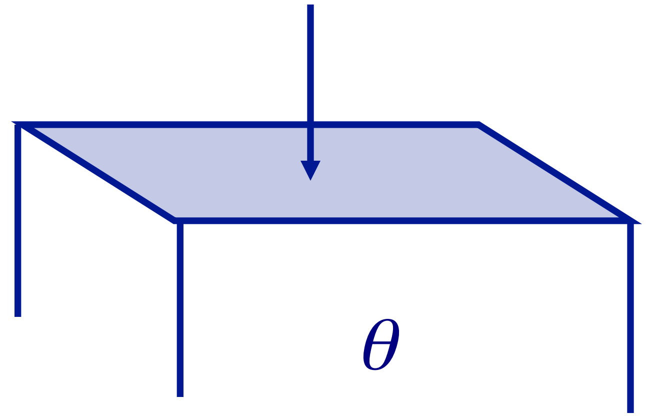
$$\sigma = \frac{-e}{A}\left[\frac{\phi}{2\pi} + \text{integer}\right]$$



ϕ is ill-defined modulo 2π

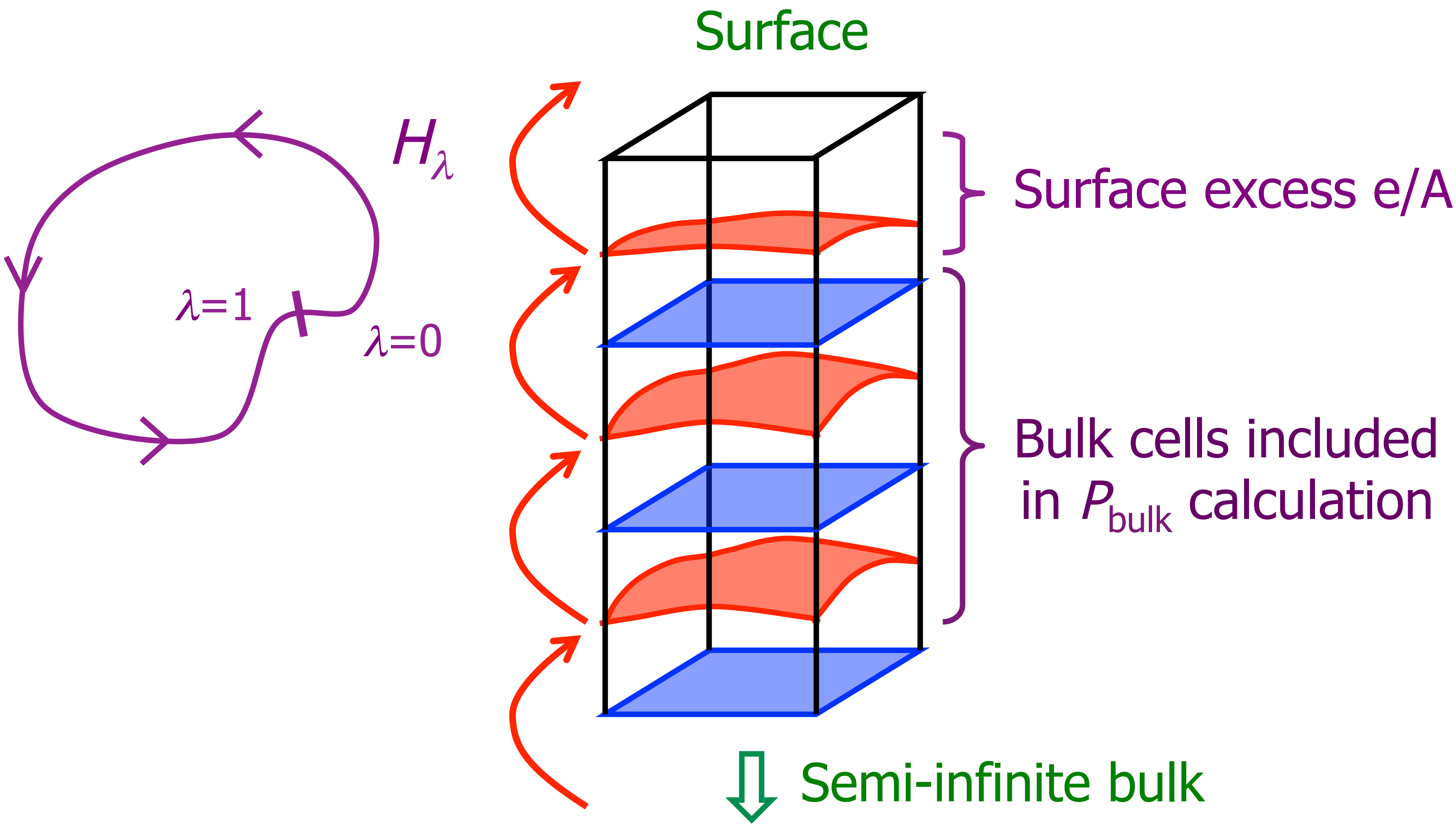
Surface AHC

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

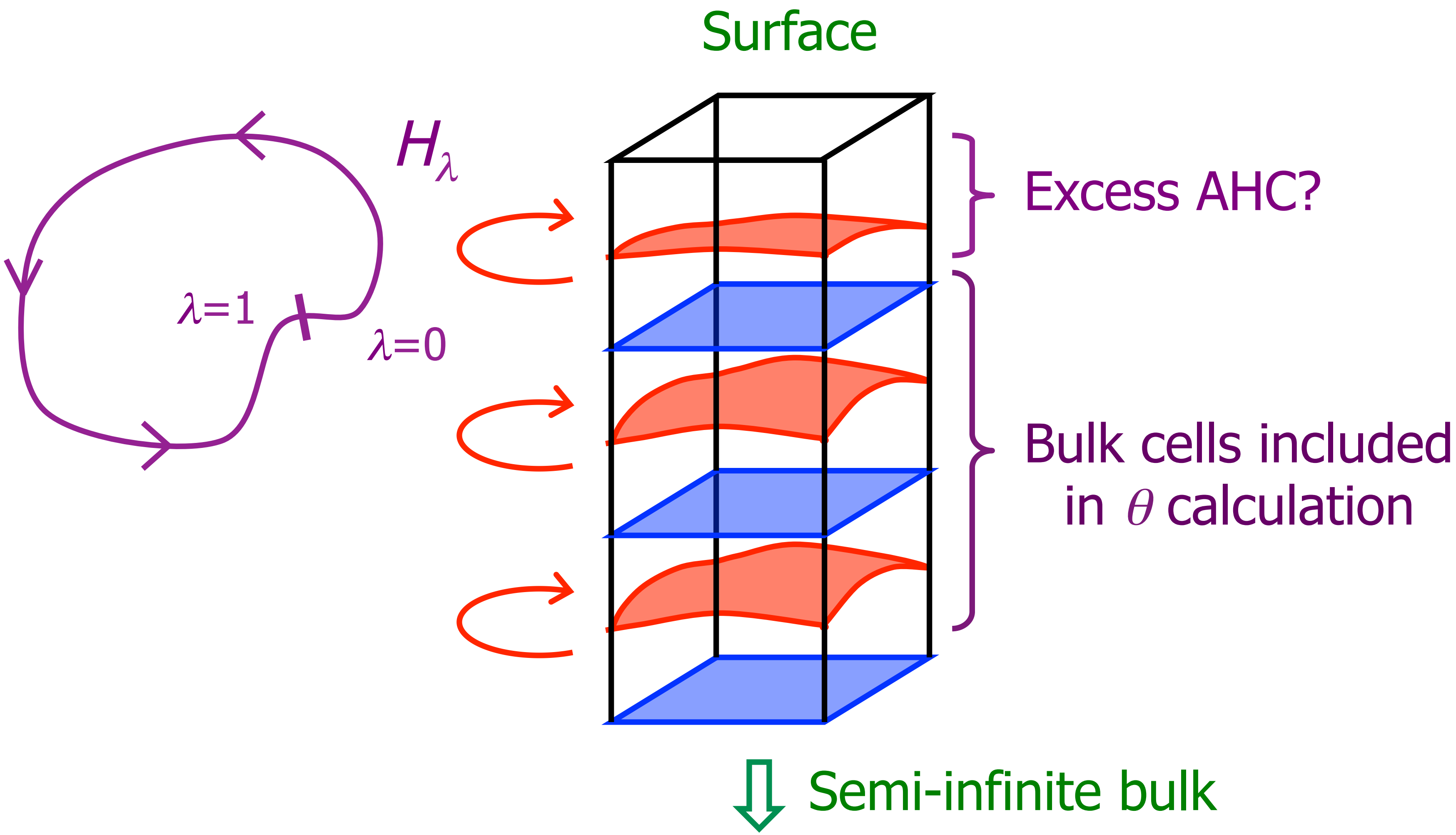


θ is ill-defined modulo 2π

Adiabatic charge pump



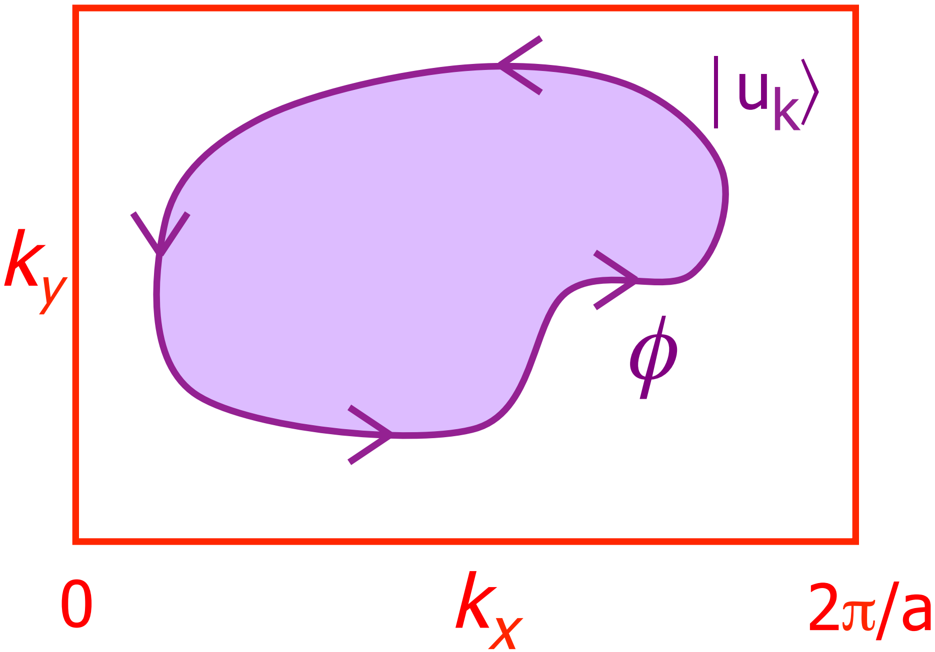
Adiabatic AHC pump ?



Outline

- Polarization in 1D
- Polarization in 3D
  - Hybrid Wannier representation
  - Surface charge theorem
- Axion magnetoelectric coupling
  - Hybrid Wannier representation
  - Surface AHC theorem
- Adiabatic loop
  - Charge pump / axion pump
- Summary & Conclusions

Berry phase and curvature in the BZ



$$u_{\mathbf{k}}(\mathbf{r}) = e^{-i\mathbf{k}\cdot\mathbf{r}}\psi_{\mathbf{k}}(\mathbf{r})$$

Bloch function

Berry potential:

$$\mathbf{A}(\mathbf{k}) = -\mathrm{Im}\,\langle u_{\mathbf{k}}|\nabla_{\mathbf{k}}|u_{\mathbf{k}}\rangle$$

Berry phase:

$$\phi = \oint \mathbf{A}(\mathbf{k})\cdot d\mathbf{k}$$

Berry curvature:

$$\Omega(\mathbf{k}) = \nabla\times\mathbf{A}$$

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

Stoke's theorem:

$$\phi = \int \Omega_z(\mathbf{k})\,d^2k$$

Gauge dependence

- Gauge change:

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

- Result:

$$\mathbf{A}(\mathbf{k}) \rightarrow \mathbf{A}(\mathbf{k}) + \nabla_{\mathbf{k}}\beta$$

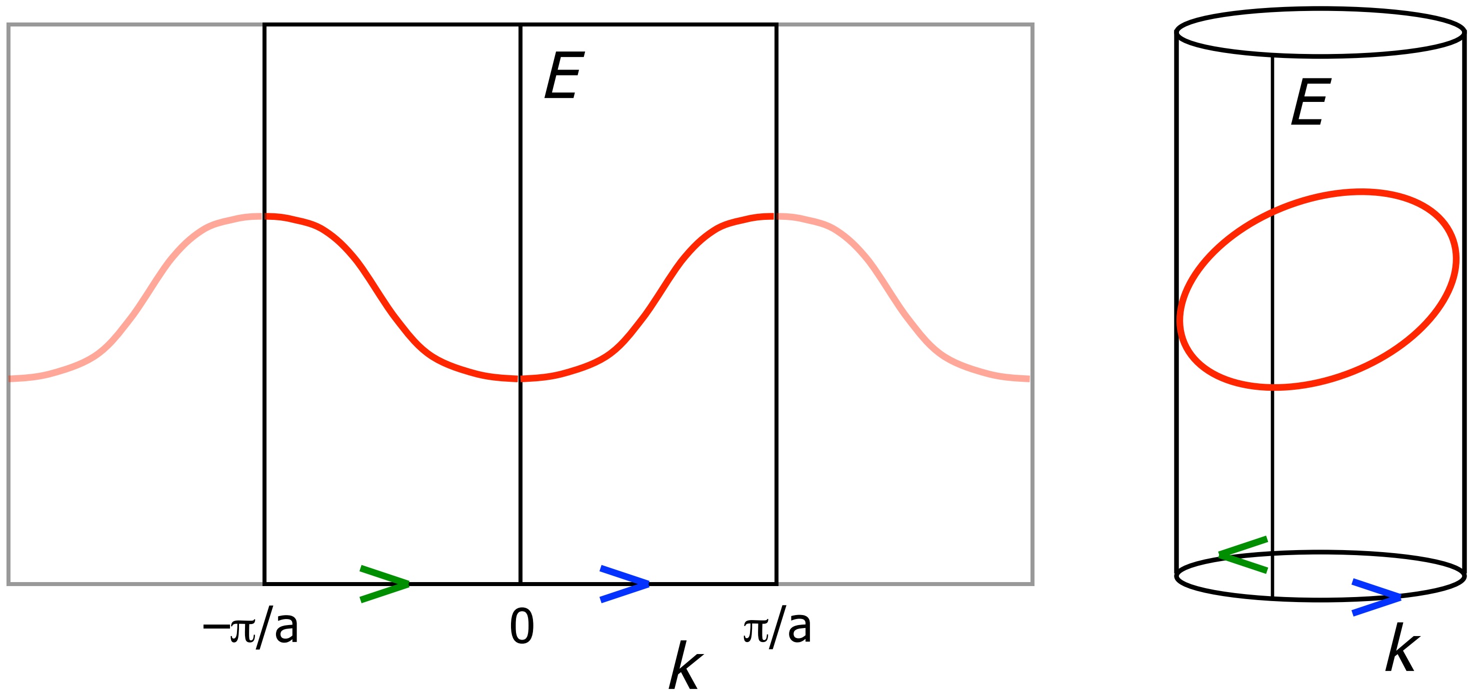
$$\phi \rightarrow \phi + 2\pi n$$

Winding of β

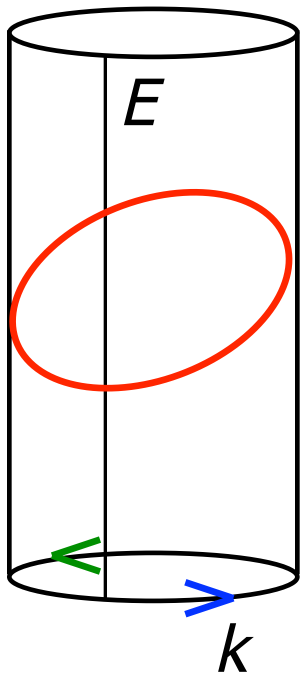
$$\Omega(\mathbf{k}) \rightarrow \Omega(\mathbf{k})$$

1D: BZ is really a loop

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



Berry phase ⟺ Wannier center



$$\phi = \oint A(k)\, dk$$

$$= \oint i \langle u_k | \partial_k u_k \rangle\, dk$$

$$x_c = \langle w_n | \hat{x} | w_n \rangle$$

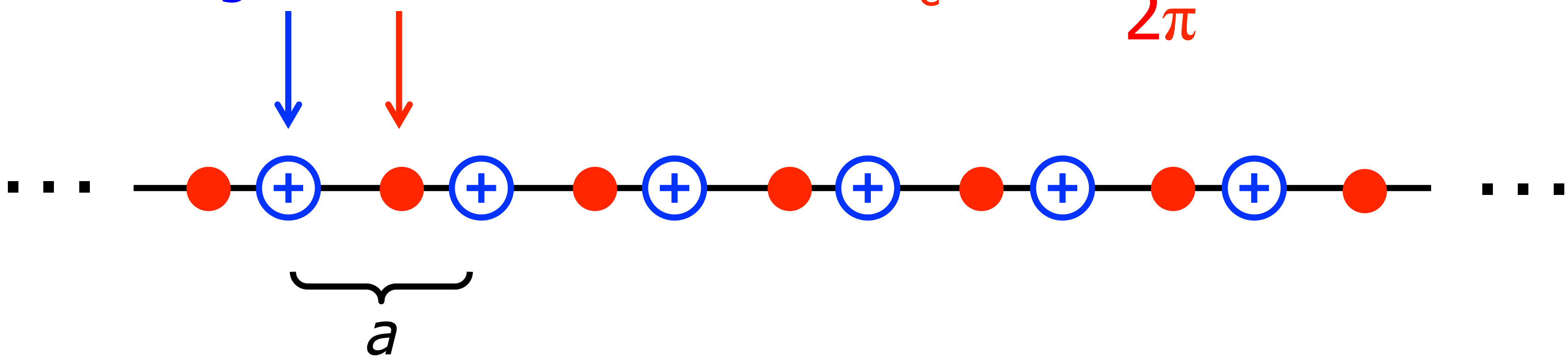
$$w_n(x-R) = \sum_k e^{ik(x-R)}\, \psi_{nk}(x)$$

$$\boxed{x_c = \frac{\phi}{2\pi}}$$

Polarization and Wannier centers (1D)

