Optically-Controlled Orbitronics on the Triangular Lattice

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Topics for today

- Motivation: Cu_2Si (Feng et al. Nature Comm. **8**, 1007 (2017)) ✓
- Model: L=1 manifold on a triangular lattice
- Anomalous Hall and Orbital Hall Effects with <u>Optical Control</u>
- More material realizations ✓

Background I: Anomalous Velocity

Equation of motion for an electron wavepacket in a band

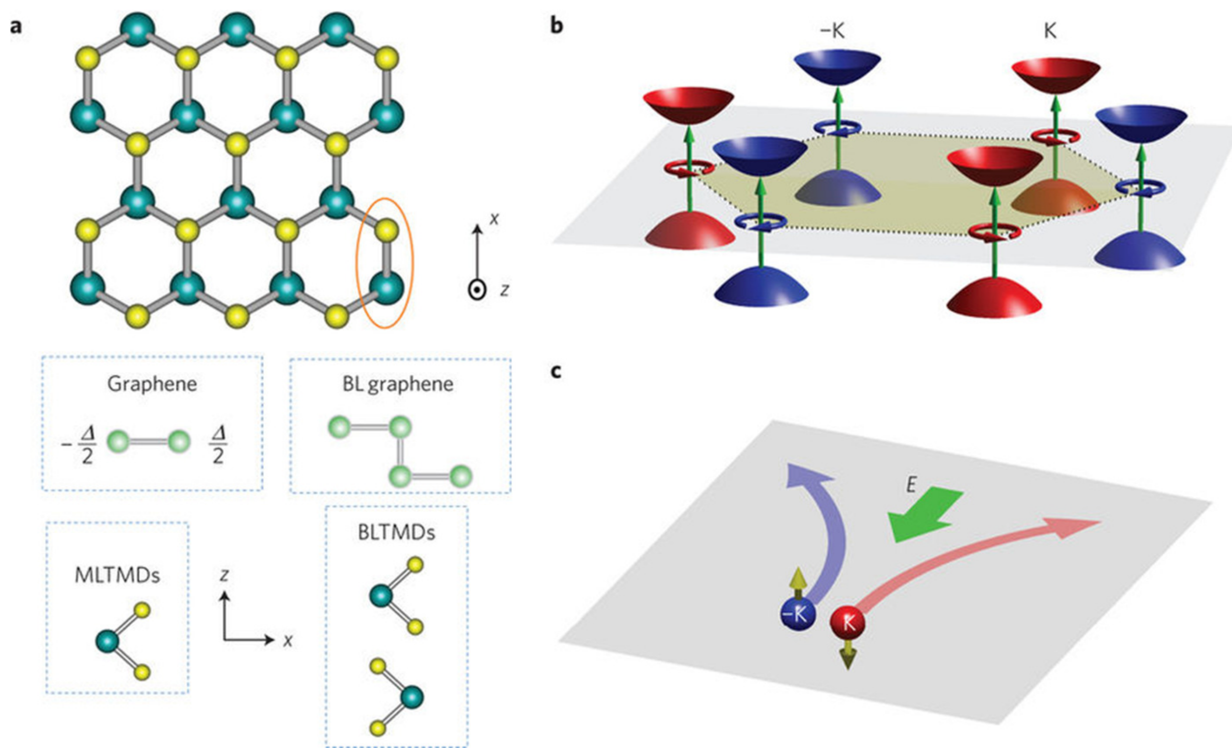
$$\hbar \dot{k} = -eE - e\dot{r} \times B \qquad \text{CM}$$

$$\dot{r} = \frac{\partial E}{\hbar \partial k} - \dot{k} \times \Omega(k) \qquad \text{QM}$$

Ω is the BERRY CURVATURE. It comes from an (<u>unremovable</u>) k-dependence of some internal degree of freedom of the w.p.

$\Omega \neq 0$ requires broken <u>time reversal symmetry</u> (anomalous Hall effect) or <u>broken inversion symmetry</u> (harder to see)

Background II (some things we already know)



Anomalous transverse transport appears in
<u>nonequilibrium states</u> with asymmetric valley population

Background III (what we'd like to do)

Population $\rightarrow$ Coherent Optical Control

- break symmetries via optical fields
- engineer Bloch k-space connections
- anomalous topological responses "on demand"

Comments:

- low-ω responses by downconverting optical fields
- frequency, phase and polarization
- intrinsically nonlinear (**estimates of intensities at end**)

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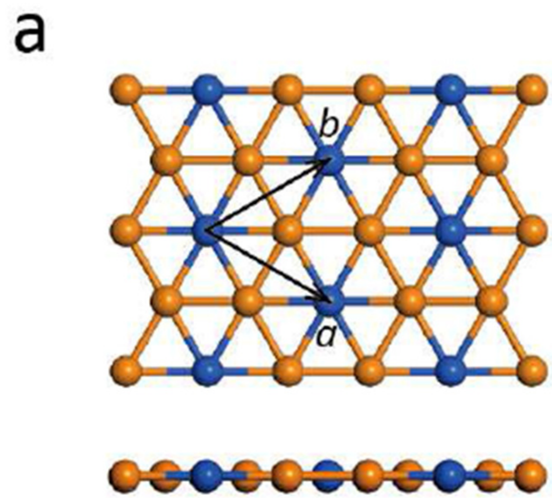
Discovery of two-dimensional Dirac nodal line fermions

Baojie Feng,[1] Botao Fu,[2] Shusuke Kasamatsu,[1] Suguru Ito,[1] Peng Cheng,[3] Cheng-Cheng Liu,[2] Sanjoy K. Mahatha,[4] Polina Sheverdyaeva,[4] Paolo Moras,[4] Masashi Arita,[5] Osamu Sugino,[1] Tai-Chang Chiang,[6] Kehui Wu,[3] Lan Chen,[3,*] Yugui Yao,[2,†] and Iwao Matsuda[1,‡]

Cu_2Si (Nature Comm. **8**: 1007 (2017))



Si (blue) embedded in a coplanar Cu honeycomb (gold)

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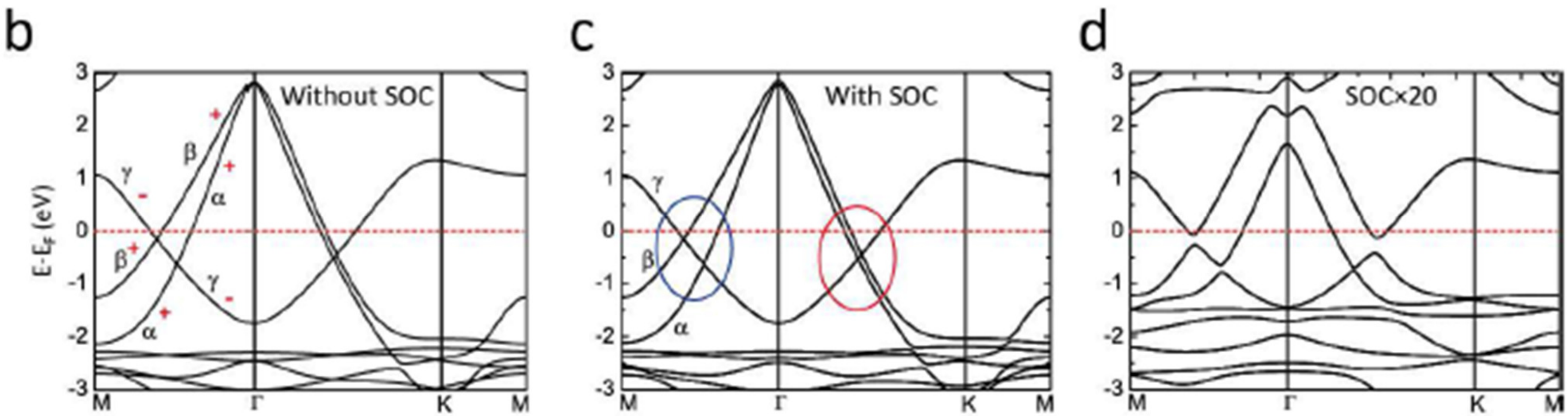