Origin

Wannier center $x_c = a \dfrac{\phi}{2\pi}$ ← Berry phase



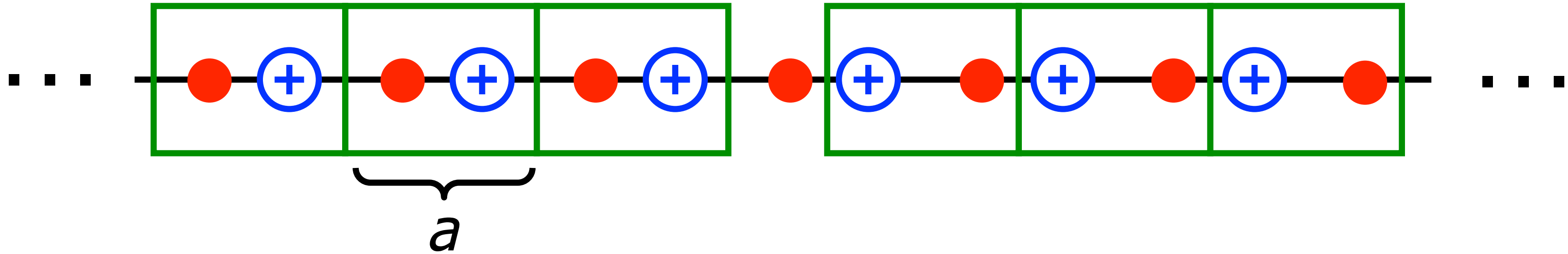
⊕ Ionic charges

● Wannier centers

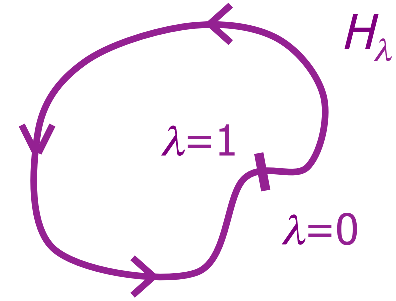
Quantum of polarization: $\Delta P = e$

$$\Delta P = e$$

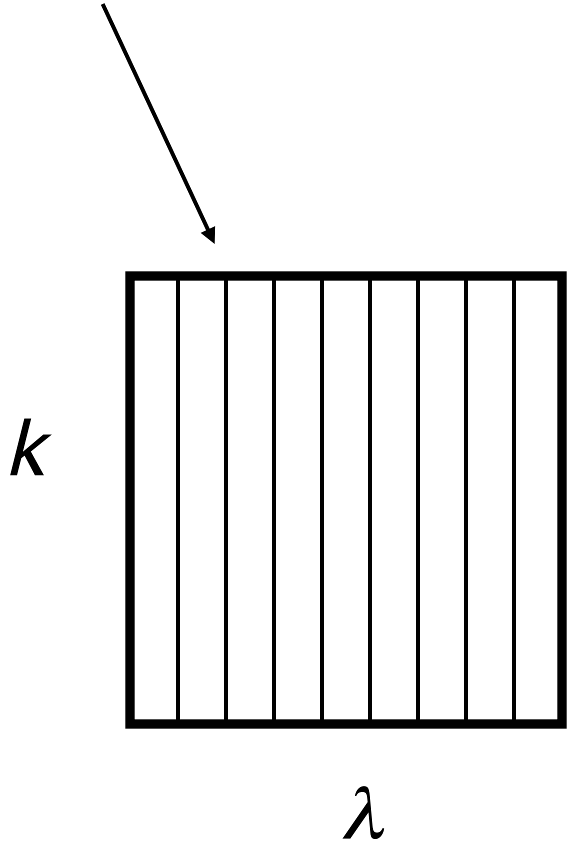
P = dipole / a $\quad$ P' = dipole / a

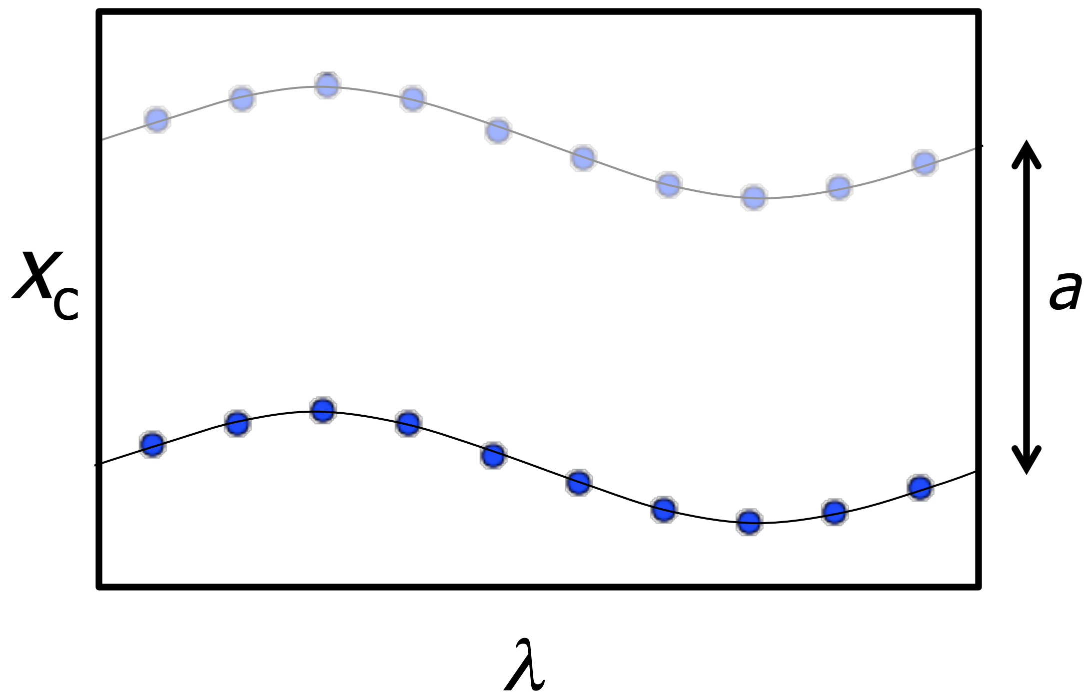


Adiabatic cycle - No pumped charge



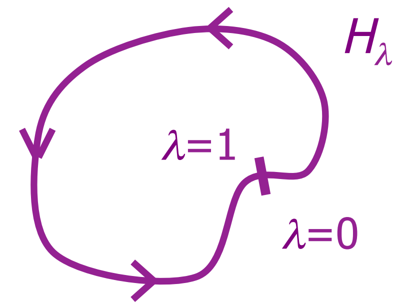
$x_c\,(\lambda)$ = Wannier center at given λ

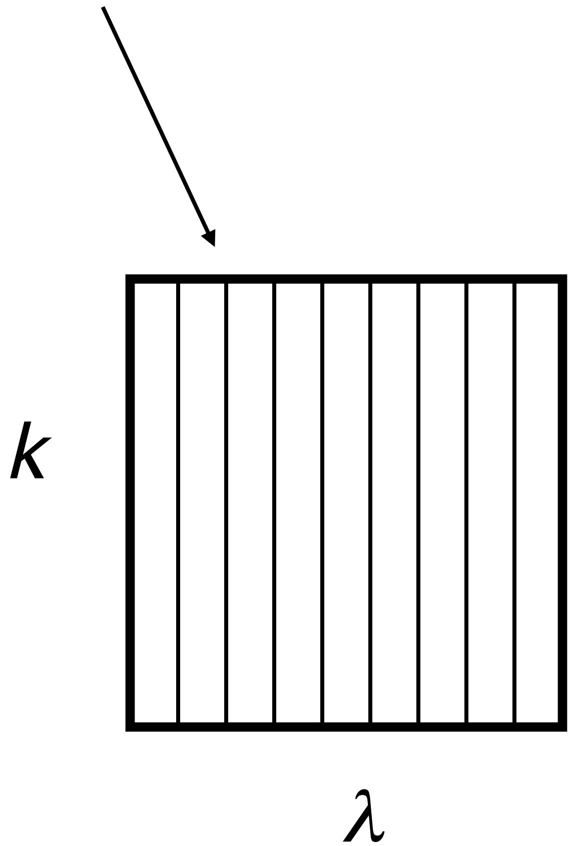


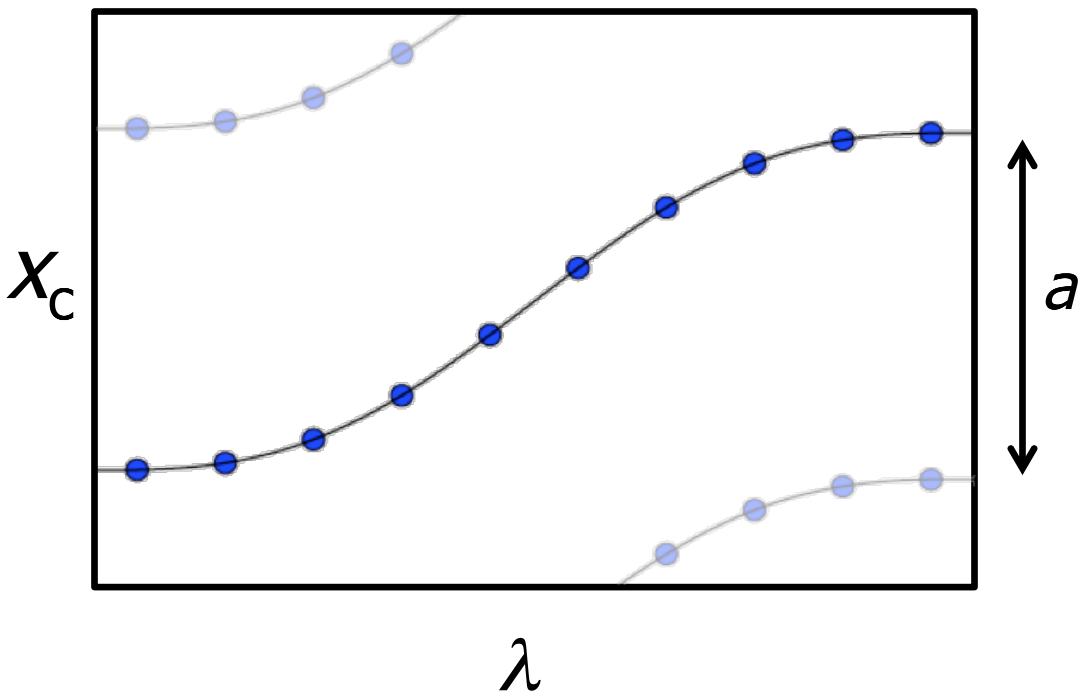


Adiabatic cycle - Quantum charge pump

$x_c(\lambda)$ = Wannier center at given λ







Wannier centers: Extended and finite

Infinite chain:

$$x_c = \frac{\phi}{2\pi}$$

Equivalently, x_c = eigenvalues of $\mathcal{P}x\mathcal{P}$ where

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

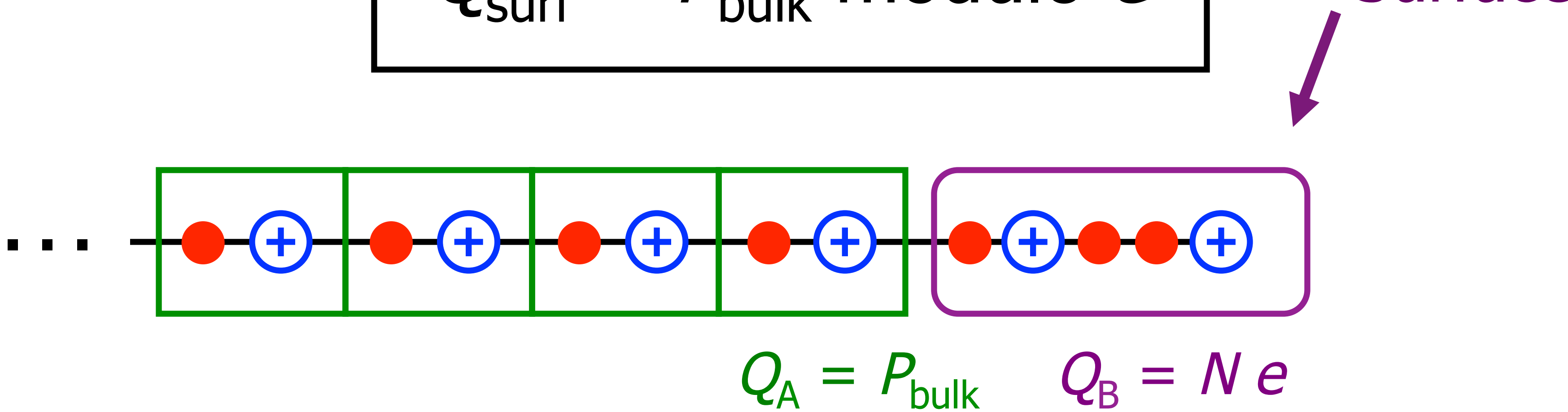
Finite chain

x_c = eigenvalues of $\mathcal{P}x\mathcal{P}$ where

$$\mathcal{P} = \sum_n^{\text{occ}} |\psi_n\rangle\langle\psi_n|$$ (finite chain eigenvectors)

Surface charge theorem: 1D

$$Q_{\text{surf}} = P_{\text{bulk}} \text{ modulo } e$$

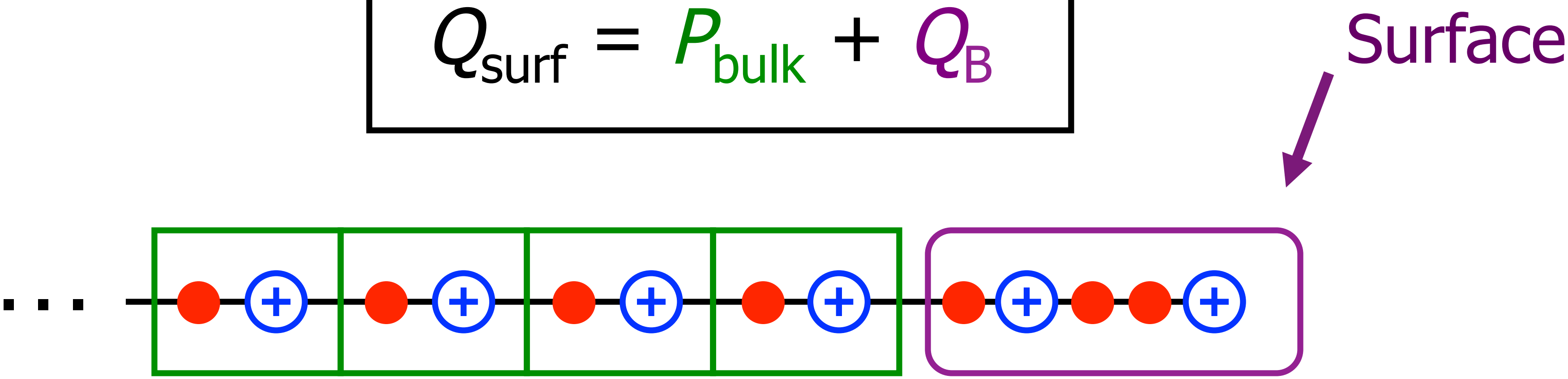


- Wannier centers: Eigenvalues of $\mathcal{P}x\mathcal{P}$

$$\mathcal{P} = \sum_n^{\text{occ}} |\psi_n\rangle\langle\psi_n|$$

Surface charge theorem: 1D

$$Q_{\text{surf}} = P_{\text{bulk}} + Q_{\text{B}}$$



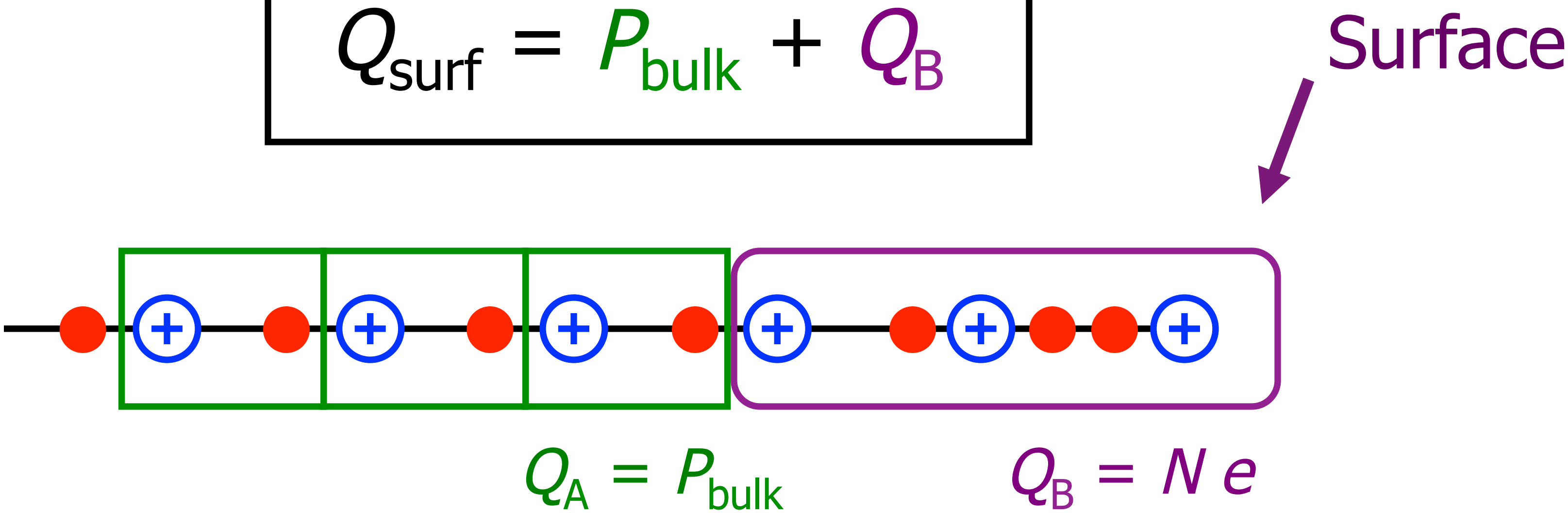
$Q_{\text{A}} = P_{\text{bulk}}$ $\quad Q_{\text{B}} = N\,e$

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

$$\mathcal{P} = \sum_{n}^{\text{occ}} |\psi_n\rangle\langle\psi_n|$$

Surface charge theorem: 1D

$$Q_{\text{surf}} = P_{\text{bulk}} + Q_B$$



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

$$\mathcal{P} = \sum_n^{\text{occ}} |\psi_n\rangle\langle\psi_n|$$

Surface charge theorem: 1D

Conclusions:

- $Q_{\text{surf}} = P_{\text{bulk}}$ modulo e
- To get correct branch choice, compute Wannier centers at the end of the chain

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

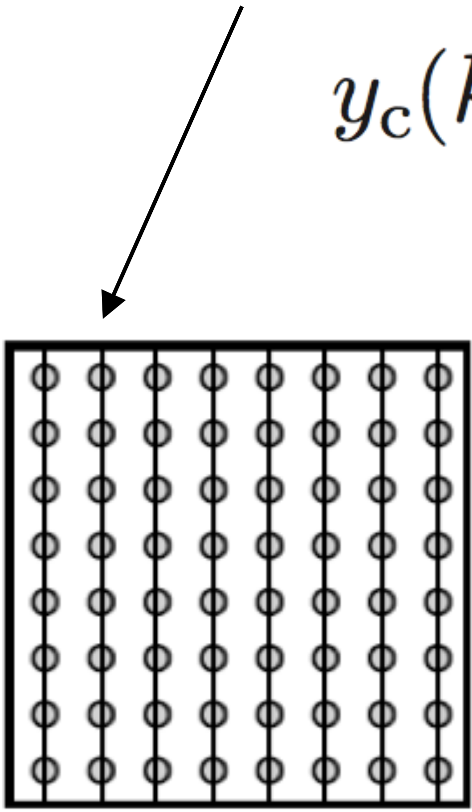
1D insulator with adiabatic parameter

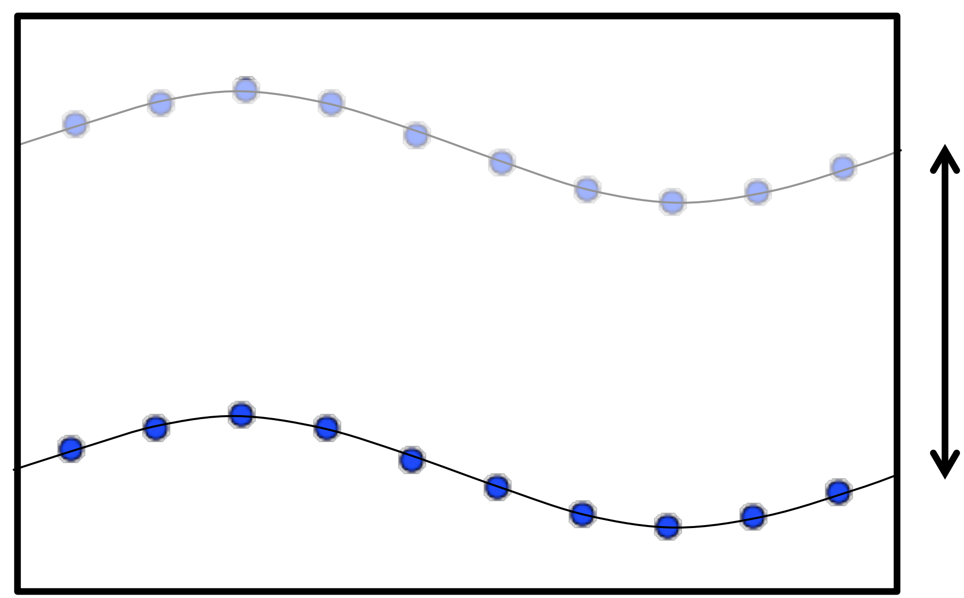
2D insulator

Hybrid Wannier centers: y_c vs. k_x

At each k_x, find 1D WF along y, and their centers

$$y_c(k_x) = \langle h_{n,k_x} | \hat{y} | h_{n,k_x} \rangle$$

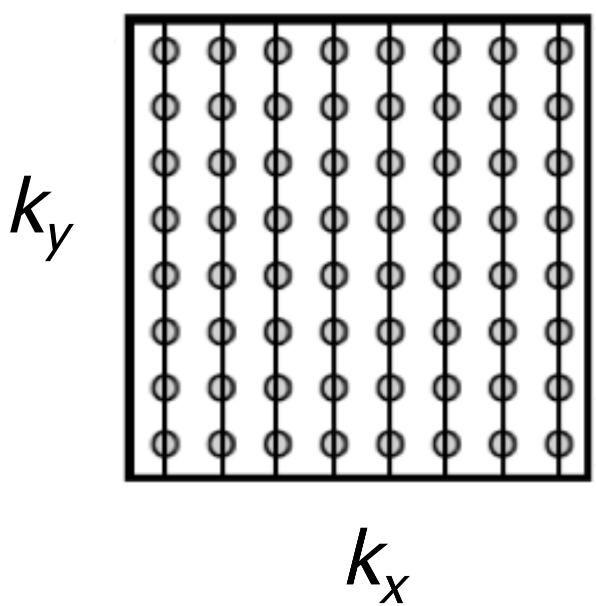


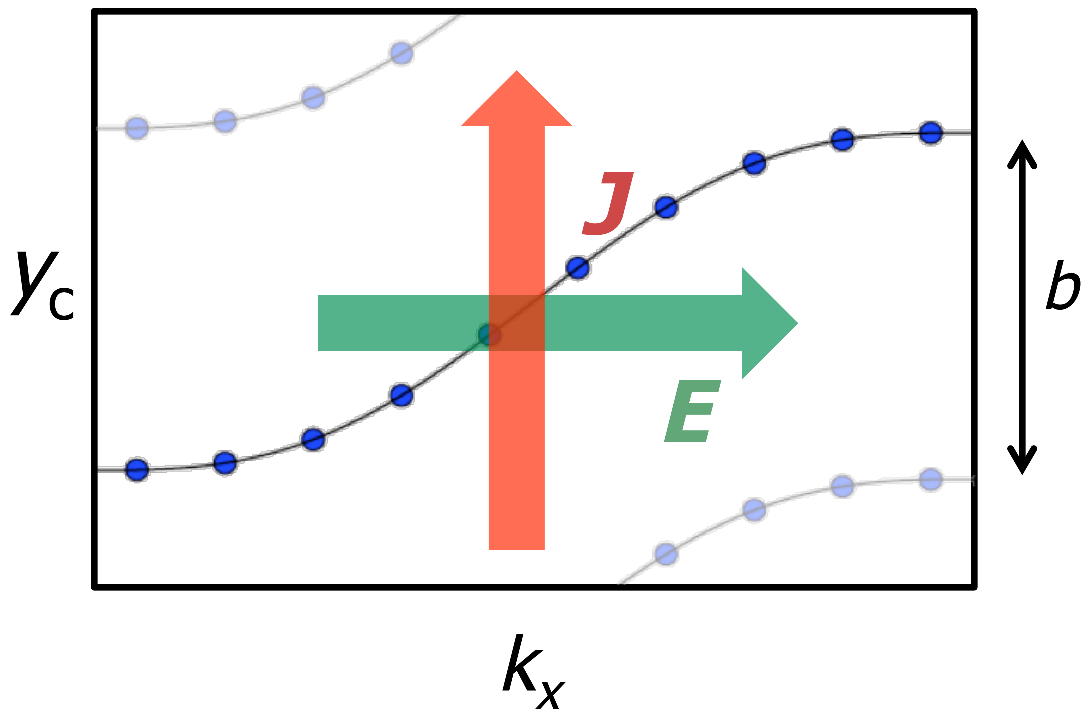


Quantum Anomalous Hall (QAH)

At each k_x, find 1D WF along y, and their centers

$$y_c(k_x) = \langle h_{n,k_x} | \hat{y} | h_{n,k_x} \rangle$$

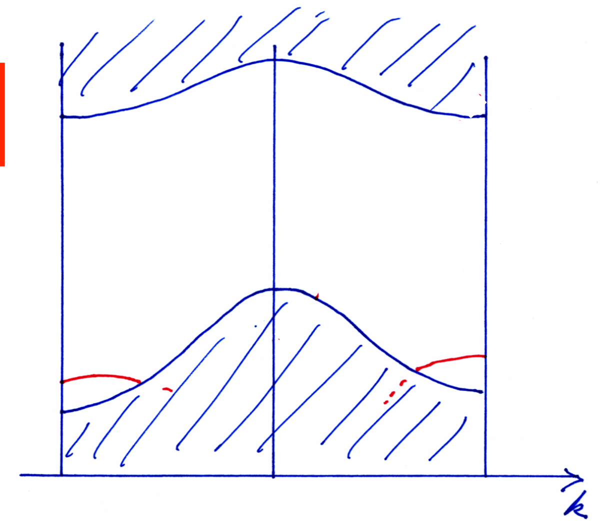




Edge states ↔ Wannier center flow

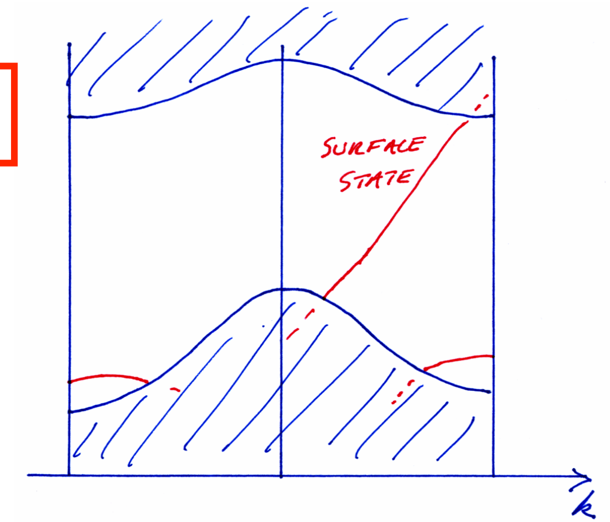
$C = 0$

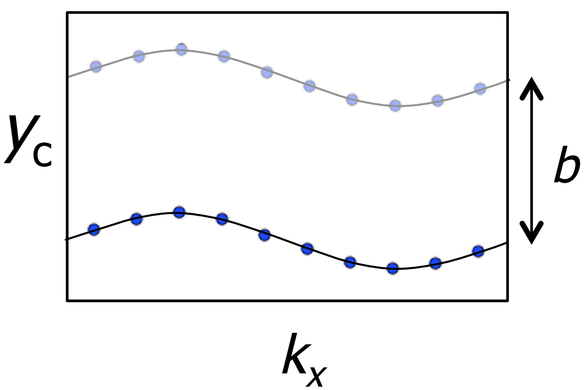
Normal

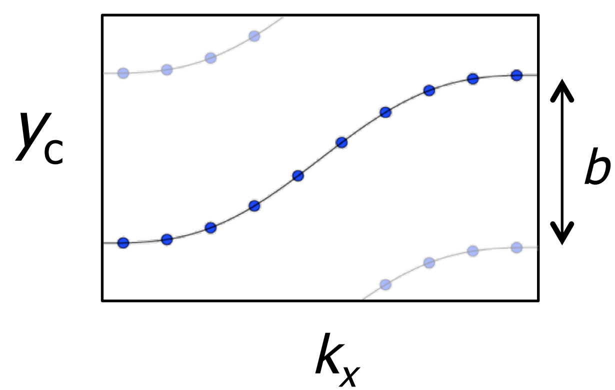


$C = +1$

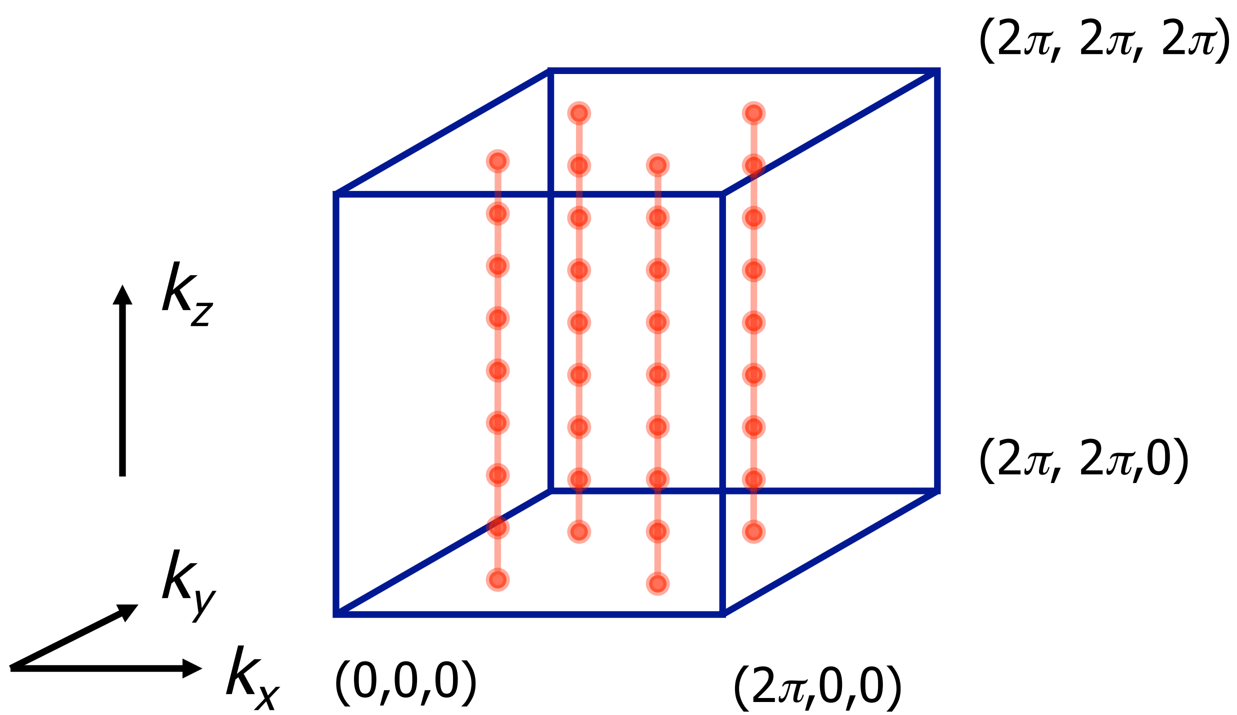
QAH (Chern ins.)







Polarization in 3D: Hybrid WFs again



Hybrid Wannier representation

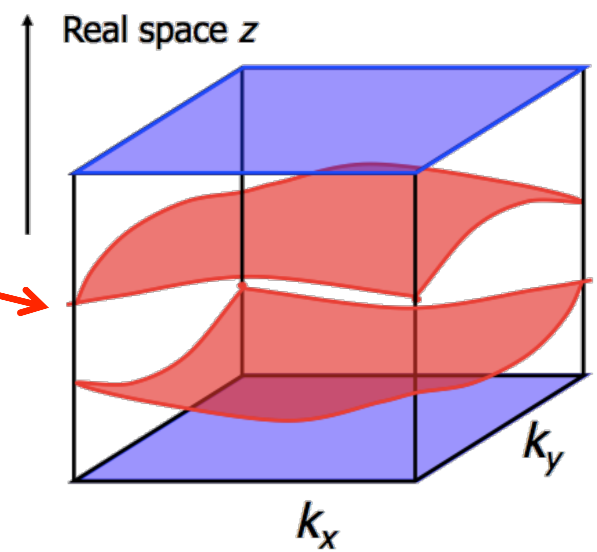
Define hybrid WFs: (maximally localized along *z*)

$$|h_{\kappa l n}\rangle = e^{-i\kappa\cdot r}\int_0^1 dk_3\, e^{-i2\pi k_3 l}\left|\psi_{(\kappa,k_3)n}\right\rangle$$

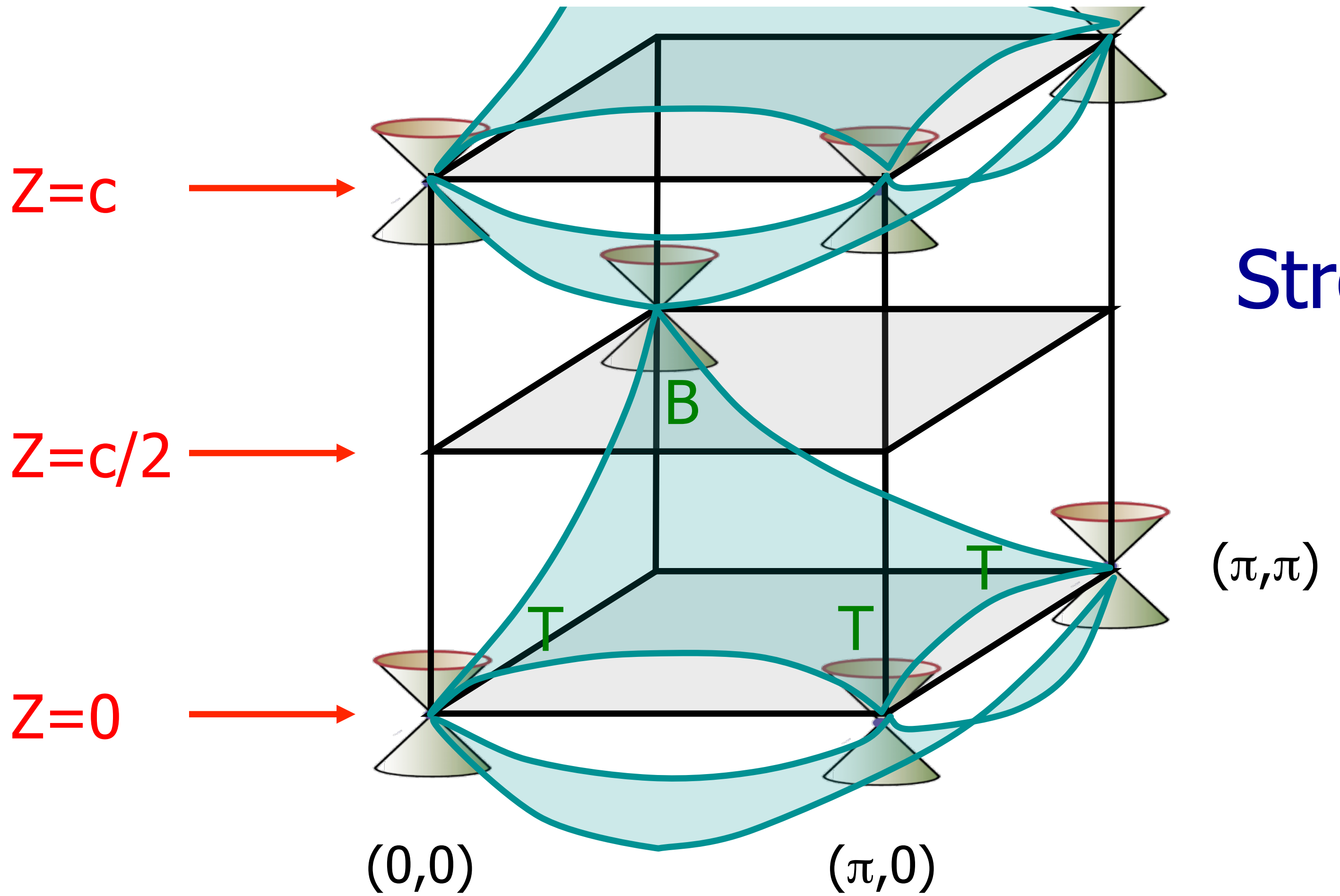
where $\kappa = k_x\hat{x} + k_y\hat{y}$

Construct hybrid WF sheets:

$$z_{\kappa l n} = \langle h_{\kappa l n}|z|h_{\kappa l n}\rangle = z_{\kappa 0 n} + lc$$