Band structures with and without spin orbit

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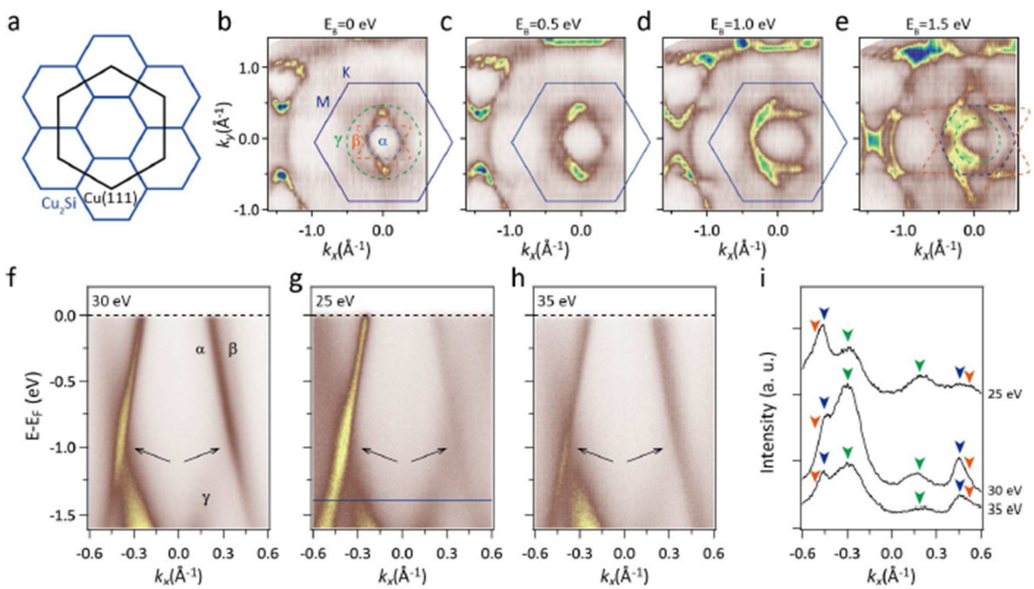
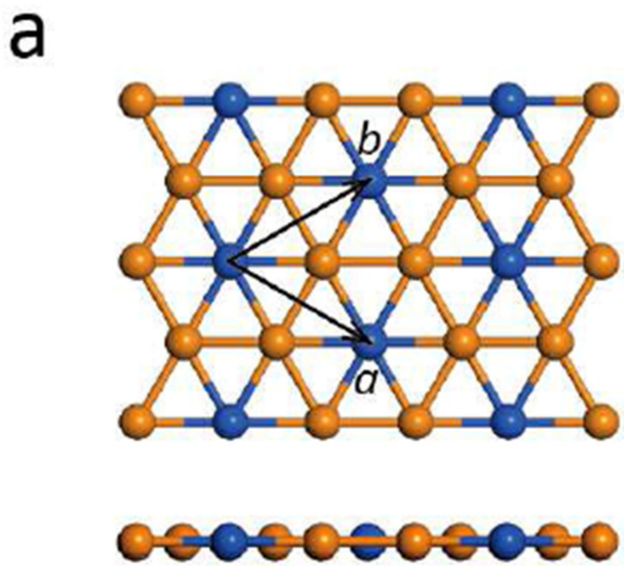
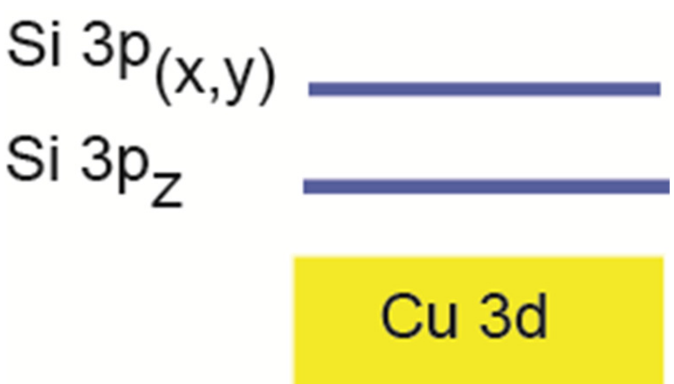


Measured in ARPES

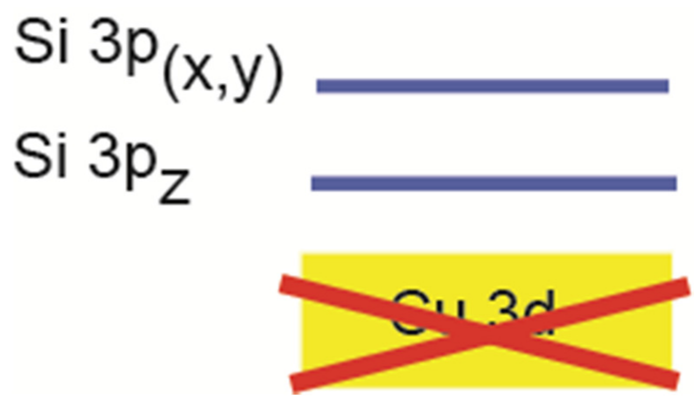
(on a Cu support)



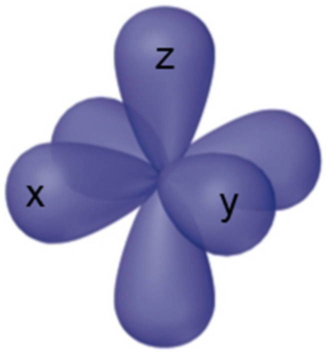
minimal model



distills to

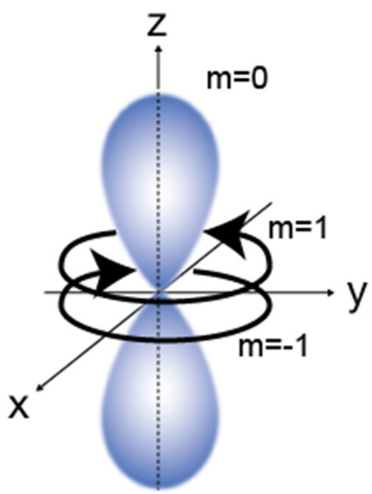


Matrix-valued intersite hopping on a primitive lattice



Cartesian

$$T_{\alpha,\beta}(\phi) = \begin{pmatrix} t_{xx} & t_{xy} & 0 \\ t_{yx} & t_{yy} & 0 \\ 0 & 0 & t_{zz} \end{pmatrix}$$

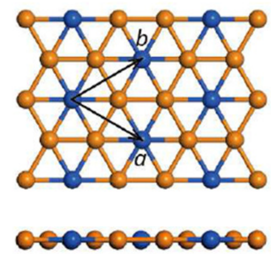


Axial

$$\Gamma_{\alpha,\beta}(\phi) = \begin{pmatrix} \gamma_{-1,-1} & 0 & \gamma_{-1,1} \\ 0 & \gamma_{oo} & 0 \\ \gamma_{1,-1} & 0 & \gamma_{1,1} \end{pmatrix}$$

In Cartesian (x,y,z) basis

a



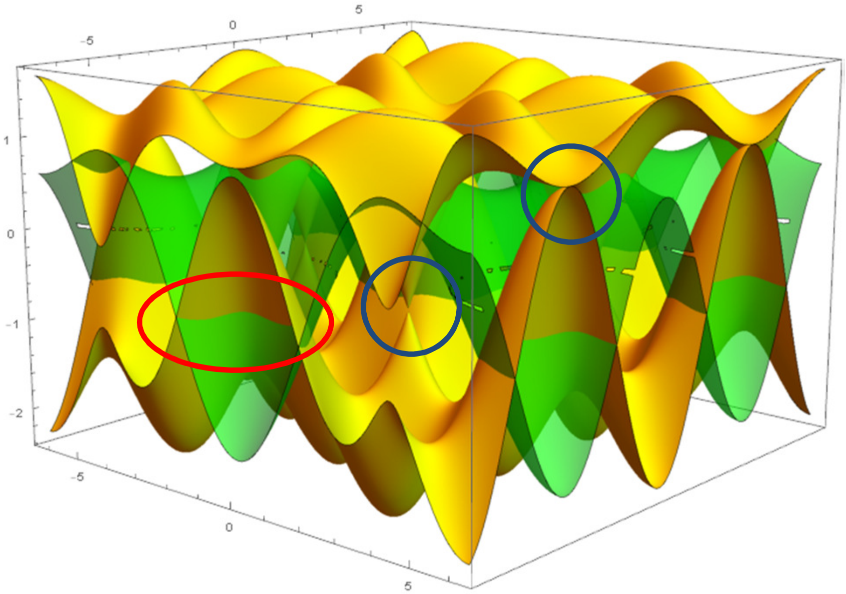
$$H_{xyz}(\vec{k}) = h_0(\vec{k})\mathrm{I}_{3\times 3} + \Delta(\vec{k})\hat{l}_z\hat{l}_z + \boxed{h(\vec{k})\cdot\hat{L}}$$

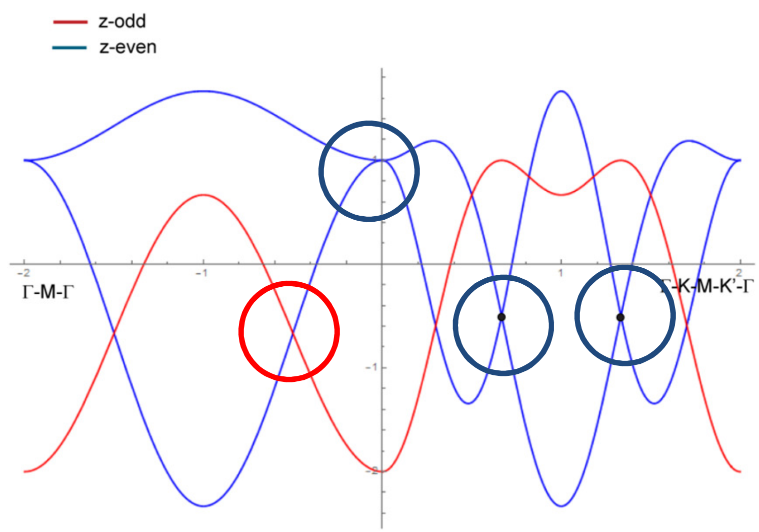
H is real : two independent control parameters
(sum of cosines in Cartesian basis) → h_y =0

Intersection of $l_z \neq 0$ and $l_z = 0$ bands are the **line nodes**
protected by z-mirror symmetry.

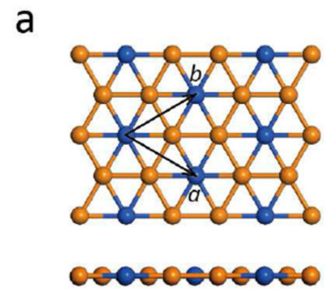
Other nodes (twofold band degeneracies in $l_z \neq 0$ sector)
occur only at **exceptional points**

Bands on primitive triangular lattice (p-states)





In axial basis (m = ±1: x ± iy)



$$H_{\text{axial}}(\vec{k}) = \begin{pmatrix} 0 & d^*(\vec{k}) \\ d(\vec{k}) & 0 \end{pmatrix}$$

Notes: d_z violates $\mathcal{T}$C_2 symmetry

C_3: requires twofold degeneracy at Γ, K.

Counting Rules for J=1

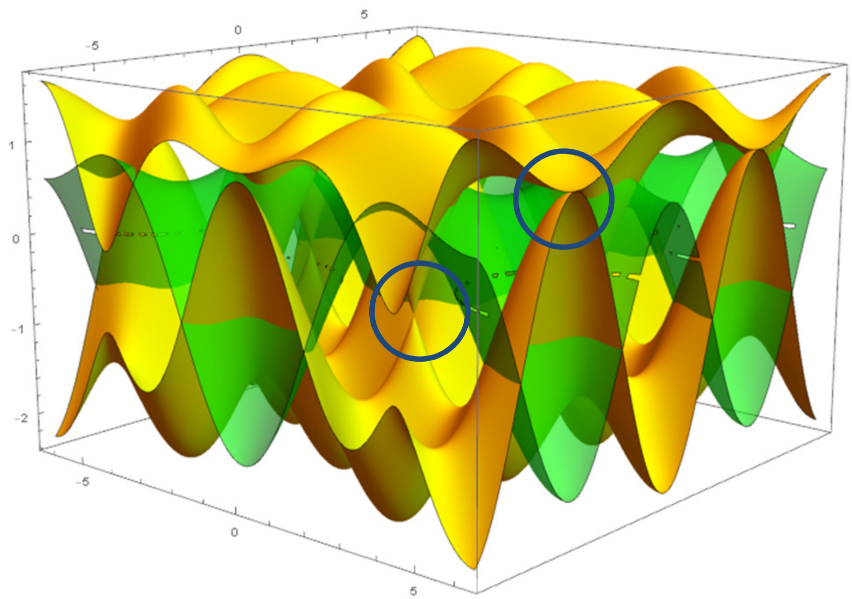
$$H_{\text{axial}}(\vec{k}) = \begin{pmatrix} 0 & d^*(\vec{k}) \\ d(\vec{k}) & 0 \end{pmatrix}$$

Δm= ±2

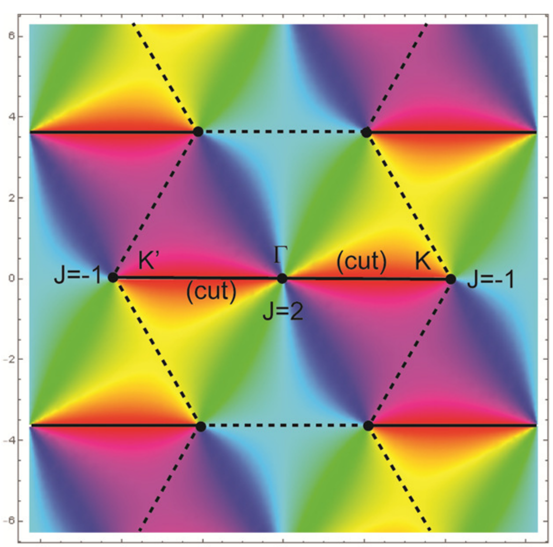
Γ: Δm= ±2 mod 6 = (**2**,-4),(**-2**,4) → J=2

K: Δm= ±2 mod **3** = (2, **-1**),(-2,**1**) → J=-1
(there are two of these in BZ)

$$H_{\text{axial}}(q) = \begin{pmatrix} 0 & q_-^2 \\ q_+^2 & 0 \end{pmatrix}_\Gamma \; ; \; \begin{pmatrix} 0 & \pm q_+ \\ \pm q_- & 0 \end{pmatrix}_{K,K'}$$



arg[d(k)]



Graphene in a pseudospin (sublattice) basis

$$H(\vec{k}) = \begin{pmatrix} 0 & d^*(\vec{k}) \\ d(\vec{k}) & 0 \end{pmatrix}$$