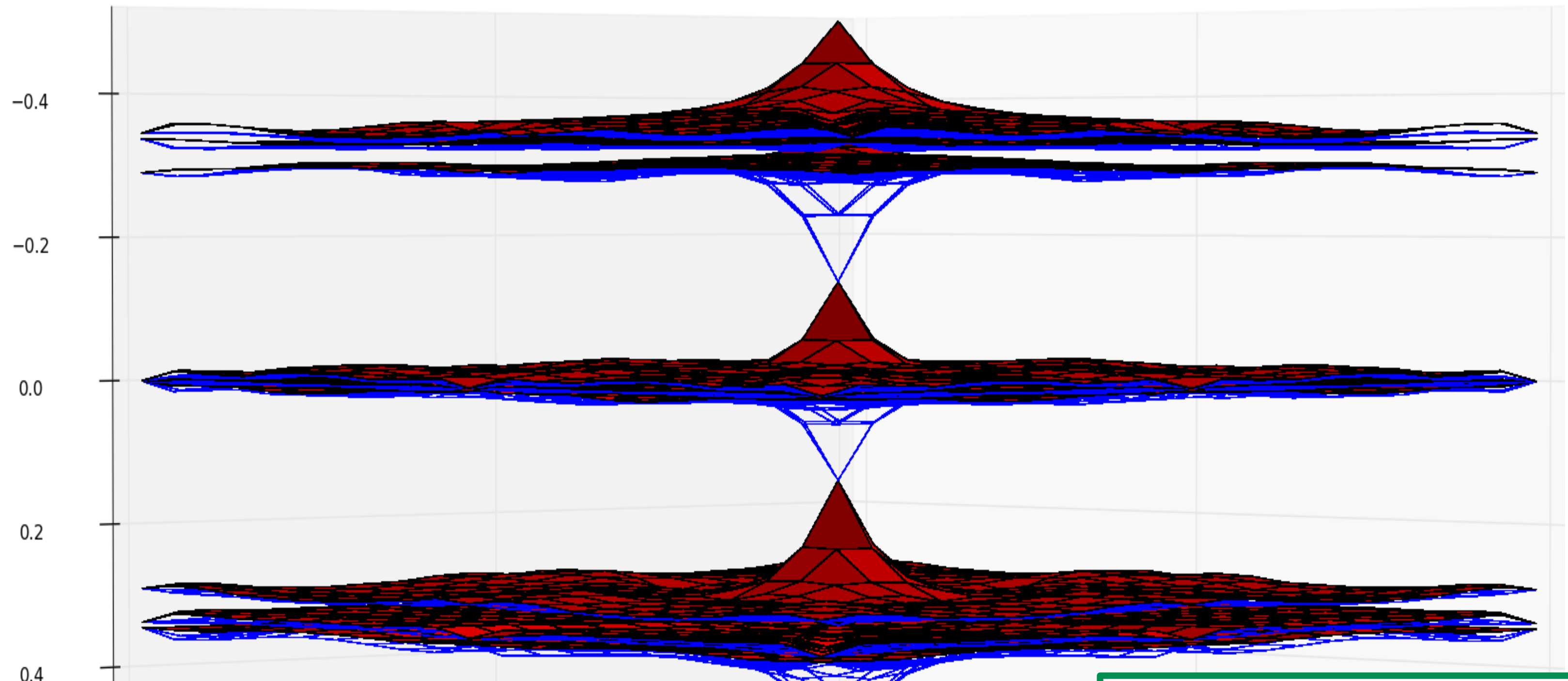


Hybrid WF sheets



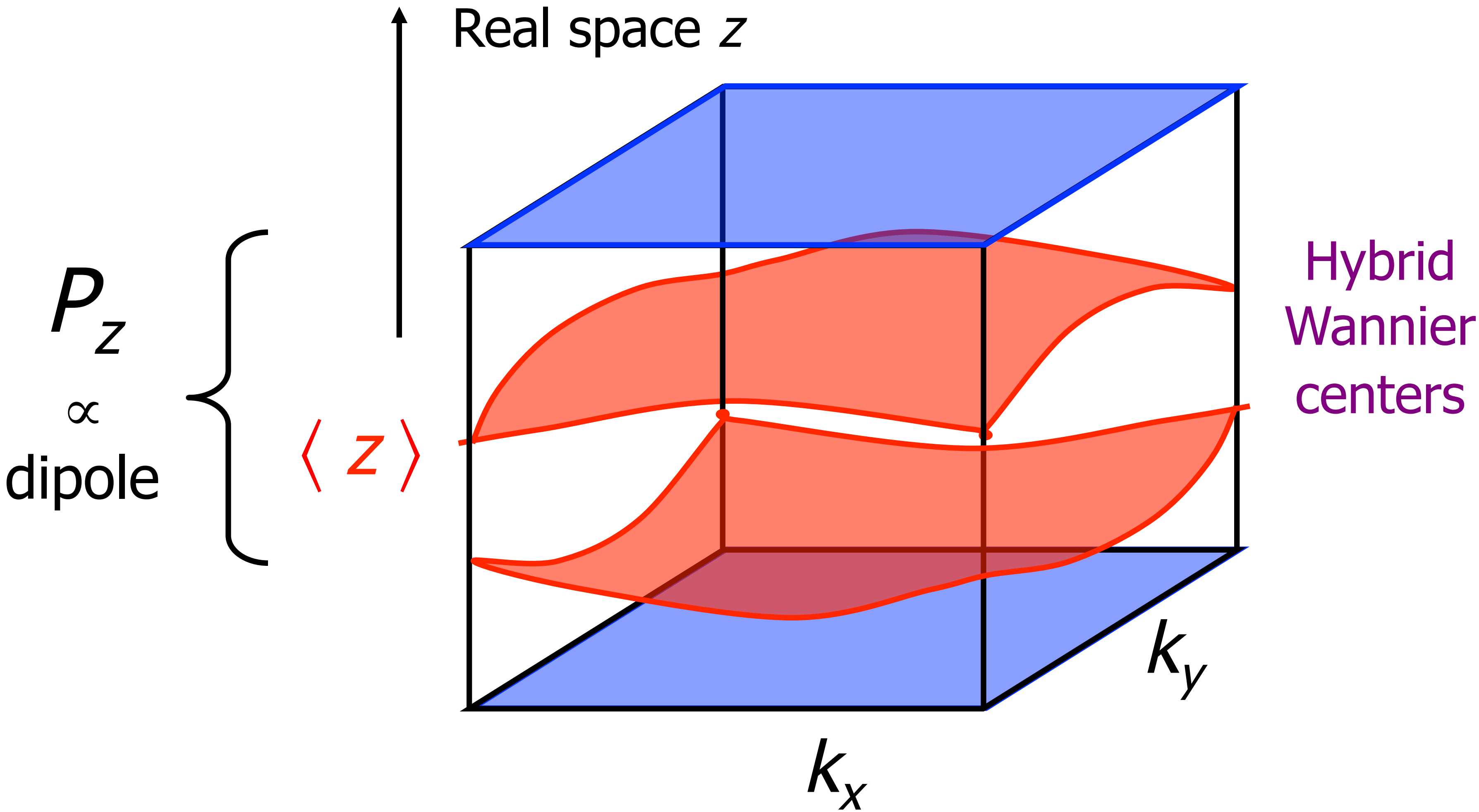
Strong TI

First-principles Bi_2Se_3 Wannier centers



Maryam Taherinejad

Polarization in 3D

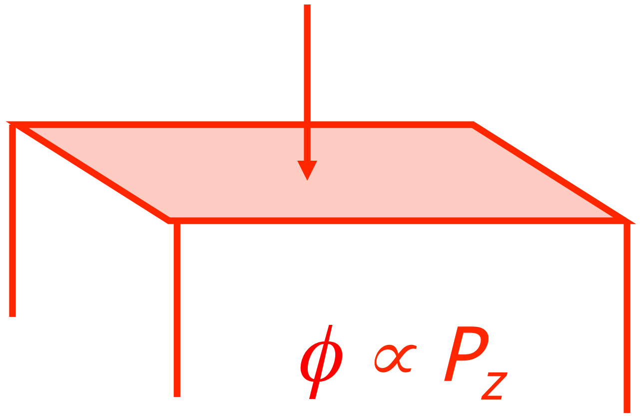


Insulating surface of bulk insulator

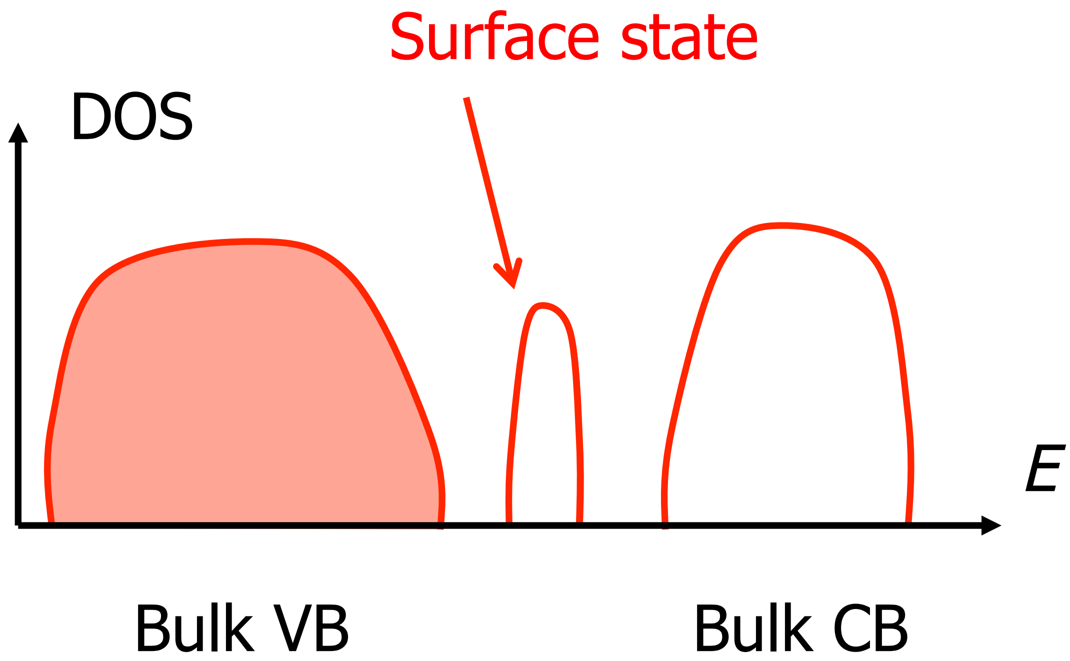
Surface charge

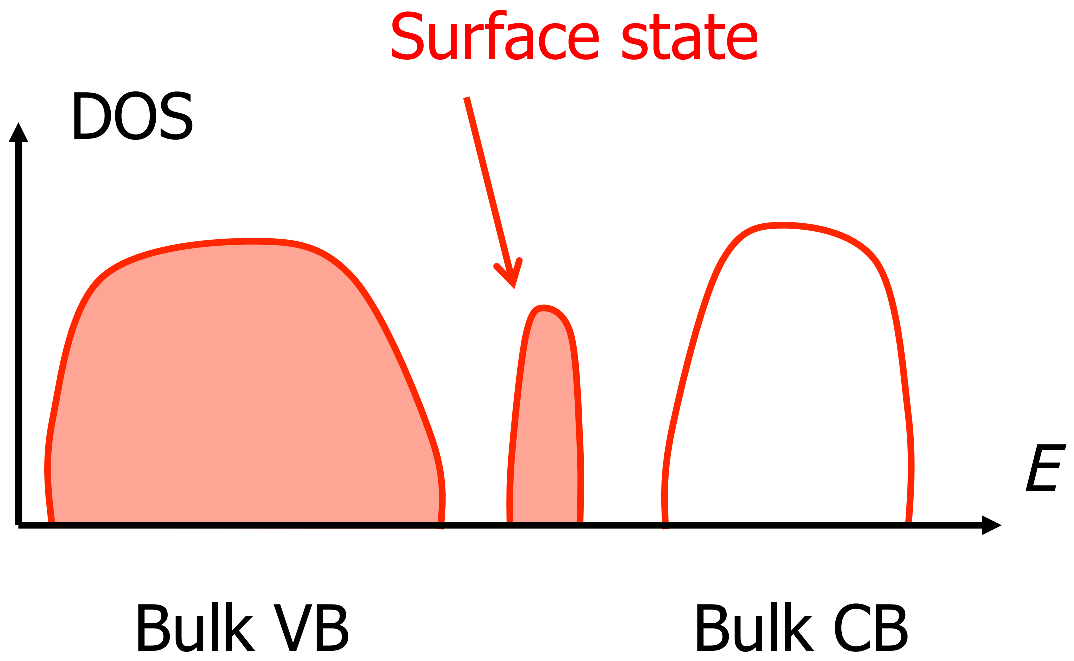
$$\sigma = \frac{-e}{A}\left[\frac{\phi}{2\pi} + \text{integer}\right]$$

?



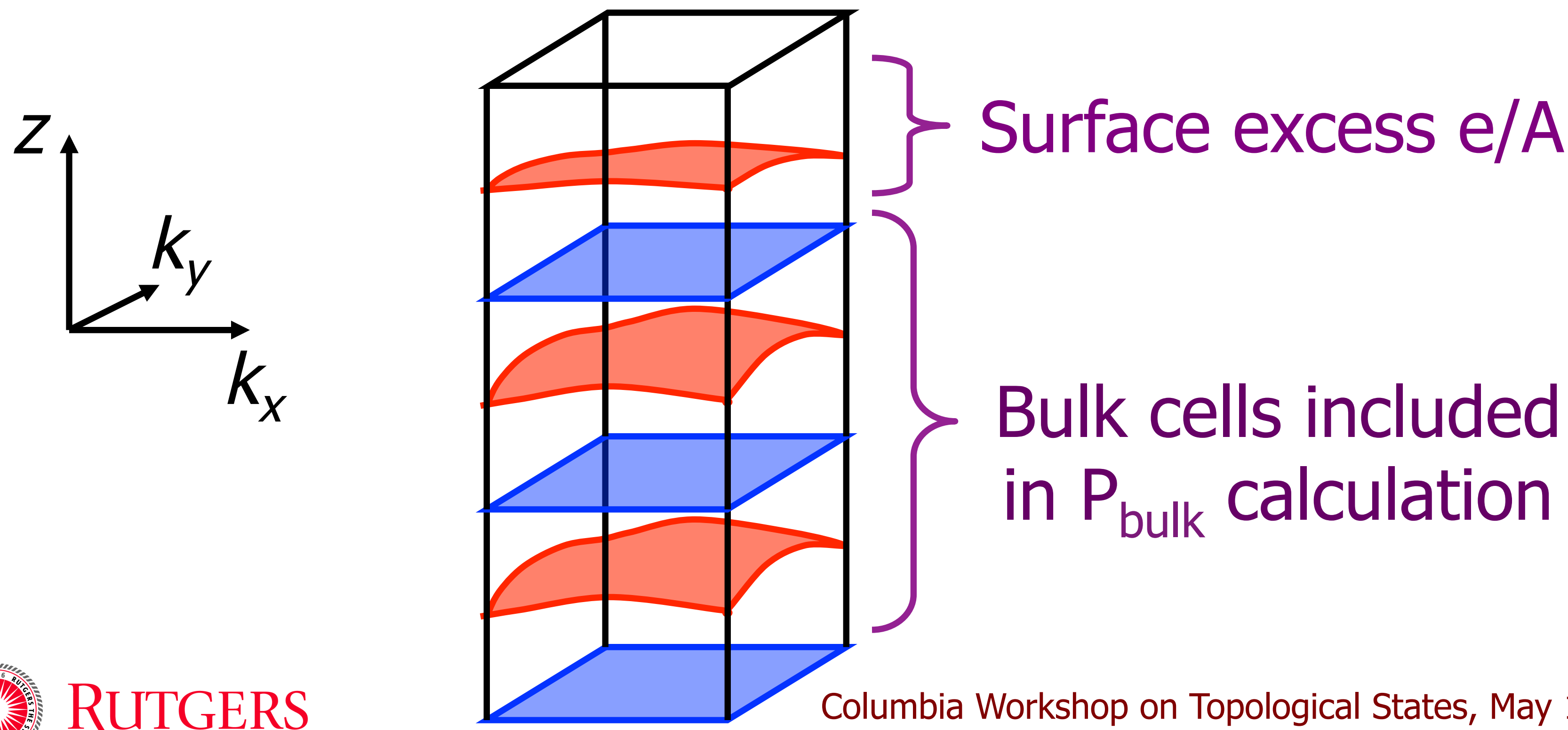
ϕ is ill-defined modulo 2π


Surface state
DOS
E
Bulk VB
Bulk CB


Surface state
DOS
E
Bulk VB
Bulk CB

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



Surface charge theorem: 3D

Conclusions:

- $\sigma_{\text{surf}} = P_{\text{bulk}}$ modulo e/A_{surf}
- To get correct branch choice, compute hybrid Wannier sheets at the surface

Outline

- Polarization in 1D
- Polarization in 3D
  - Hybrid Wannier representation
  - Surface charge theorem
- Axion magnetoelectric coupling
  - Hybrid Wannier representation
  - Surface AHC theorem
- Adiabatic loop
  - Charge pump / axion pump
- Summary & Conclusions

Linear magnetoelectric coupling (MEC)

$$\alpha_{ij} = \frac{-\partial^2 E}{\partial \mathcal{E}_i \partial B_j} = \frac{dP_i}{dB_j} = \frac{dM_j}{d\mathcal{E}_i}$$

$$\alpha = \alpha_{\text{lattice}} + \alpha_{\text{frozen-ion}}$$

$$\rightarrow \alpha^{\text{Zeeman}}_{\text{frozen-ion}} + \alpha^{\text{orbital}}_{\text{frozen-ion}}$$

Remainder of this talk:

Only orbital contribution to frozen-ion MEC.

Full theory of orbital MEC

$$\alpha_{da} = \alpha_{da}^{\rm LC} + \alpha_{da}^{\rm IC} + \alpha_{da}^{\rm geom}$$

NG = non-geometric

$$\alpha_{da}^{\rm LC} = -\frac{e}{\hbar c}\epsilon_{abc}\int\frac{d^3k}{(2\pi)^3}\sum_n^N {\rm Im}\langle\widetilde{\partial}_b u_{n{\rm k}}|(\partial_c H_{\rm k})|\widetilde{\partial}_{\mathcal{E}_d} u_{n{\rm k}}\rangle$$

$$\alpha_{da}^{\rm IC} = -\frac{e}{\hbar c}\epsilon_{abc}\int\frac{d^3k}{(2\pi)^3}\sum_{mn}^N {\rm Im}\Big\{\langle\widetilde{\partial}_b u_{n{\rm k}}|\widetilde{\partial}_{\mathcal{E}_d} u_{m{\rm k}}\rangle\langle u_{m{\rm k}}|(\partial_c H_{\rm k})|u_{n{\rm k}}\rangle\Big\}$$

$$\alpha_{da}^{\rm geom} = \frac{\theta}{2\pi}\frac{e^2}{hc}\delta_{da}$$

$$\theta_{\rm geom} = -\frac{1}{4\pi}\int d^3k\,\epsilon_{abc}{\rm tr}\left[A_a\partial_b A_c - \frac{2i}{3}A_a A_b A_c\right]$$

CS = Chern-Simons

Theory of geometric orbital MEC

$$\theta = -\frac{1}{4\pi}\int d^3k\, \epsilon_{abc} \mathrm{tr}\left[A_a \partial_b A_c - \frac{2i}{3} A_a A_b A_c\right]$$

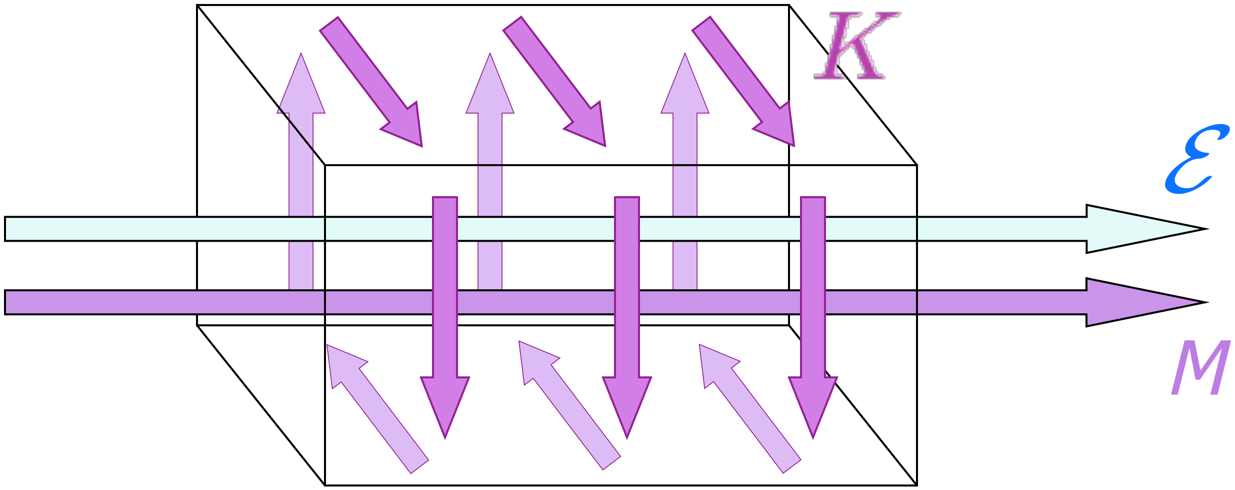
Berry connection: $\mathcal{A}^a_{nn'}(\mathbf{k}) = i\langle u_{n\mathbf{k}} | \partial_{k_a} u_{n'\mathbf{k}}\rangle$

Qi, Hughes and Zhang, PRB ***78****, 195424 (2008)*
Essin, Moore and Vanderbilt, PRL ***120****,146805 (2009)*

- Integrand is not gauge-invariant
- But integral over 3D BZ *is* gauge-invariant, modulo 2π

Physical understanding of "modulo 2π"?