Nodes (i.e. d=0) also occur on exceptional points

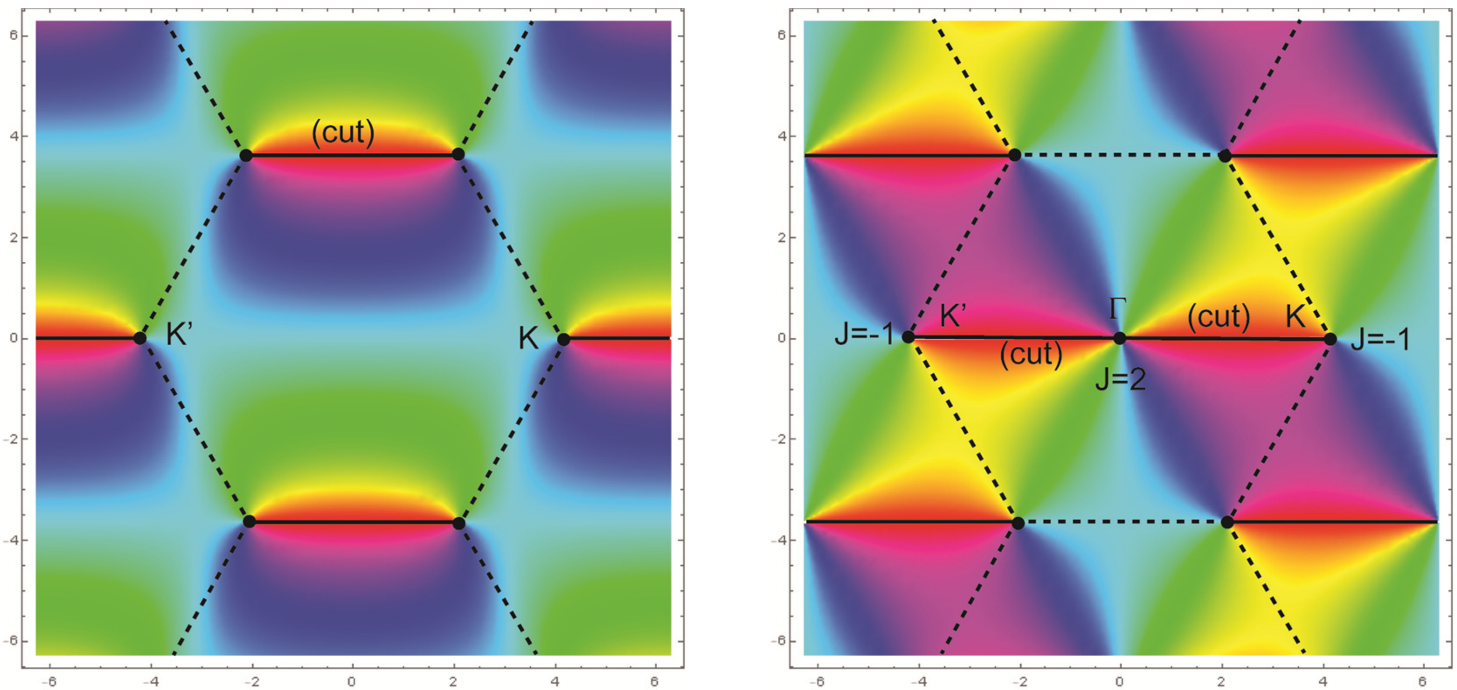
$$H_{\text{axial}}(q) = \begin{pmatrix} 0 & q_- \\ q_+ & 0 \end{pmatrix}_K \; ; \; \begin{pmatrix} 0 & -q_+ \\ -q_- & 0 \end{pmatrix}_{K'}$$

Compensated partners on opposite valleys

Momentum Space Phase Profiles

Graphene: J = ±1 nodes

T-lattice J = -1,2 nodes



Partners at +/- K

Partners at K, Γ

Counting Rules Redux

Graphene: $1_K + (-1)_{K'} = 0$

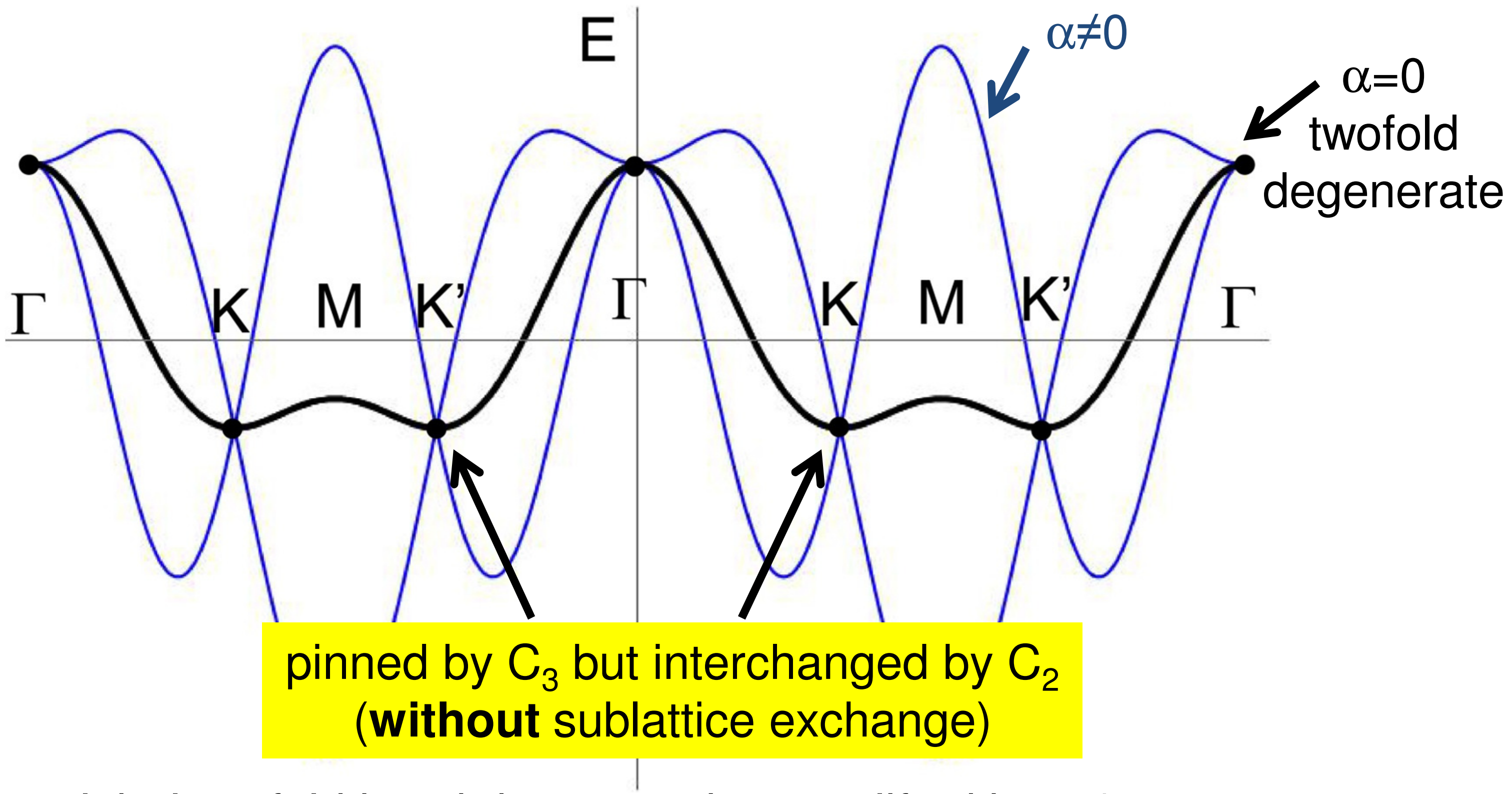
Cu_2Si: $2_\Gamma + (-1)_K + (-1)_{K'} = 0$[a]

uncompensated pair

[a] Note: energies at Γ and K are generically unequal

Sign selection with a twist

$$H_{ij} = \alpha_{ij}(L_i \bullet \hat{d}_{ij})(L_j \bullet \hat{d}_{ij}) + \beta_{ij}(L_i \bullet L_j)$$



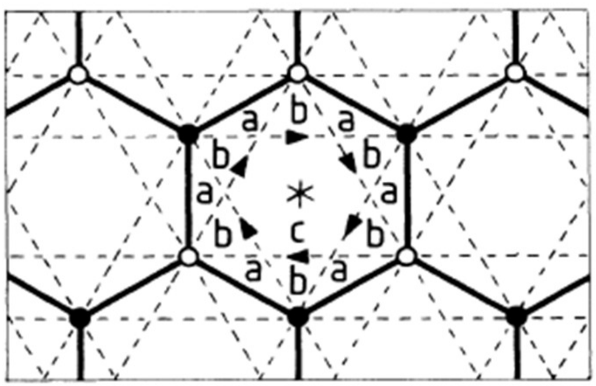
- global twofold band degeneracies get lifted by $\alpha \neq 0$
- **sgn(αβ):** velocity reversal at $\alpha=0$ is the critical point
- choice is **revealed in its gapped variants**