Orbital MEC ↔ Surface dissipationless σ_{xy}



Interpret magnetization = M = K

$$-\mathbf{K} = \sigma_{\mathbf{yx}} \vec{\mathcal{E}} \times \hat{\mathbf{n}}$$

$$\sigma_{yx}^{\text{surf}} = -\alpha^{\text{CS}} = \frac{-e^2}{h} \frac{\theta}{2\pi}$$

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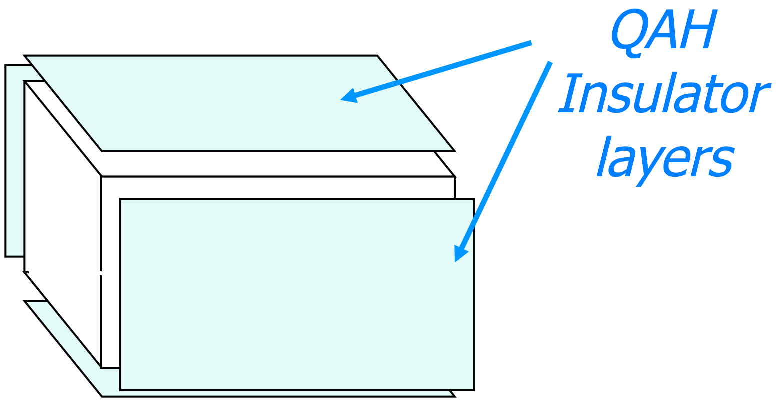
α^{CS} only defined modulo 2π

Suppose we start with crystal having α^{CS} given by θ.

Now glue to each surface an extra 2D QAH insulator layer having C=1:

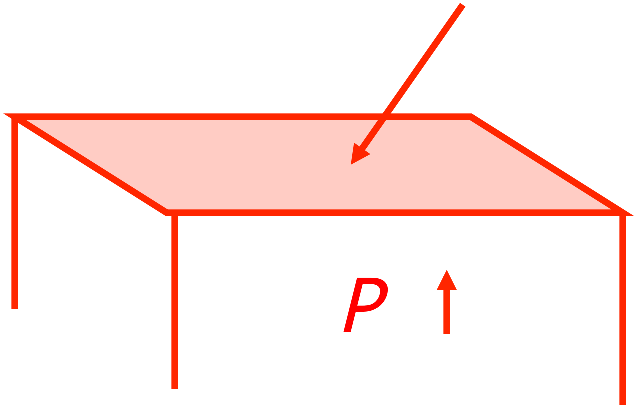
$$\alpha^{CS} = \frac{e^2}{h}\frac{\theta}{2\pi}$$

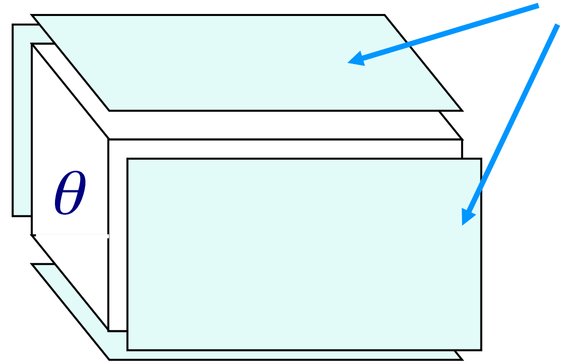


This increments $\sigma_{xy}^{\rm surf}$ by $\dfrac{e^2}{h}$, i.e., $\theta_{\rm new} = \theta + 2\pi$

So θ as a bulk property is ill-defined modulo 2π !

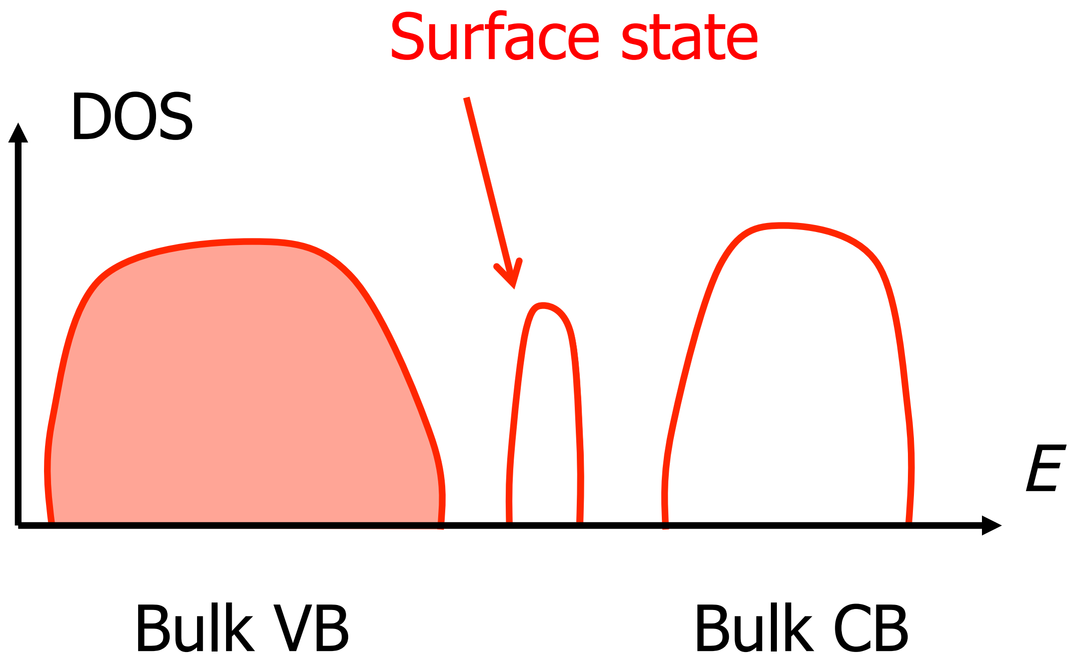
Indeterminacy modulo 2π





P is ill-defined modulo 2π

θ is ill-defined modulo 2π


Surface state
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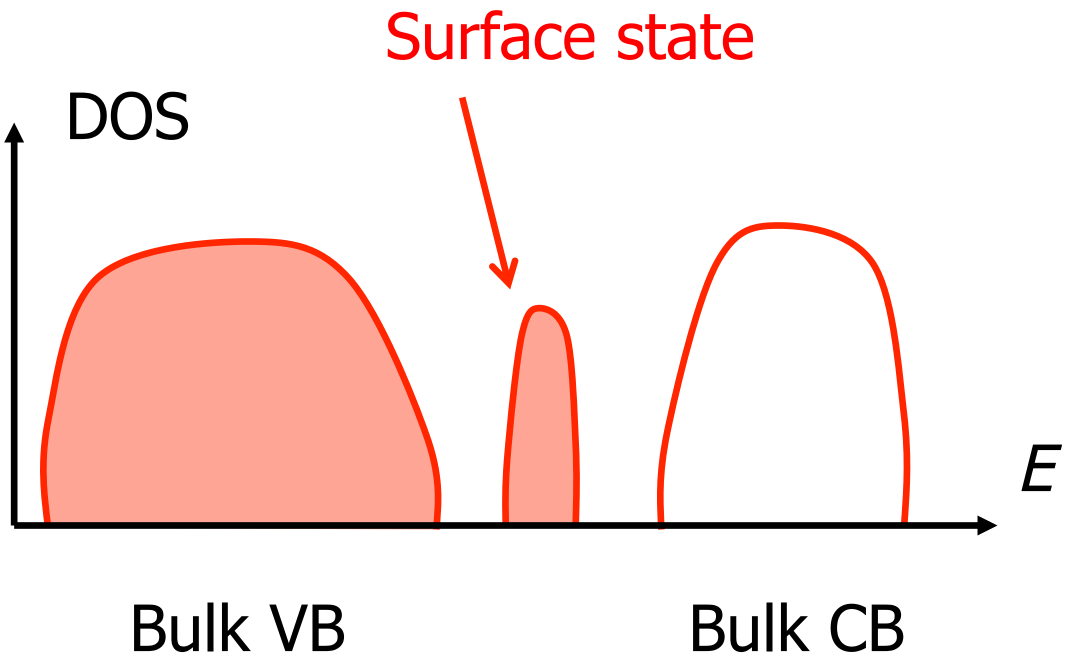
Surface state
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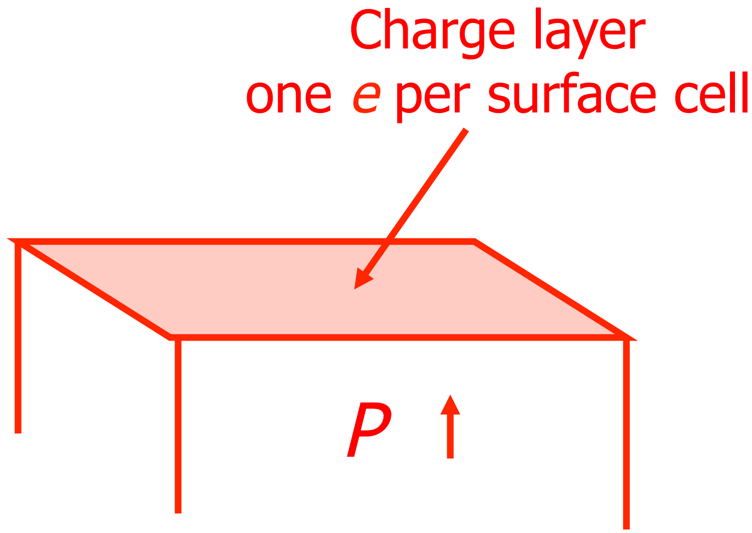
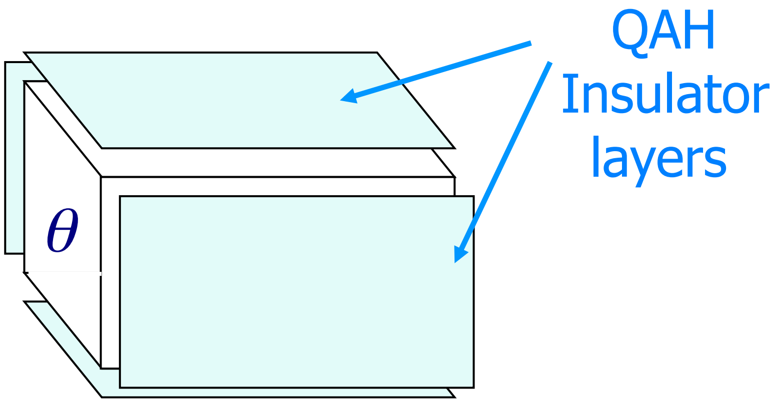
Indeterminacy modulo 2π





P is ill-defined modulo 2π

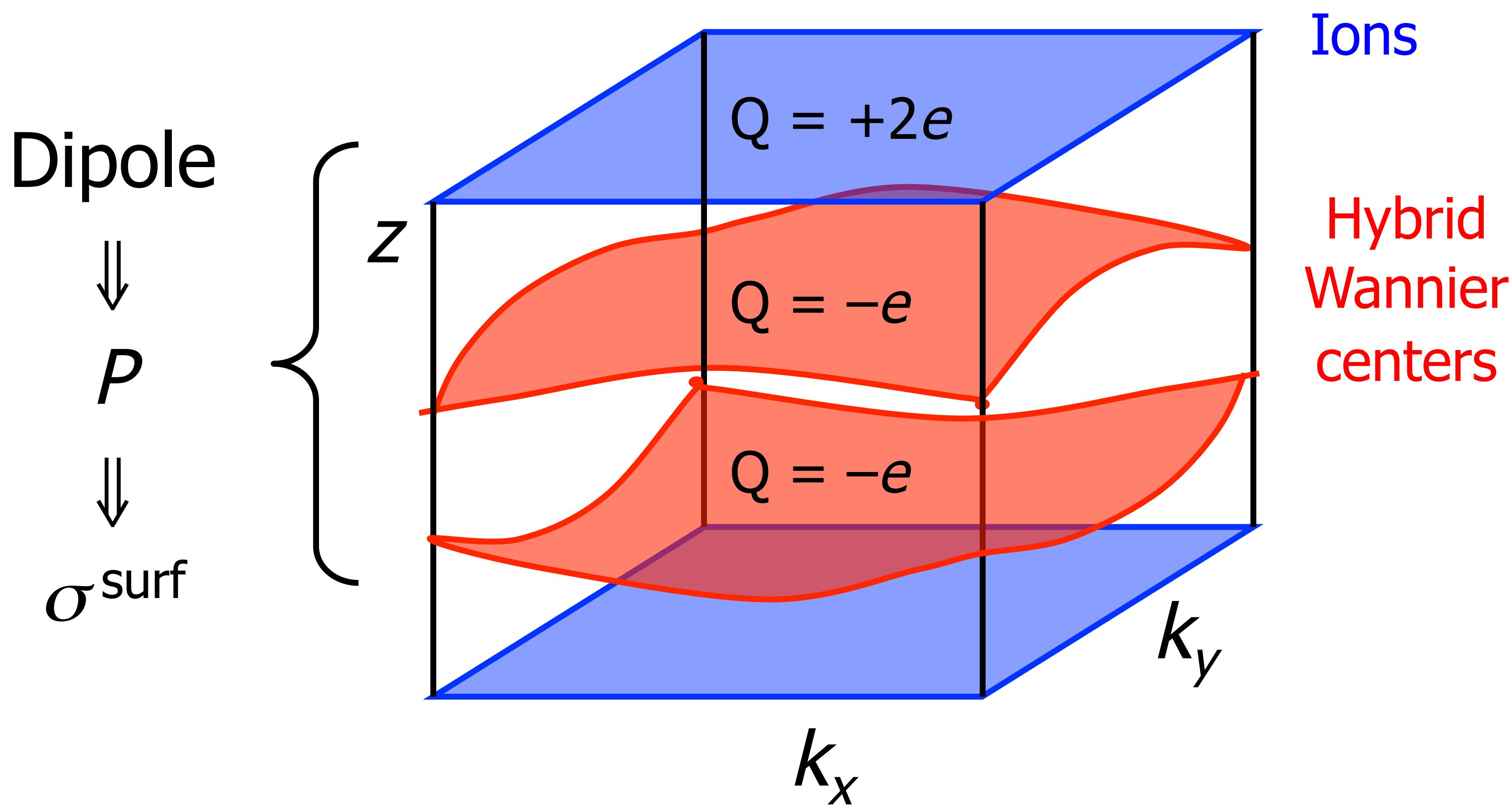
θ is ill-defined modulo 2π

ME coupling of TR-invariant insulator

- The T symmetry operator maps θ into $-\theta$
- But θ is only well defined modulo 2π
- Case of $\theta=0$ $\Leftrightarrow$ normal insulator
- Case of $\theta=\pi$ $\Leftrightarrow$ strong topological insulator!

*Qi, Hughes and Zhang, PRB **78**, 195424 (2008)*
Essin, Moore and Vanderbilt, PRL 120,146805 (2009)

Polarization and surface charge



CS coupling and surface AHC

Dipole

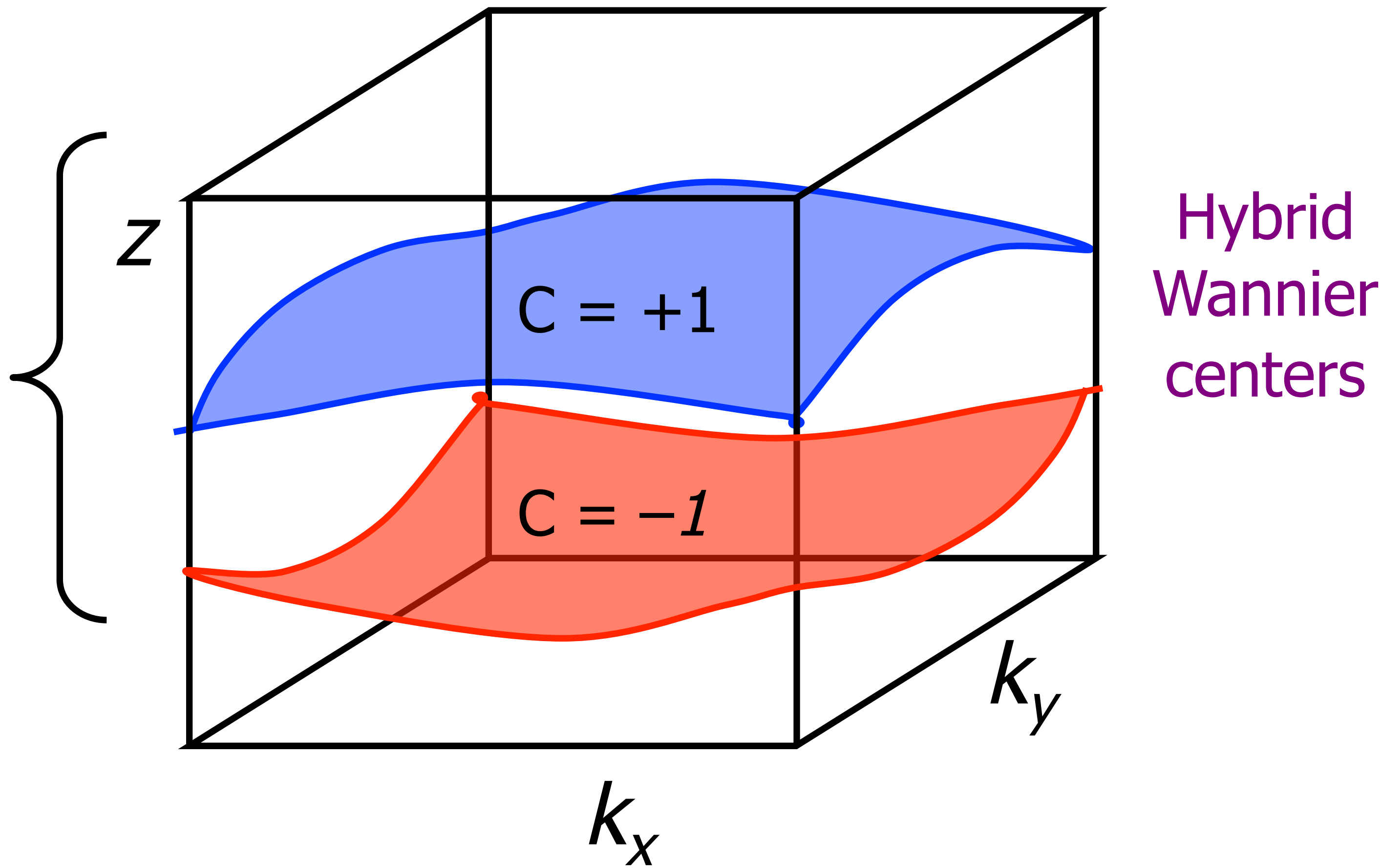
$\Downarrow$

θ

$\Downarrow$

$\sigma^{\text{AH,surf}}$

?