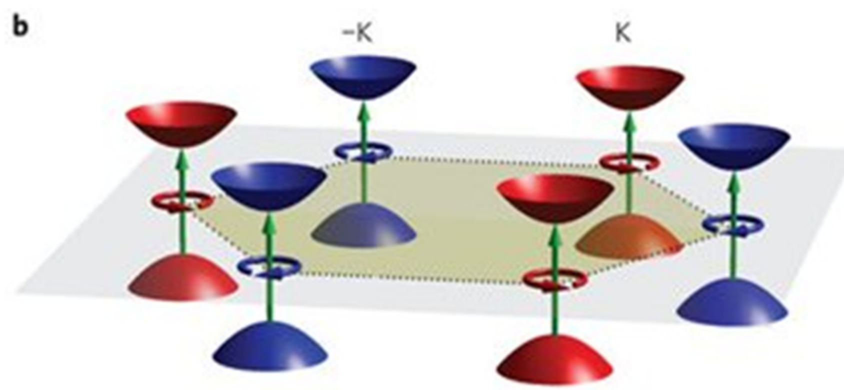
Precedents and Observables

➡ Gapping out the point nodes liberates the Berry curvature

But, on the honeycomb lattice (and its heteropolar variants) this can be accessed in transport only for **valley antisymmetric** mass terms (which eat the minus sign: FDMH-Chern insulator, K-M QSH-state)

or… possibly by forcing a valley asymmetric nonequilibrium state





Instead this physics is directly accessed using valley symmetric **(e.g. local and spatially uniform)** fields**.**

Examples

- **Break T**: couple to T-odd pseudovector:
  gaps WP's, LN protected by z-mirror
  (magnetism, CPL at normal incidence)

- **Break z-mirror (I)**: couple to a T-even tensor
  partially gaps LN $\rightarrow$ Weyl Pair
  (buckling, strain)

- **Break z-mirror (II)**: couple to T-odd tensor
  fully gap LN
  (axial state, noncollinear magnetism)

Examples

- **Break T**: couple to T-odd pseudovector:
  gaps WP's, LN protected by z-mirror
  *(magnetism, **CPL at normal incidence**)*

- **Break z-mirror (I)**: couple to T-even tensor
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  fully gap LN
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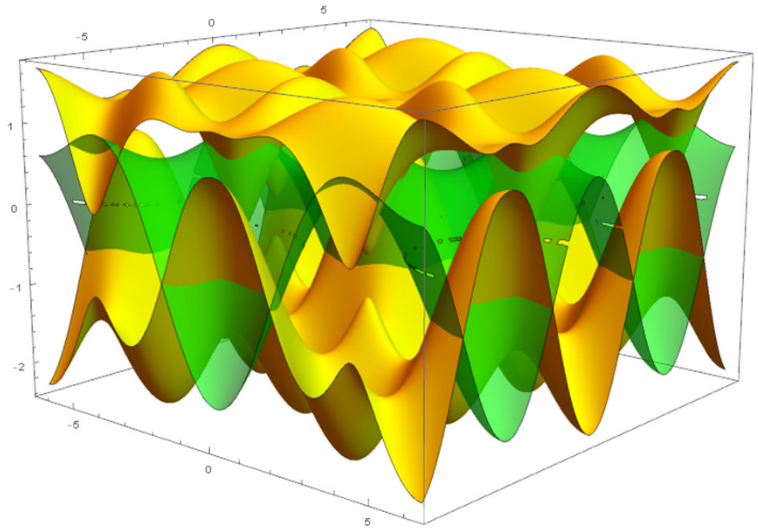
Anomalous Hall from Curvature

$$\sigma_{\alpha\beta} = \frac{e^2}{\hbar} \frac{1}{N\Omega} \sum_{k,n} F_{\alpha\beta,n} f(\varepsilon_n(k) - \mu)$$

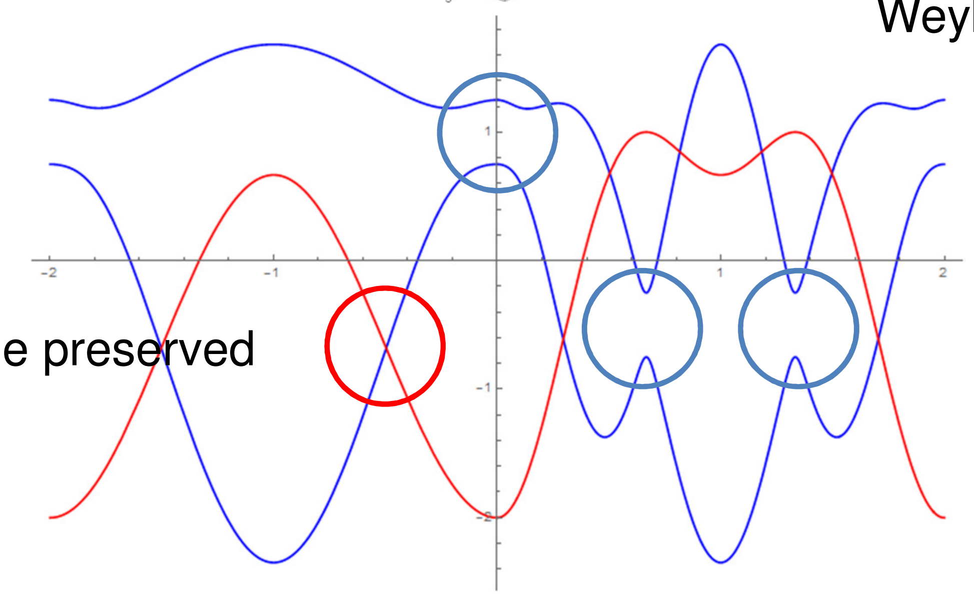
$$F_{\alpha\beta,n} = \partial_{k_\alpha} A_{\beta,n} - \partial_{k_\beta} A_{\alpha,n}$$

$$A_{\alpha,n} = -i \left\langle u_n(k) \,|\, \partial_{k_\alpha} u_n(k) \right\rangle$$

Gapping by **on site σ_z** (orbital Zeeman field)