Hybrid Wannier representation

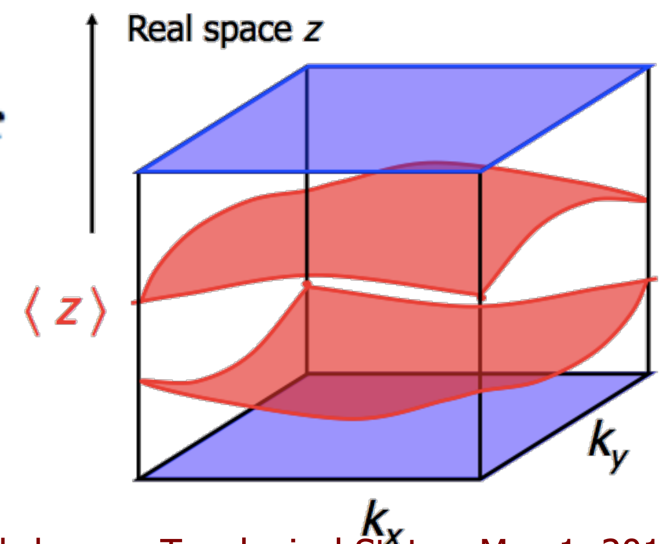
Define hybrid WFs: (maximally localized along *z*)

$$|h_{\kappa l n}\rangle = e^{-i\kappa\cdot r}\int_0^1 dk_3\, e^{-i2\pi k_3 l}\left|\psi_{(\kappa,k_3)n}\right\rangle$$

where $\kappa = k_x\hat{x} + k_y\hat{y}$

Construct hybrid WF sheets:

$$z_{\kappa l n} = \langle h_{\kappa l n}|z|h_{\kappa l n}\rangle = z_{\kappa 0 n} + lc$$



Hybrid Wannier representation

Define Berry connection and curvature on the sheets:

$$A^i_{ln,l'm} = i\langle h_{ln} | \partial_{k_i} h_{l'm} \rangle = A^i_{0n,(l'-l)m},$$

$$\Omega^{ij}_{ln,l'm} = \partial_{k_i} A^j_{ln,l'm} - \partial_{k_j} A^i_{ln,l'm} = \Omega^{ij}_{0n,(l'-l)m}$$

$$i, j = x, y$$

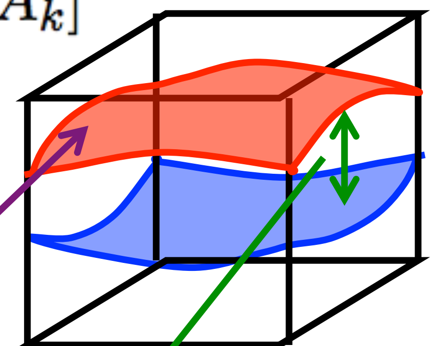
Chern number of each sheet:

$$C_{ln} = \frac{1}{2\pi} \int d\kappa \, \Omega^{xy}_{ln,ln}$$

Axion coupling in the HWF representation

Bulk Bloch represenatation

$$\theta = -\frac{1}{4\pi}\int d^3k\,\epsilon^{ijk}\,\mathrm{Tr}[A_i\partial_j A_k - i\frac{2}{3}A_iA_jA_k]$$



HWF represenatation

Berry curvature on *n*'th sheet

$$\theta = \theta_{z\Omega} + \theta_{\Delta xy}$$

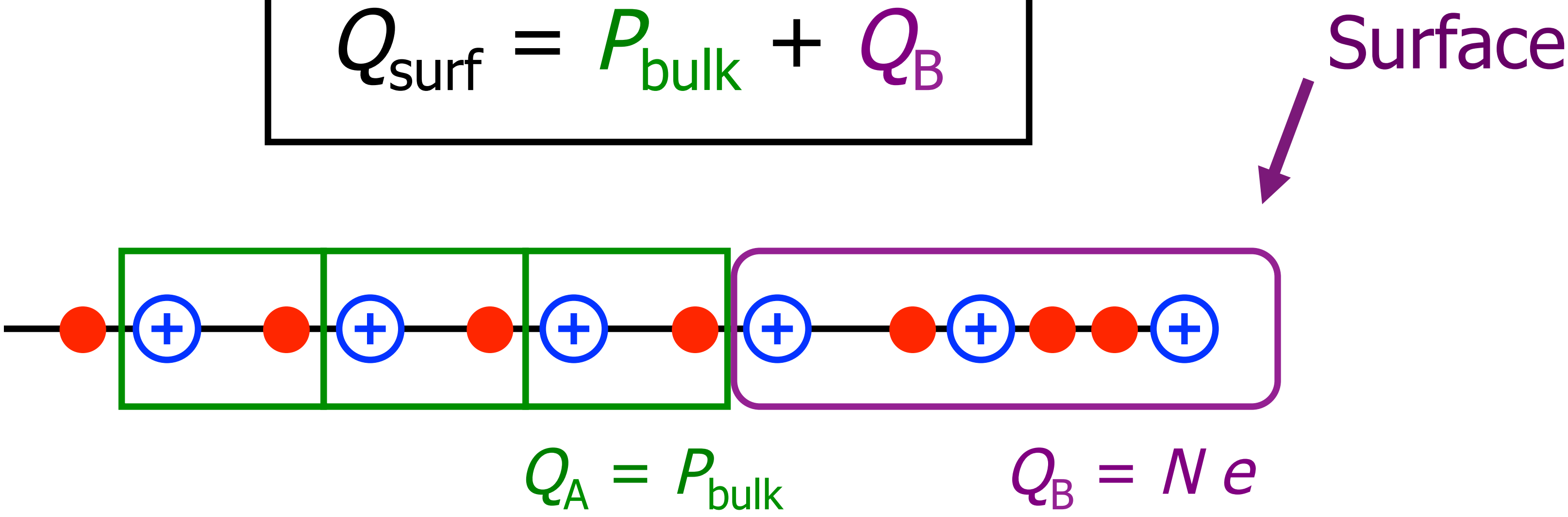
$$\theta_{z\Omega} = -\frac{1}{c}\int d^2k \sum_n \bar{z}_n \Omega_{xy,0n,0n}$$

Berry potential between sheets

$$\theta_{\Delta xy} = -\frac{i}{c}\int d^2k \sum_{lmn} (\bar{z}_{lm} - \bar{z}_{0n}) A_{x,0n,lm} A_{y,lm,0n}$$

Surface charge theorem: 1D

$$Q_{\text{surf}} = P_{\text{bulk}} + Q_{\text{B}}$$

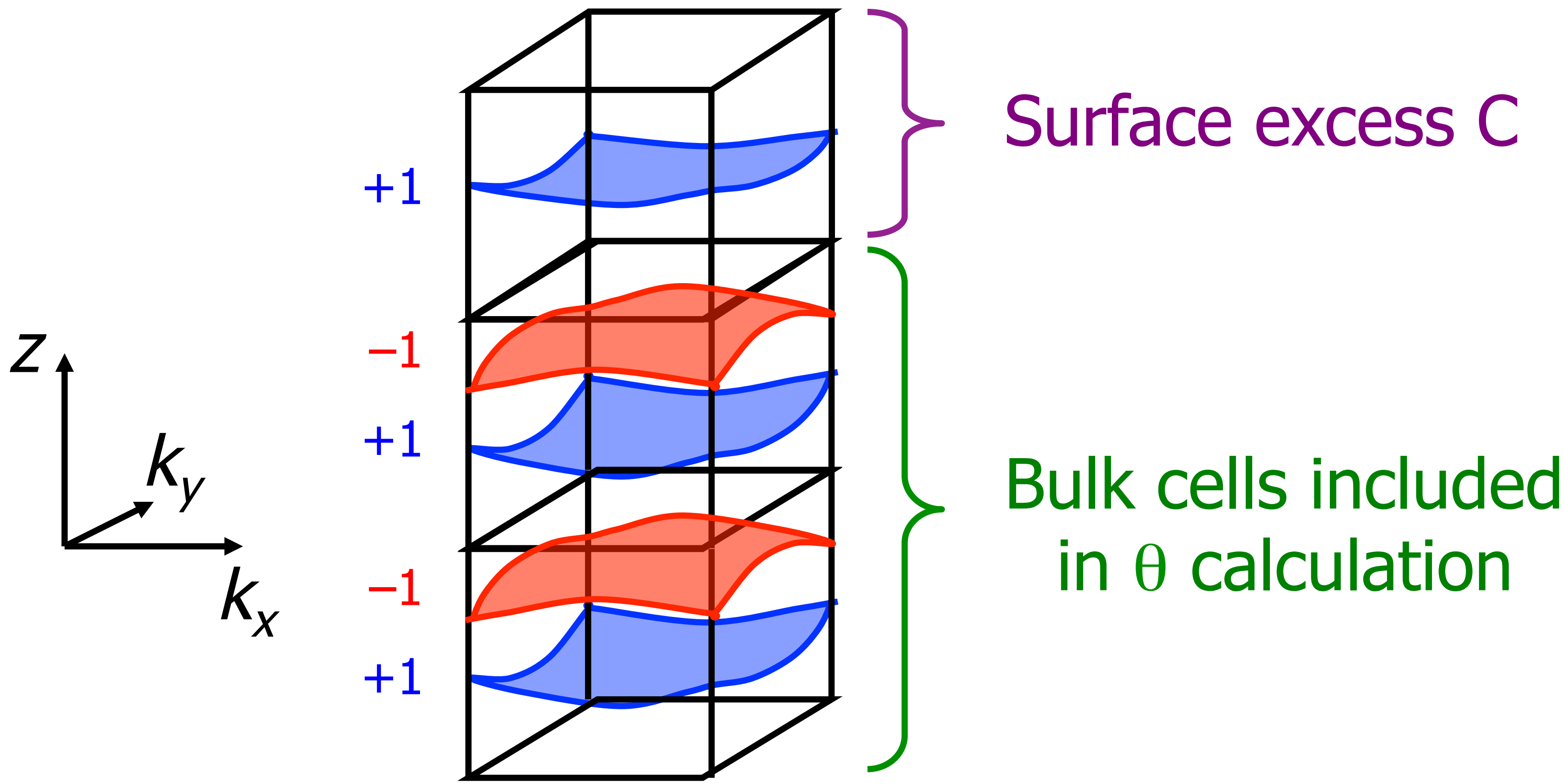


- Wannier centers: Eigenvalues of $\mathcal{P} x \mathcal{P}$

$$\mathcal{P} = \sum_n^{\text{occ}} |\psi_n\rangle\langle\psi_n|$$

Surface σ^{AH} theorem

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

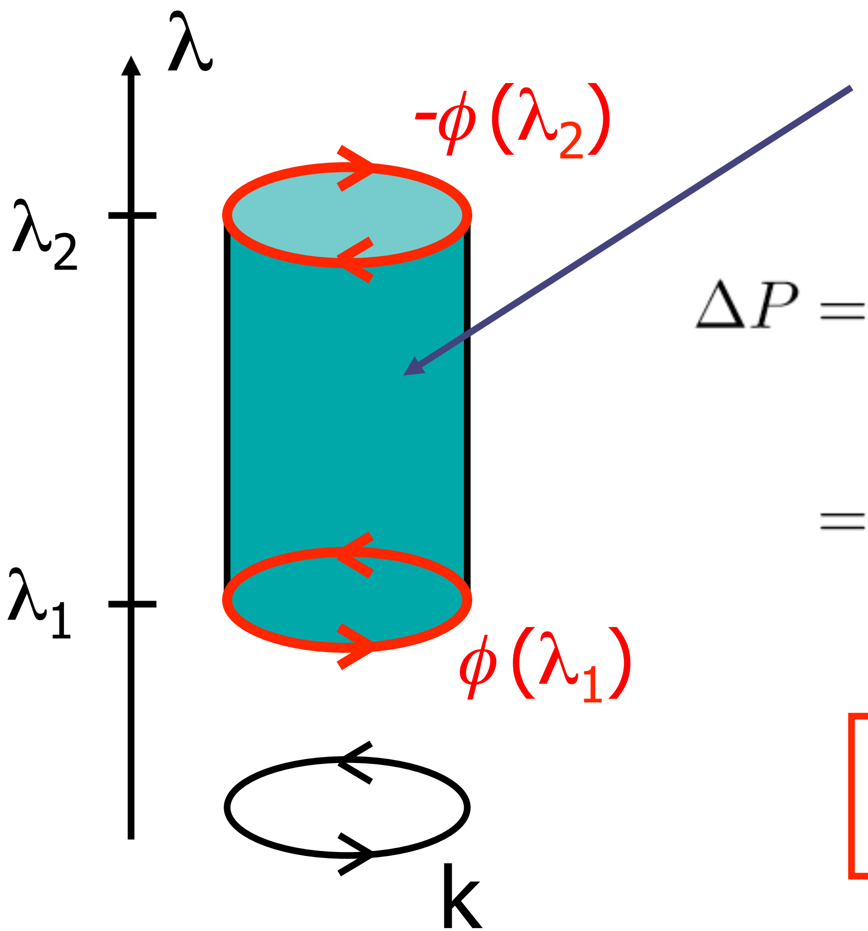


RUTGERS

Outline

- Polarization in 1D
- Polarization in 3D
  - Hybrid Wannier representation
  - Surface charge theorem
- Axion magnetoelectric coupling
  - Hybrid Wannier representation
  - Surface AHC theorem
- Adiabatic loop
  - Charge pump / axion pump
- Summary & Conclusions

Parametric 1D Ham. (Open path)



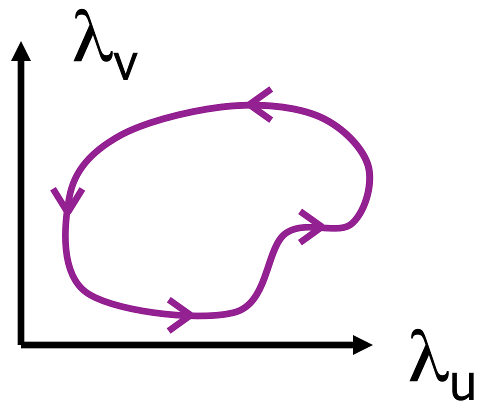
$$\Delta P = -\frac{e}{2\pi}\oint dk \int_{\lambda_1}^{\lambda_2} d\lambda \;\Omega^{(k\lambda)}$$

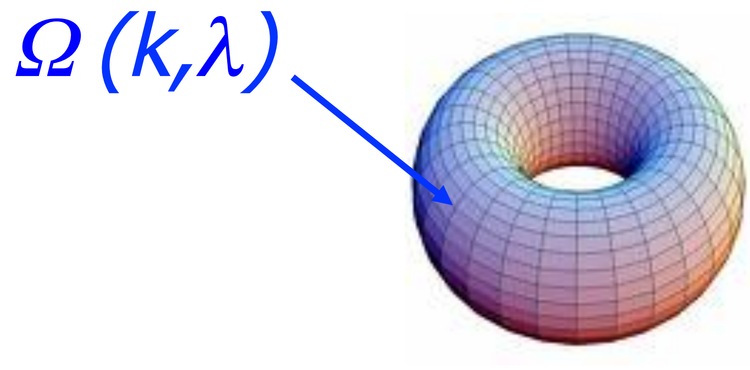
$$= \frac{e}{2\pi}\phi(\lambda_2) - \frac{e}{2\pi}\phi(\lambda_1)$$

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

(modulo e)

Parametric 1D Ham. (Closed path)





(k, λ) space

Under an adiabatic cycle,

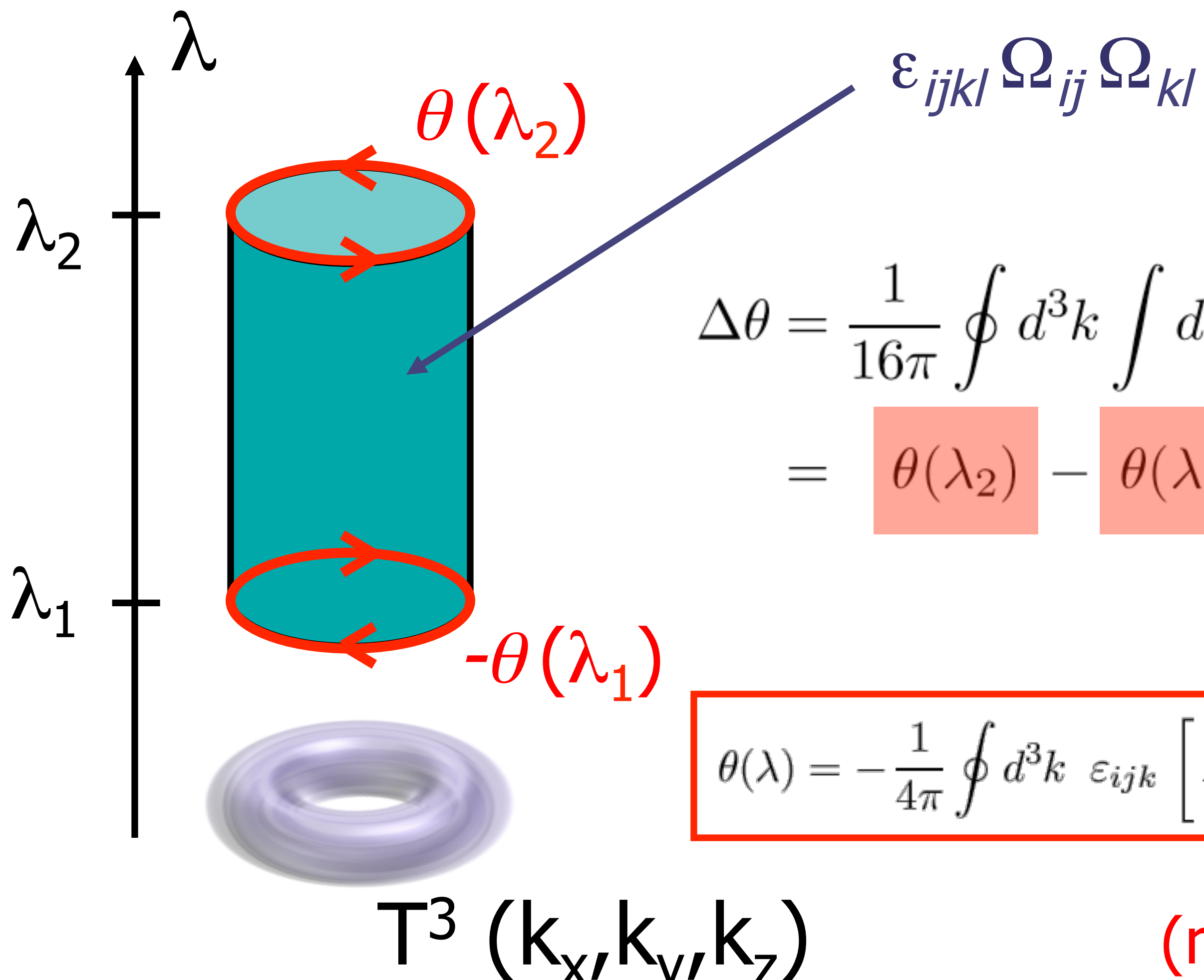
$$\Delta P = \frac{e}{2\pi} \oint d\lambda \oint dk \;\; \Omega(k, \lambda)$$

By Chern theorem,

$$\Delta P = n\,e$$

(n = TKNN invariant = integer)

Parametric 3D Ham. (Open path)



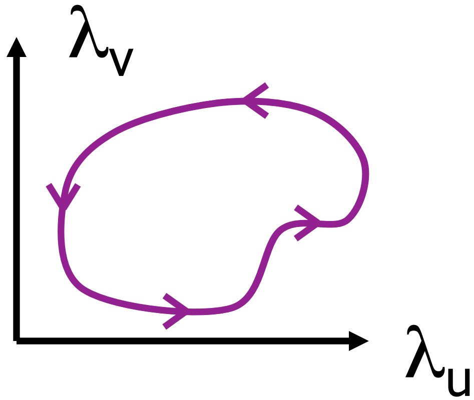
$$\Delta\theta = \frac{1}{16\pi}\oint d^3k \int d\lambda \;\; \varepsilon_{ijkl}\,\Omega_{ij}\,\Omega_{kl}$$

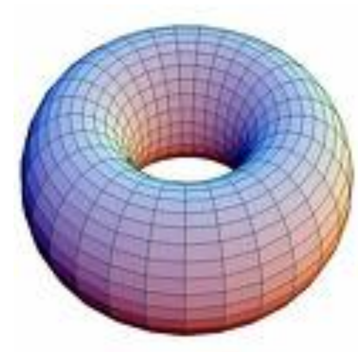
$$= \;\; \theta(\lambda_2) \; - \; \theta(\lambda_1)$$

$$\theta(\lambda) = -\frac{1}{4\pi}\oint d^3k \;\; \varepsilon_{ijk}\left[A_i\,\partial_j A_k - \frac{2i}{3}A_i\,A_j\,A_k\right]$$

(modulo 2π)

Parametric 3D Ham. (Closed path)





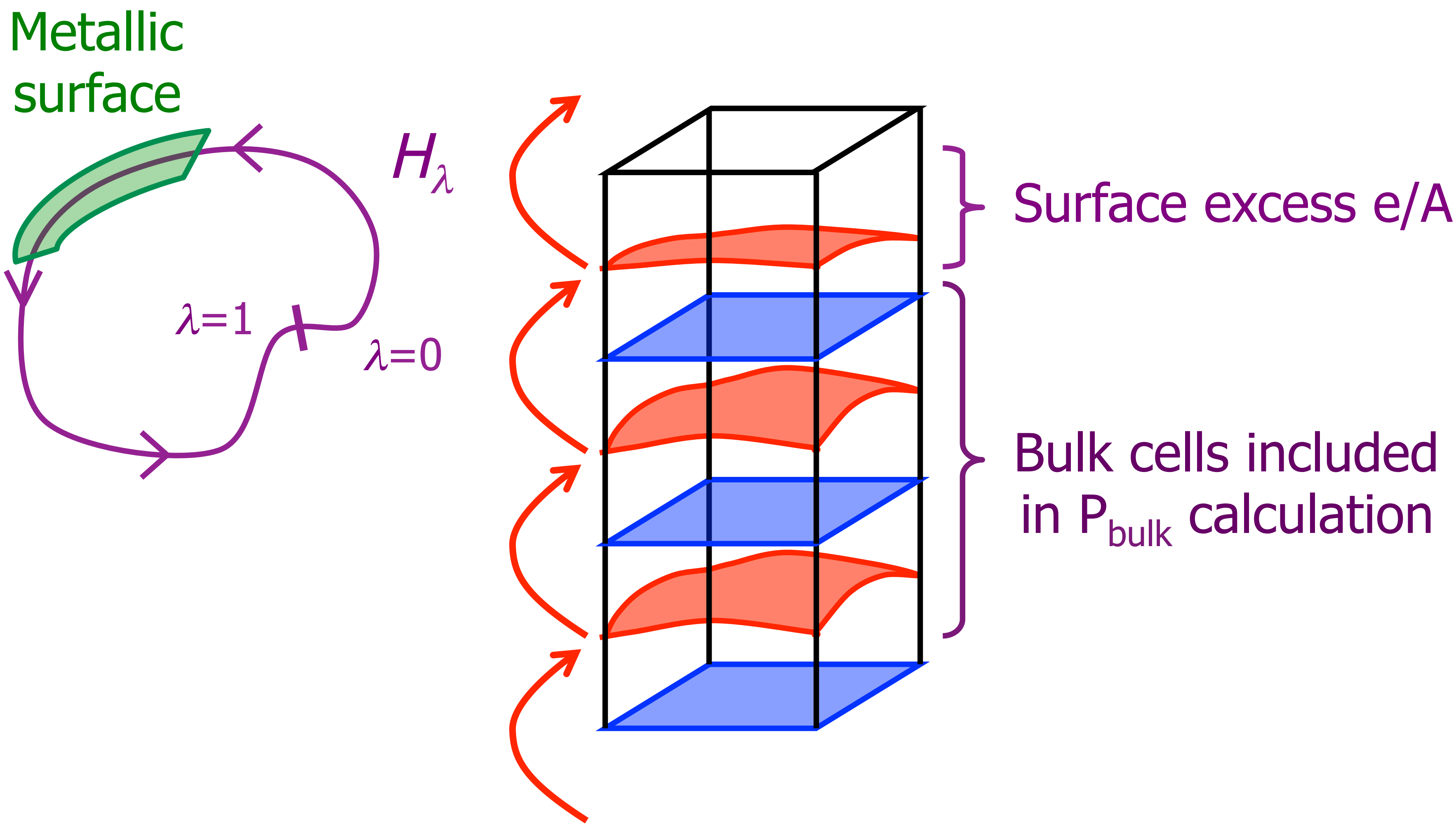
(k_x,k_y,k_z,λ) space

Under an adiabatic cycle,

$$\Delta\theta = 2\pi N_2$$

where N_2 = “second Chern number”

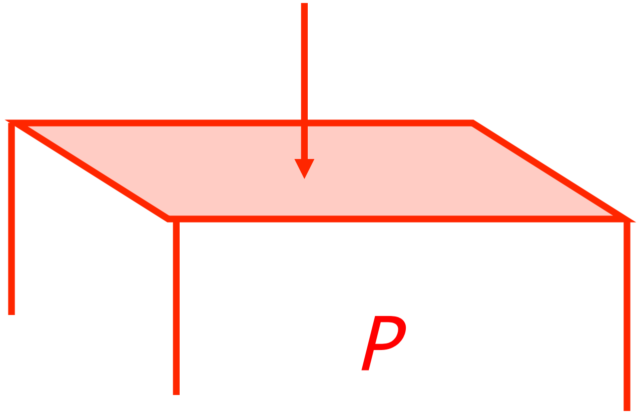
Adiabatic charge pump



Metallic surface of bulk insulator

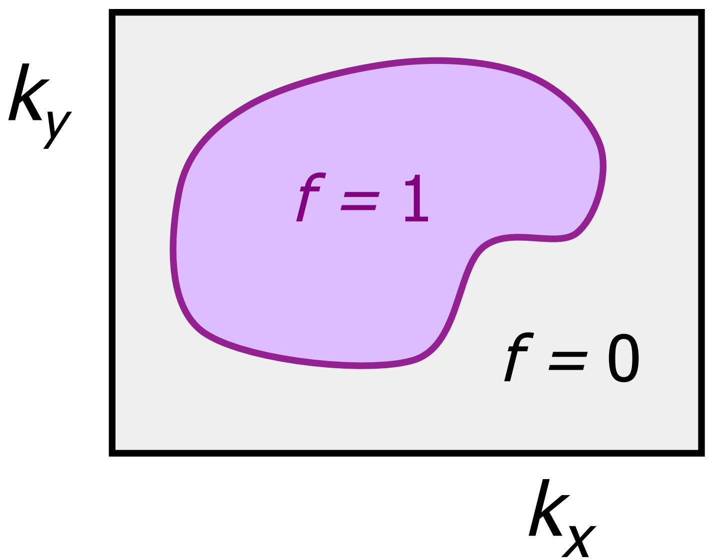
Surface charge

$$\sigma = \frac{-e}{A}\left[\frac{\phi}{2\pi} + \text{int} + \frac{A}{(2\pi)^2}\int d^2k\, f(\mathbf{k})\right]$$



ϕ is ill-defined modulo 2π

Surface BZ

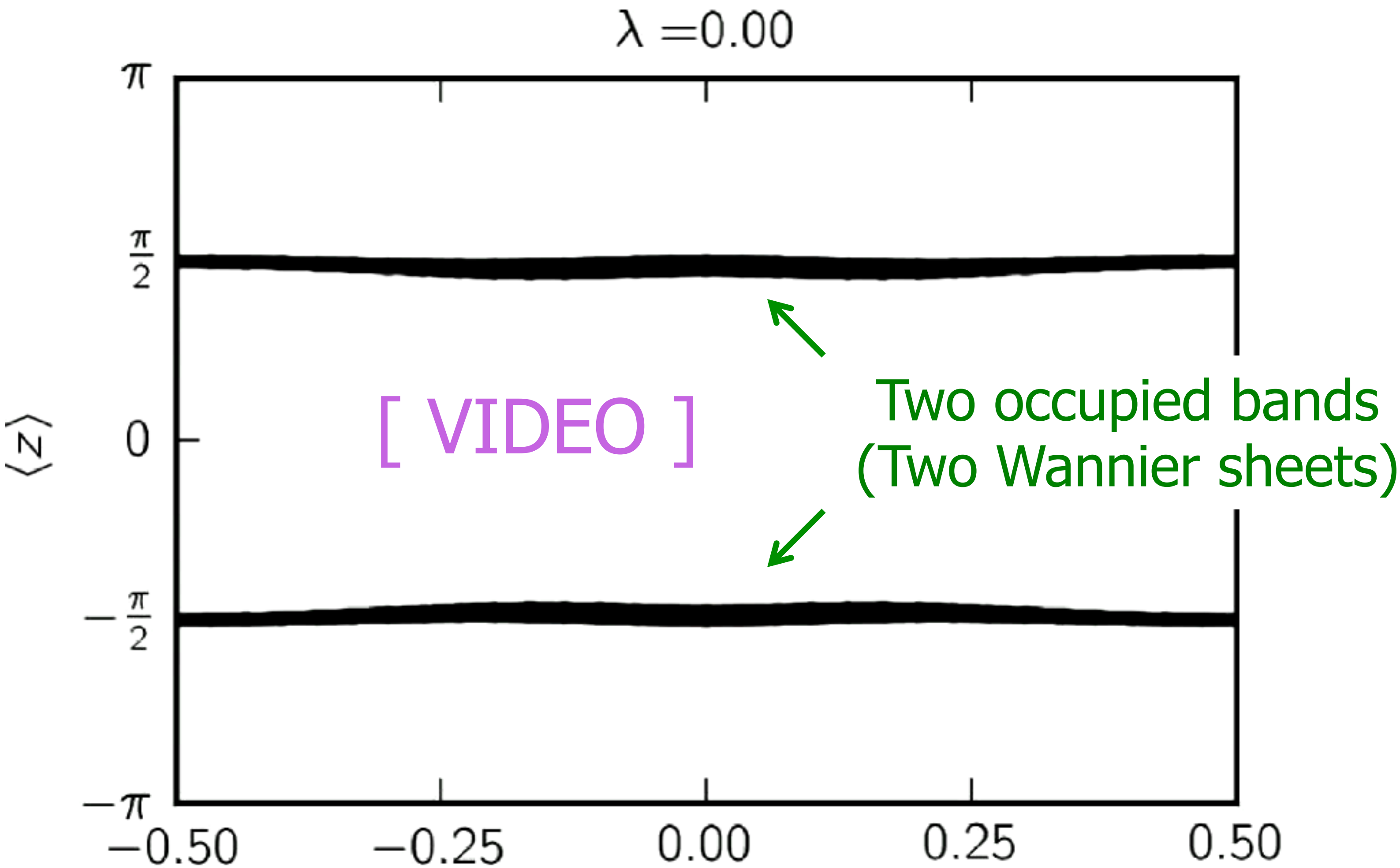


Adiabatic axion pump

- Bulk *H* undergoes cyclic evolution: $\theta \to \theta/2\pi$ without gap closure
- What happens to bulk Wannier sheets?