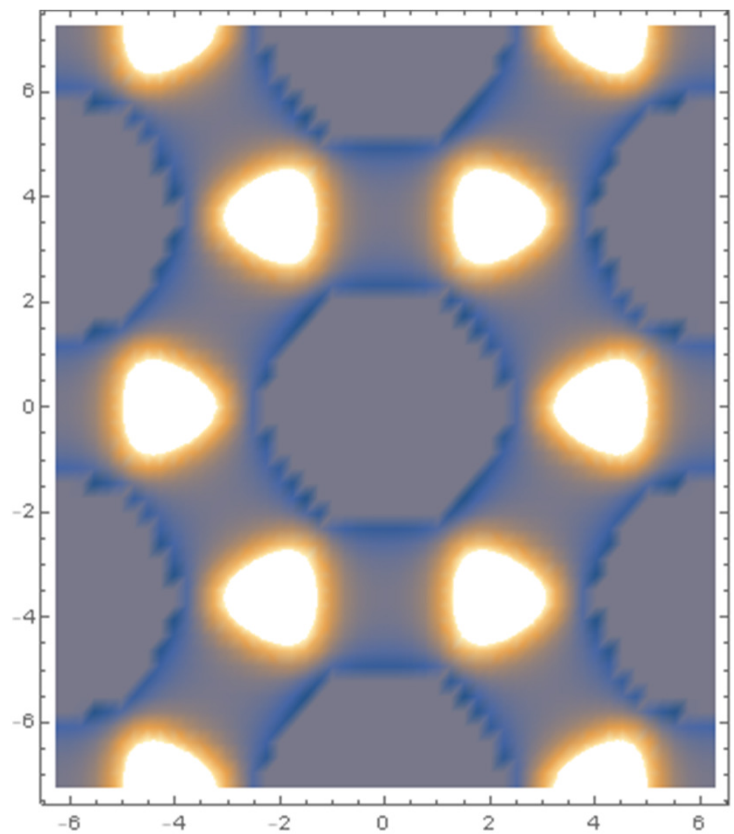


Weyl points gapped

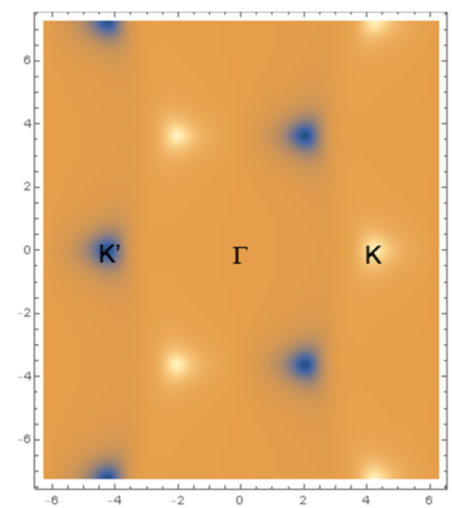


Line node preserved

Berry curvature from **site localized T-breaking** term

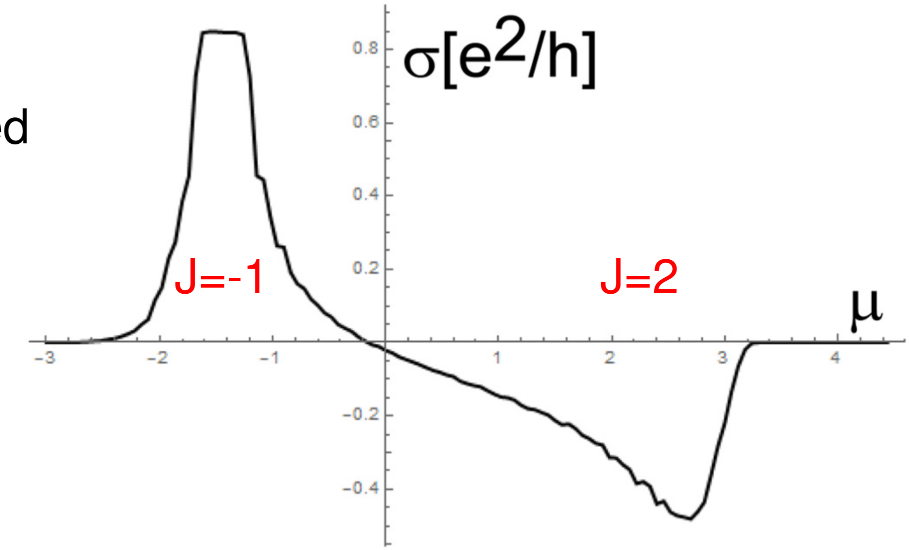


Recall: on honeycomb:
σ_z staggered sublattice

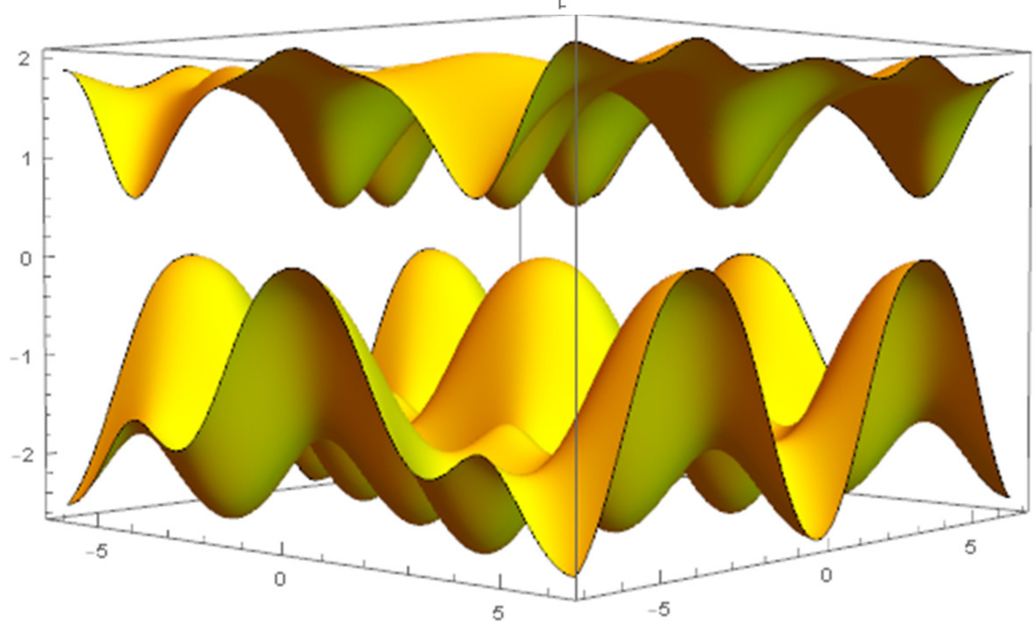


Hall conductance vs. band filling

Weak coupling:
AHE weakly screened



Strong coupling:
fully gapped



Hall conductance vs. band filling

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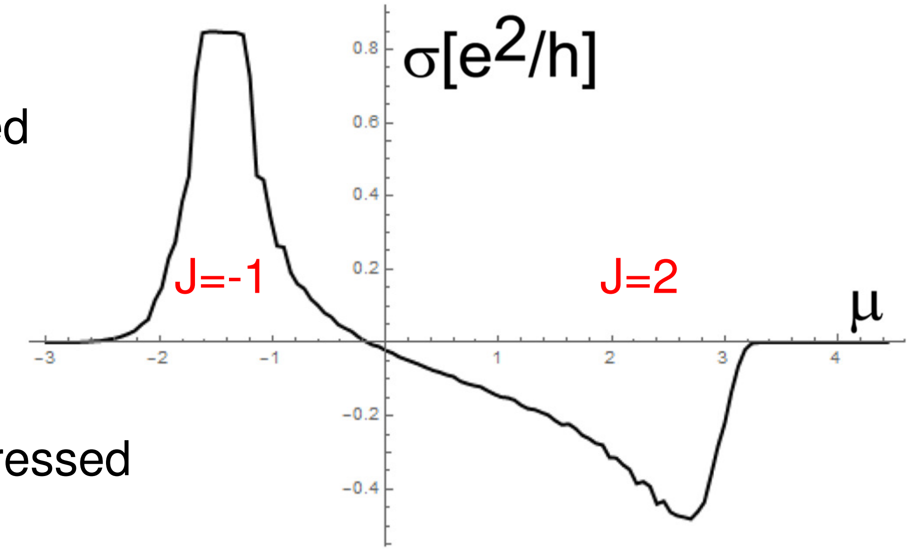
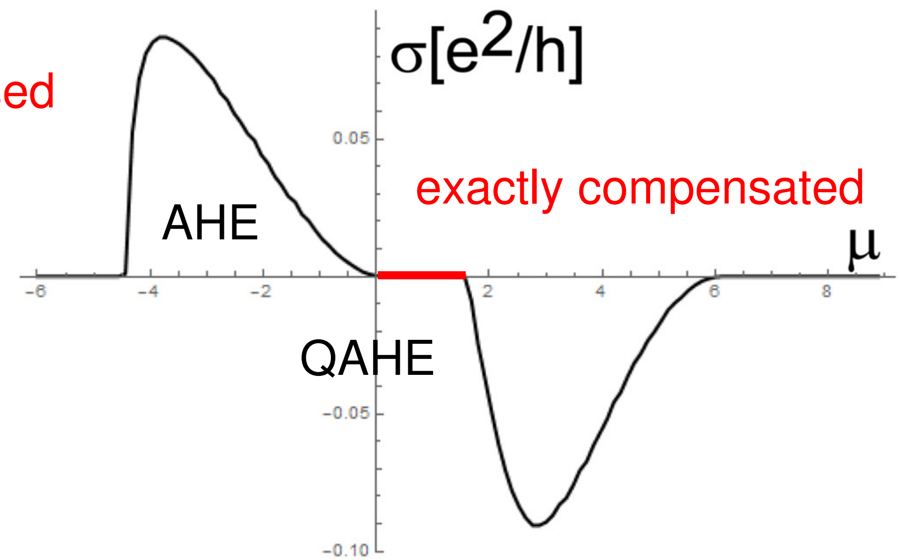


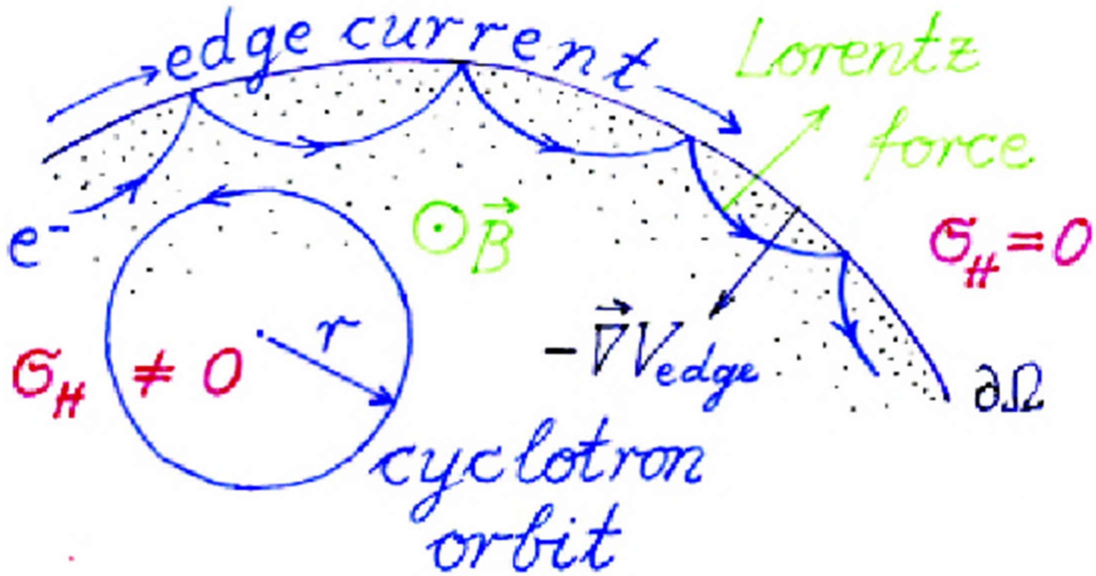
Anomalous Hall suppressed
& nulled in the gap

suppressed



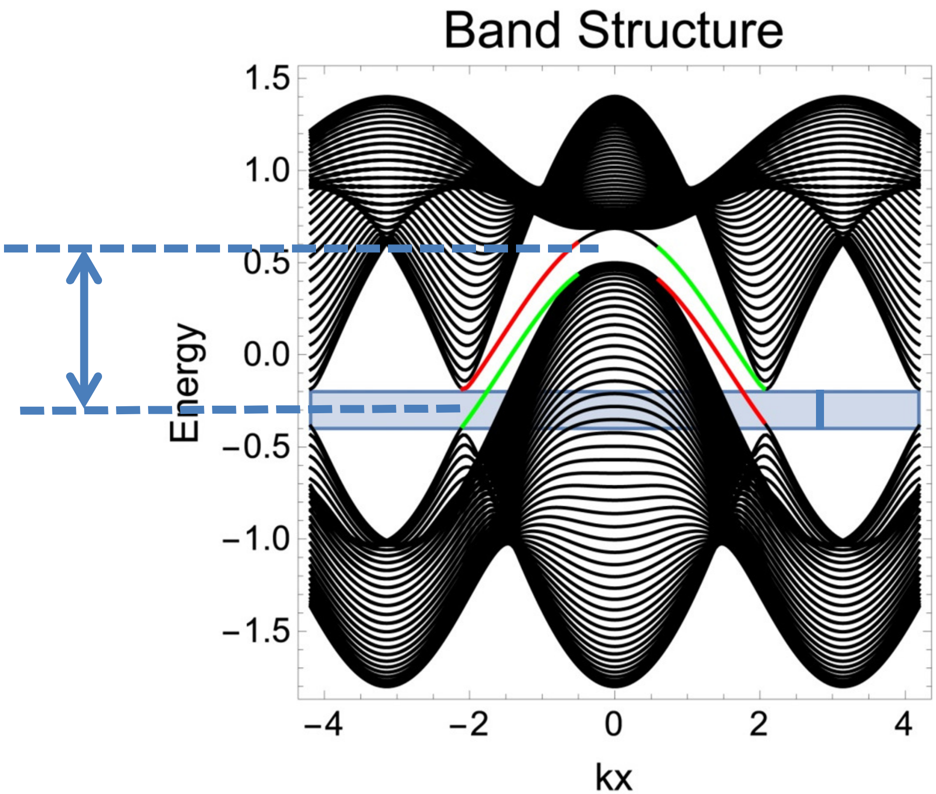
Bulk or Boundary ?

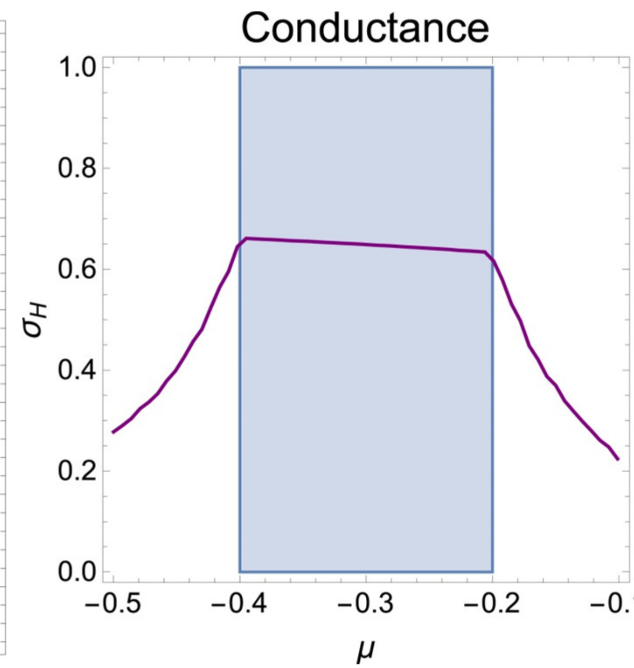
Both (*viz.* either)

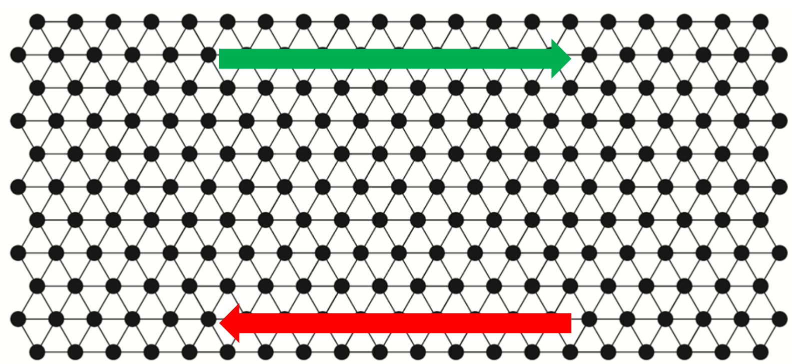


(borrowed from hep lecture notes)