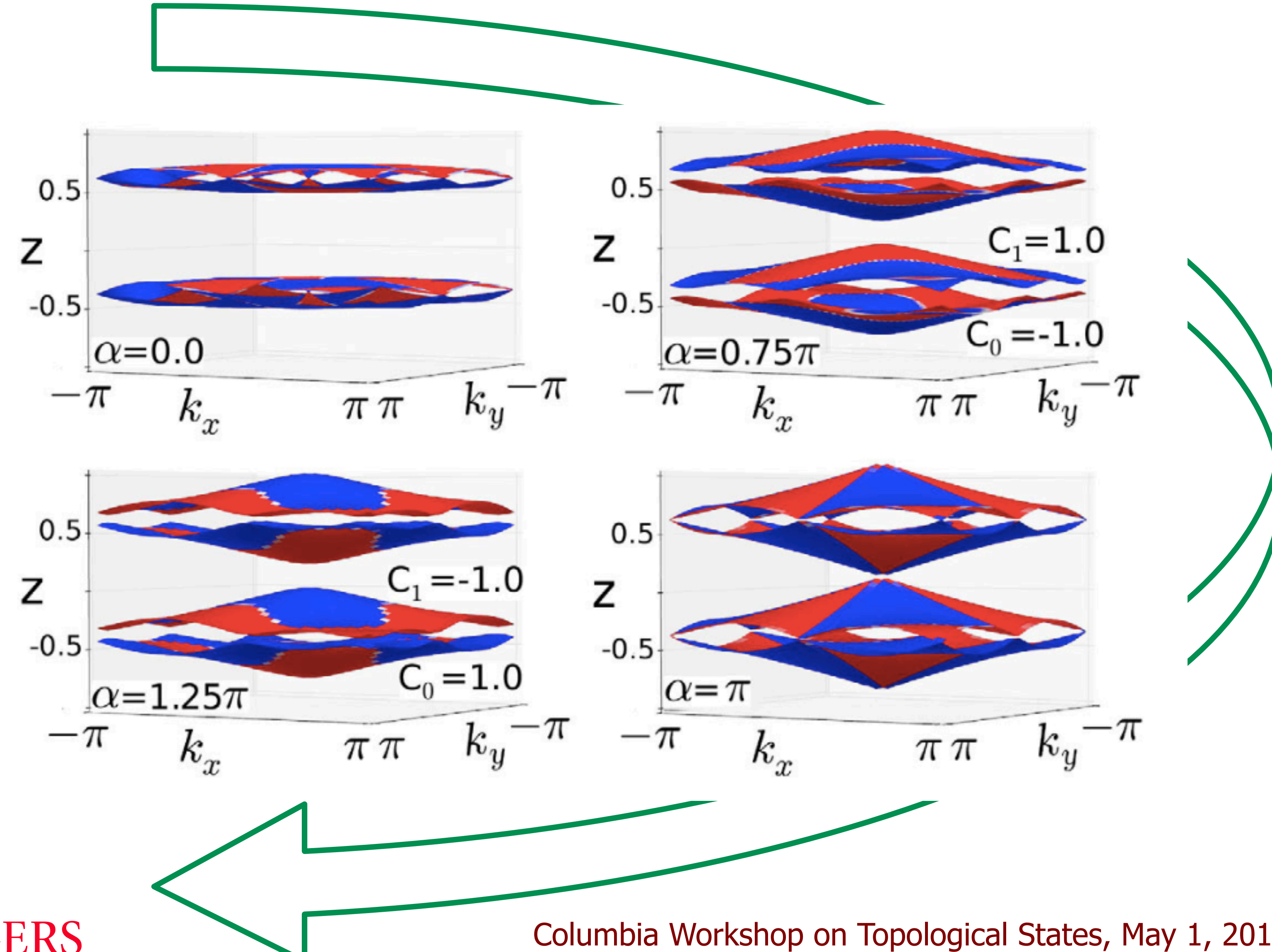
Modified TB model of Qi, Hughes & Zhang

Sinisa Coh



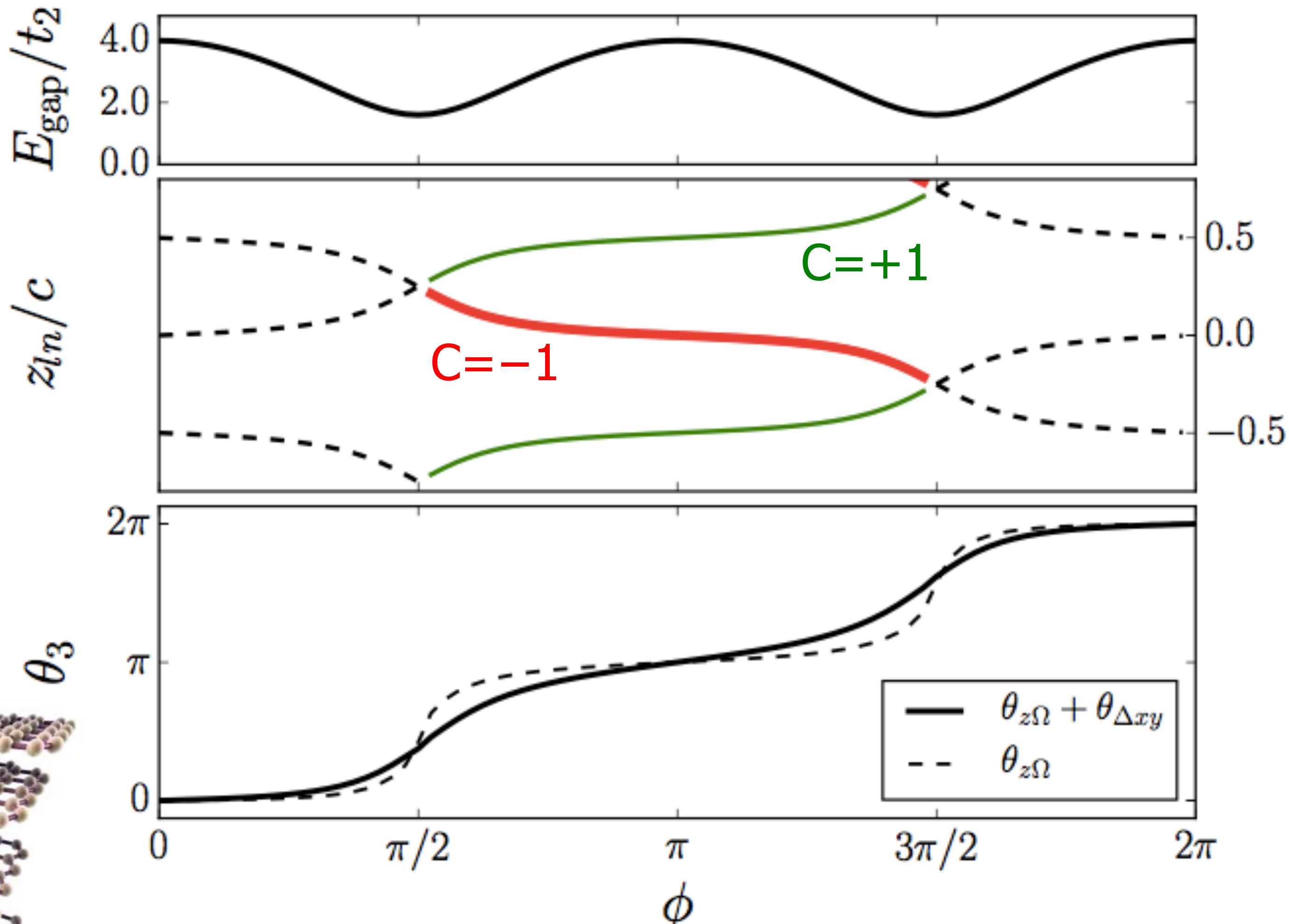
TB model of Fu, Kane & Mele

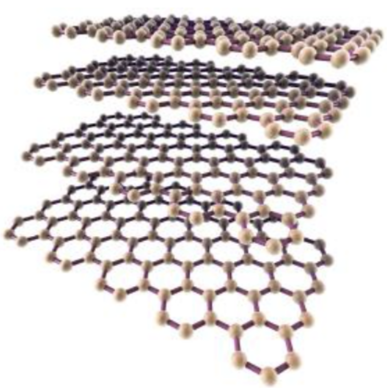
Maryam Taherinejad



TB model of coupled Haldane layers: Bulk

Thomas Olsen

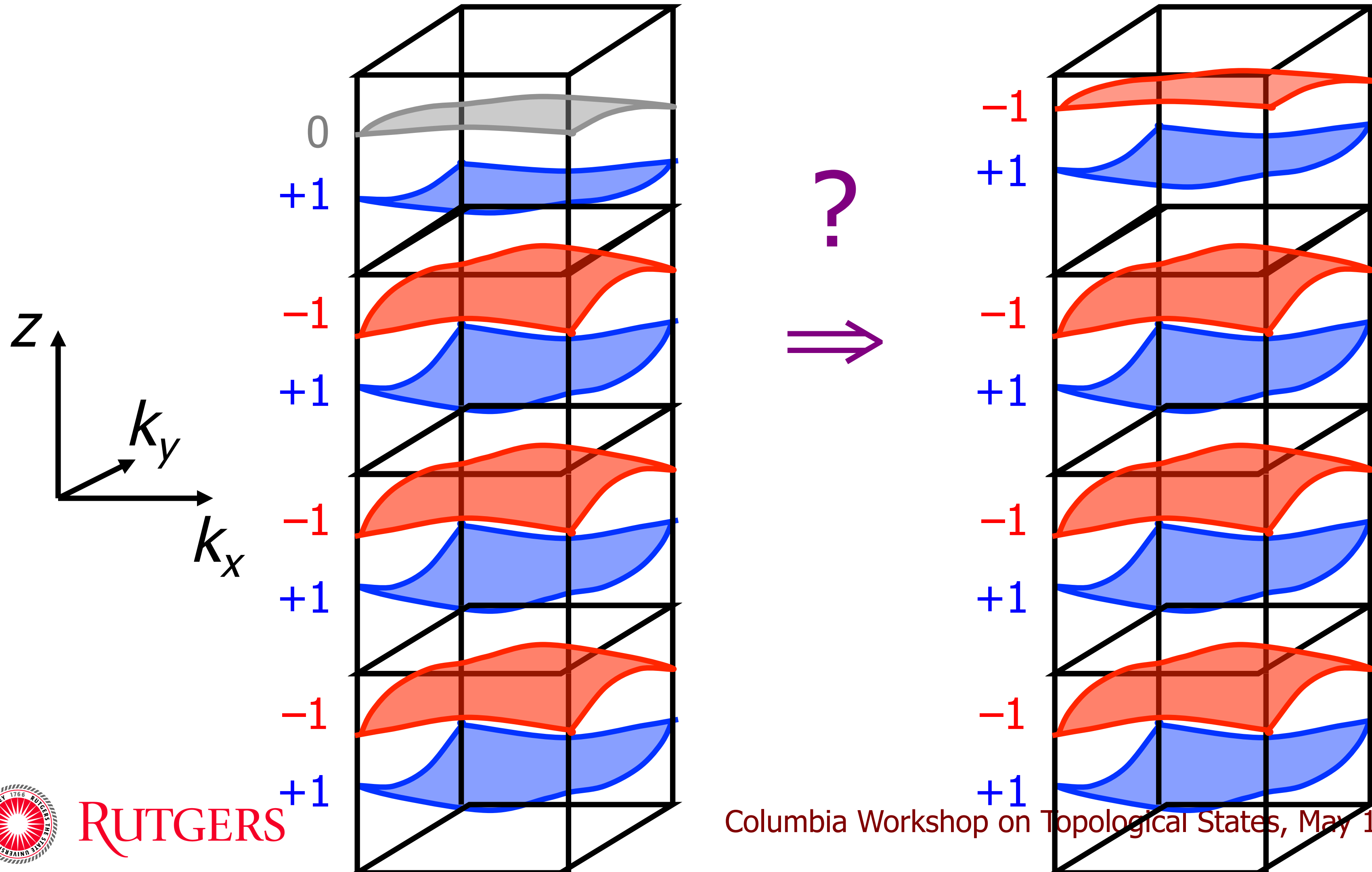




Axion charge pump

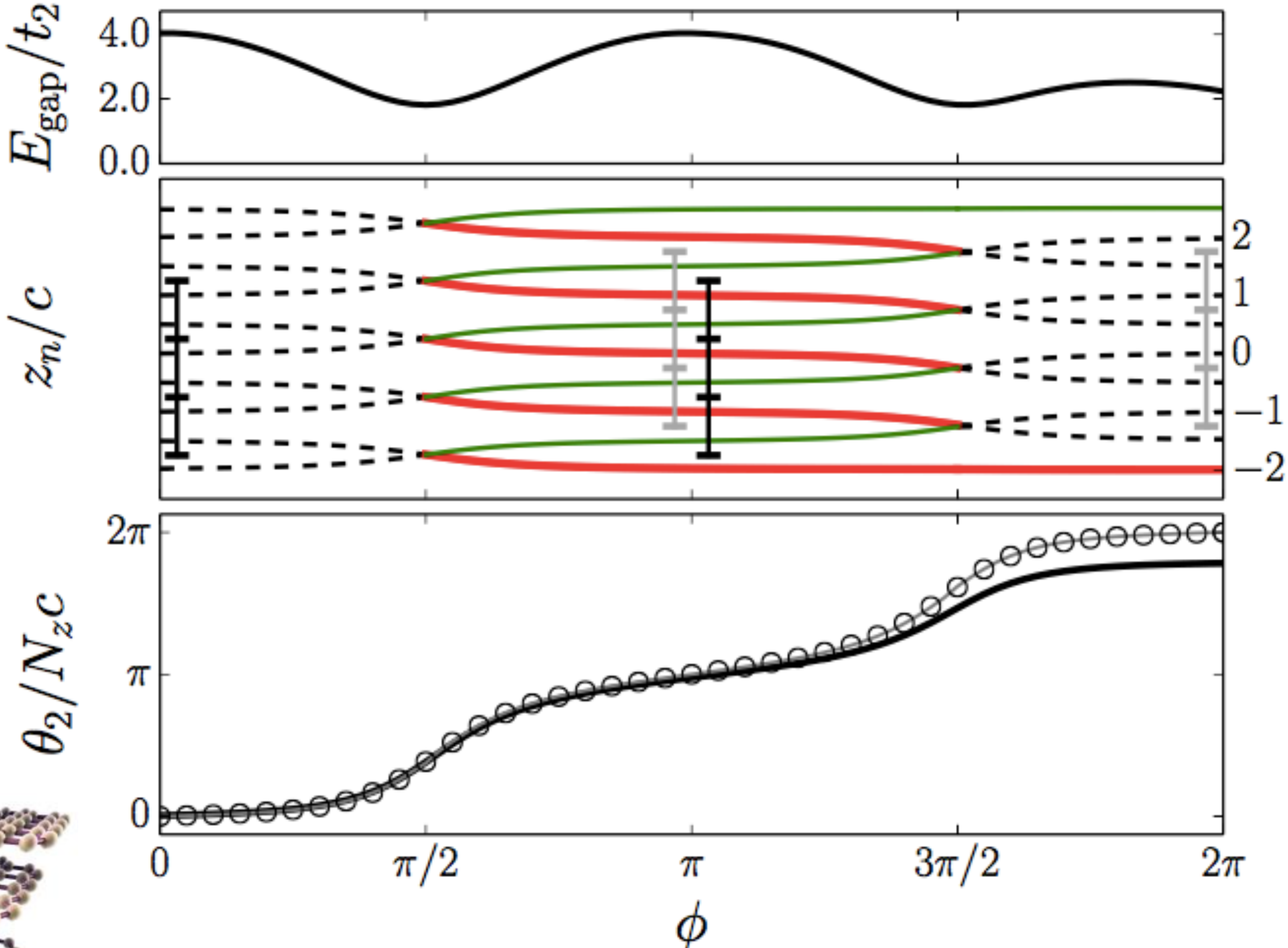
- Bulk H undergoes cyclic evolution: $\theta \rightarrow \theta/2\pi$ without gap closure
- What happens to surface AHC?
- Two scenarios to consider:
  - H_{surf} changes so as to keep surface insulating
  - H_{surf} returns to itself

Adiabatic evolution of surface AHC



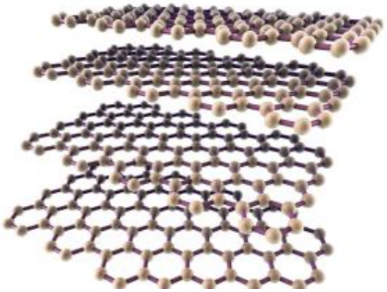
TB model of coupled Haldane layers: Slab

Thomas Olsen



C=+1

C=−1



Adiabatic axion pump

- Bulk H undergoes cyclic evolution: $\theta \rightarrow \theta/2\pi$ without gap closure
- What happens to surface AHC?
- Two scenarios to consider:
  - H_{surf} changes so as to keep surface insulating
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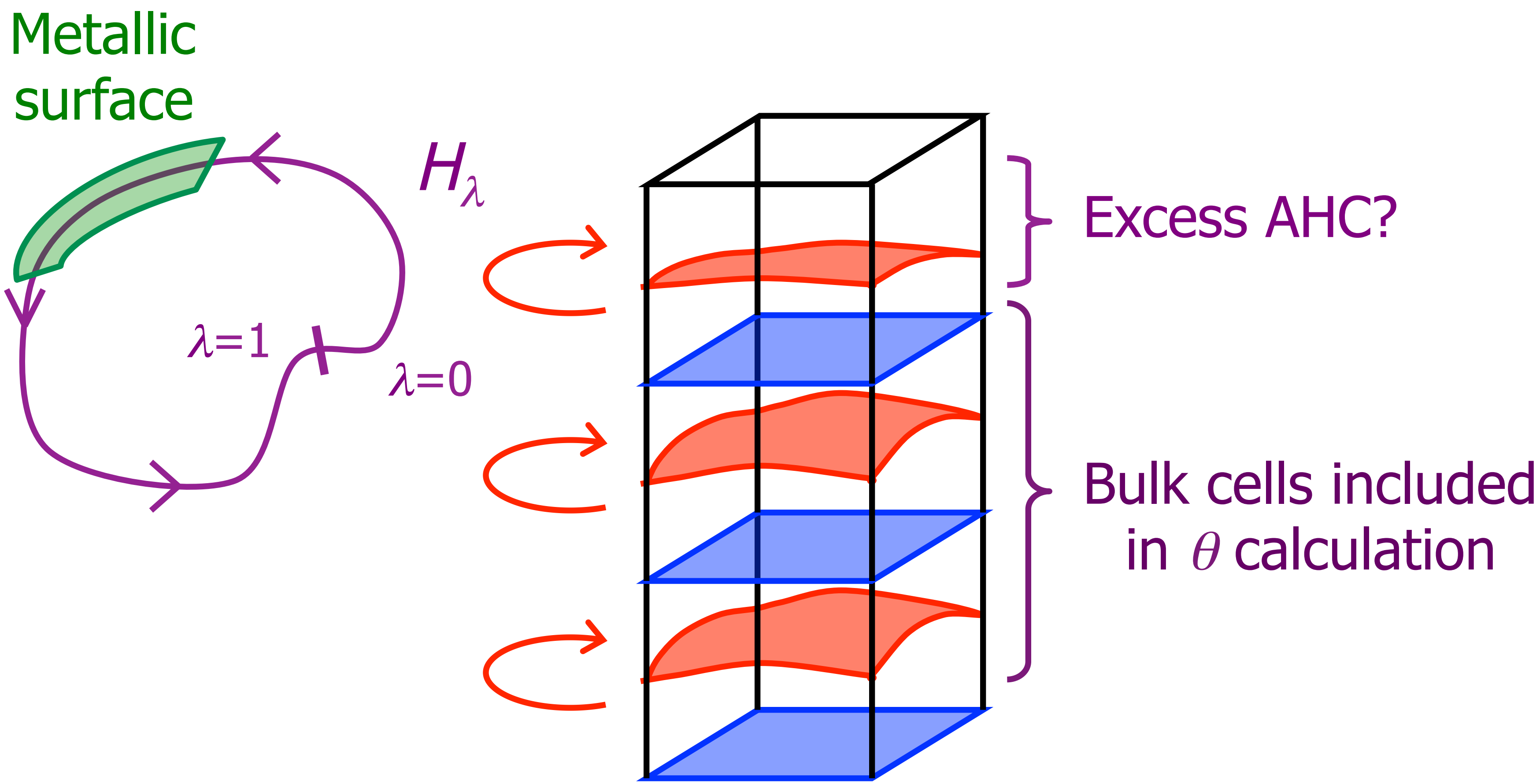
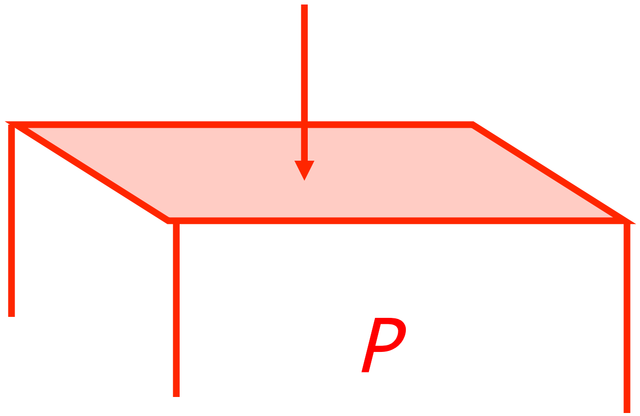
Adiabatic axion pump



Metallic surface of bulk insulator

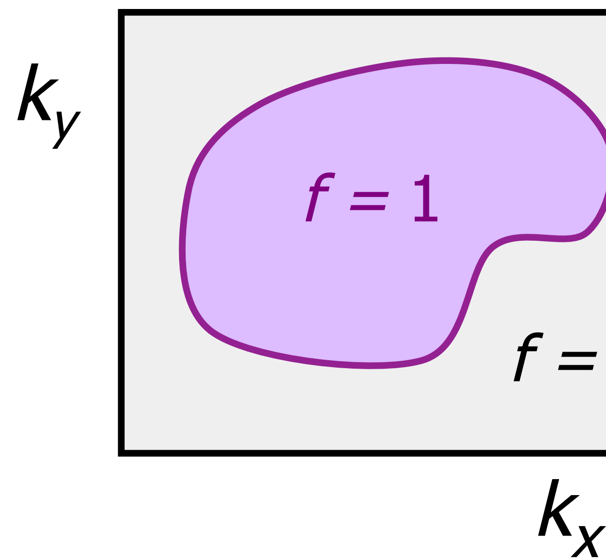
Surface charge

$$\sigma = \frac{-e}{A}\left[\frac{\phi}{2\pi} + \text{int} + \frac{A}{(2\pi)^2}\int d^2k\, f(\mathbf{k})\right]$$



ϕ is ill-defined modulo 2π

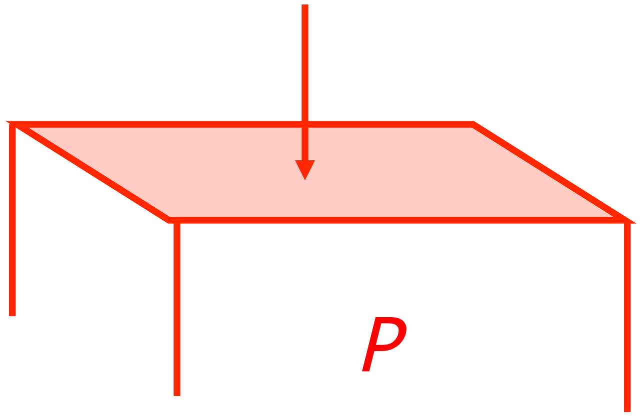
Surface BZ



Metallic surface of bulk insulator

Surface charge

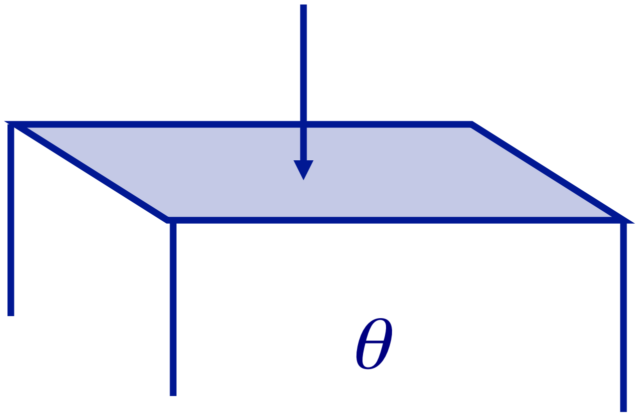
$$\sigma = \frac{-e}{A}\left[\frac{\phi}{2\pi} + \text{int} + \frac{A}{(2\pi)^2}\int d^2k\, f(\mathbf{k})\right]$$



ϕ is ill-defined modulo 2π

Anom. Hall conductivity

$$\sigma^{\text{AH}} = \frac{e^2}{h}\left[\frac{\theta}{2\pi} + \text{int} + \frac{1}{2\pi}\int d^2k\, f(\mathbf{k})\,\Omega(\mathbf{k})\right]$$



θ is ill-defined modulo 2π

Summary: Analogy

Polarization	Orbital ME coupling
Berry phase ϕ	Axion angle θ
Surface charge	Surface AHC
Adiabatic charge pump	Adiabatic axion pump
First Chern number	Second Chern number

References

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Adiabatic Pumping of Chern-Simons Axion Coupling

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Surface theorem for the Chern-Simons axion coupling

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