Edge State Picture







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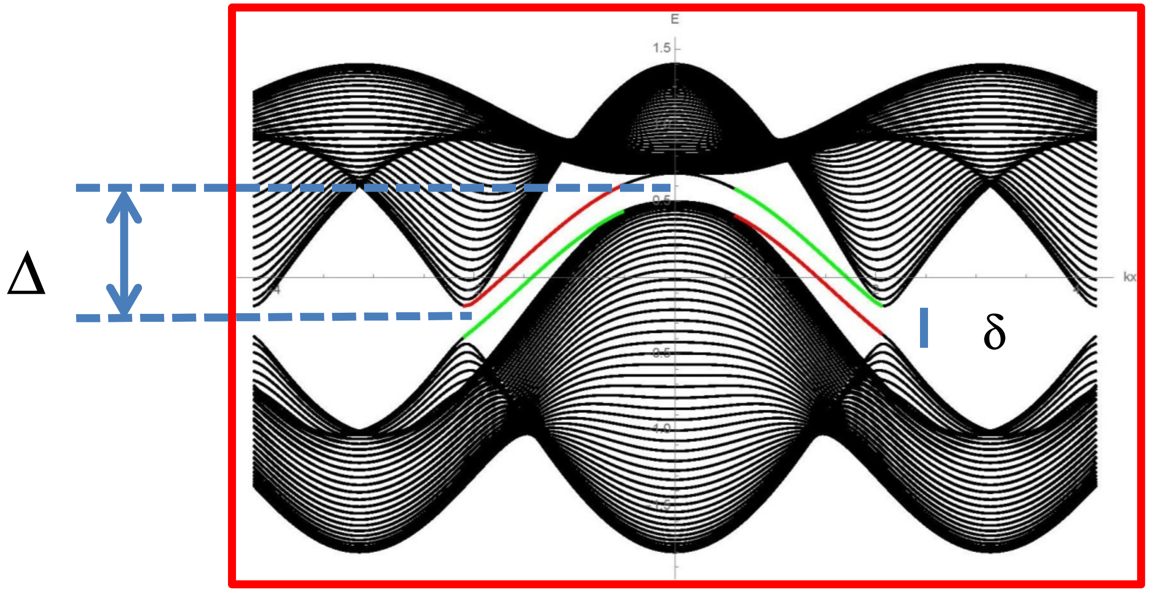
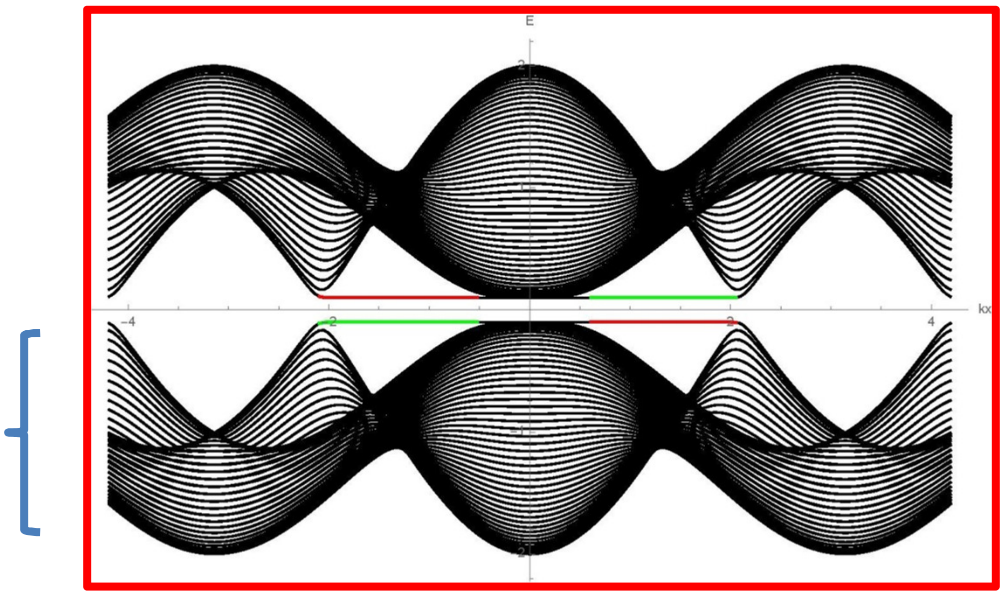


weak coupling
$\delta < \Delta$



strong coupling
$\delta > \Delta$

adiabatically connected to trivial insulator

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Optical control

Orbital Zeeman field can be imposed optically

Couple to circularly polarized light

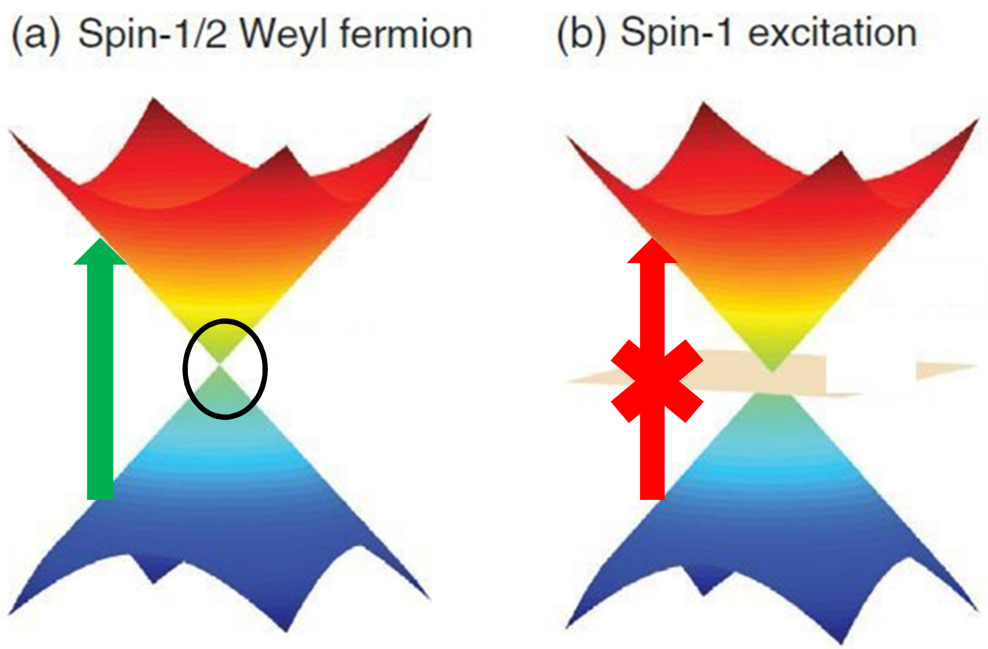
$$\mathcal{H}_{\rm int} = \mathbf{r} \cdot \mathbf{E} \, \cos \omega t - s \, \hat{n} \cdot (\mathbf{r} \times \mathbf{E}) \, \sin \omega t$$

and integrate out the first Floquet bands

$$\mathrm{Tr}[L_z \cdot \mathcal{H}_{\rm eff}] = \left[\frac{\omega}{\Delta(\mathbf{k})^2 - \omega^2} \right] \mathcal{E}_+(\omega) \mathcal{E}_+(-\omega)$$

Odd in ω, proportional to intensity and can be spatially modulated

Interband Selection Rules



mixing <u>with</u> population inversion **mixing <u>without</u> population inversion**

Floquet-Magnus Expansion

$$\mathcal{H}_{\text{eff}}(\mathbf{k}) = \mathcal{P}\mathcal{H}_0(\mathbf{k})\mathcal{P} + \frac{\hbar^2\omega_1^2}{\Delta(\mathbf{k}) - \hbar\omega}\mathcal{P}L_+\mathcal{Q}L_-\mathcal{P} + \frac{\hbar^2\omega_1^2}{\Delta(\mathbf{k}) + \hbar\omega}\mathcal{P}L_-\mathcal{Q}L_+\mathcal{P}$$

$$= \begin{pmatrix} h_0(\mathbf{k}) + \Delta(\mathbf{k}) + \frac{\hbar^2\omega_1^2}{\Delta(\mathbf{k})-\hbar\omega} & h_1(\mathbf{k}) \\ h_1^*(\mathbf{k}) & h_0(\mathbf{k}) + \Delta(\mathbf{k}) + \frac{\hbar^2\omega_1^2}{\Delta(\mathbf{k})+\hbar\omega} \end{pmatrix}.$$

$$\delta(\mathbf{k}) = \frac{e^2\alpha^2 I\hbar\omega}{c\epsilon_0(\Delta(\mathbf{k}) - \hbar\omega)(\Delta(\mathbf{k}) + \hbar\omega)}.$$

δ~100 meV: E~10^8 (10^9) on(off) resonance @ crystal field Δ

Lindenberg (2011), Nelson (2013), Rubio (2015), Averitt (2017)

Can we induce a k-space tilt?

untilted **tilted Type I** **tiltedType II**

<u>FLO(quet)-NO-GO</u>:
linear-in-intensity terms $\rightarrow$ constant
(absence of linear-in-q terms)

Closing Comments and Open Items

✓ • **More material realizations** (Cu_2Si is not optimal, but the model is generic[1])

• Spin (magnetism, spin orbit, etc)

• Quenched orbital angular momentum at boundaries (anomalous transport without edge states)

[1]**Closely related models on a 2D <u>honeycomb:</u>**

Topological bands for optical lattices: C. Wu *et al.* (2007-8)
Low energy models for small angle moire t-BLG (2018)

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