Bulk-edge correspondence in topological materials – Dirac fermions beyond chiral states (Part 2)

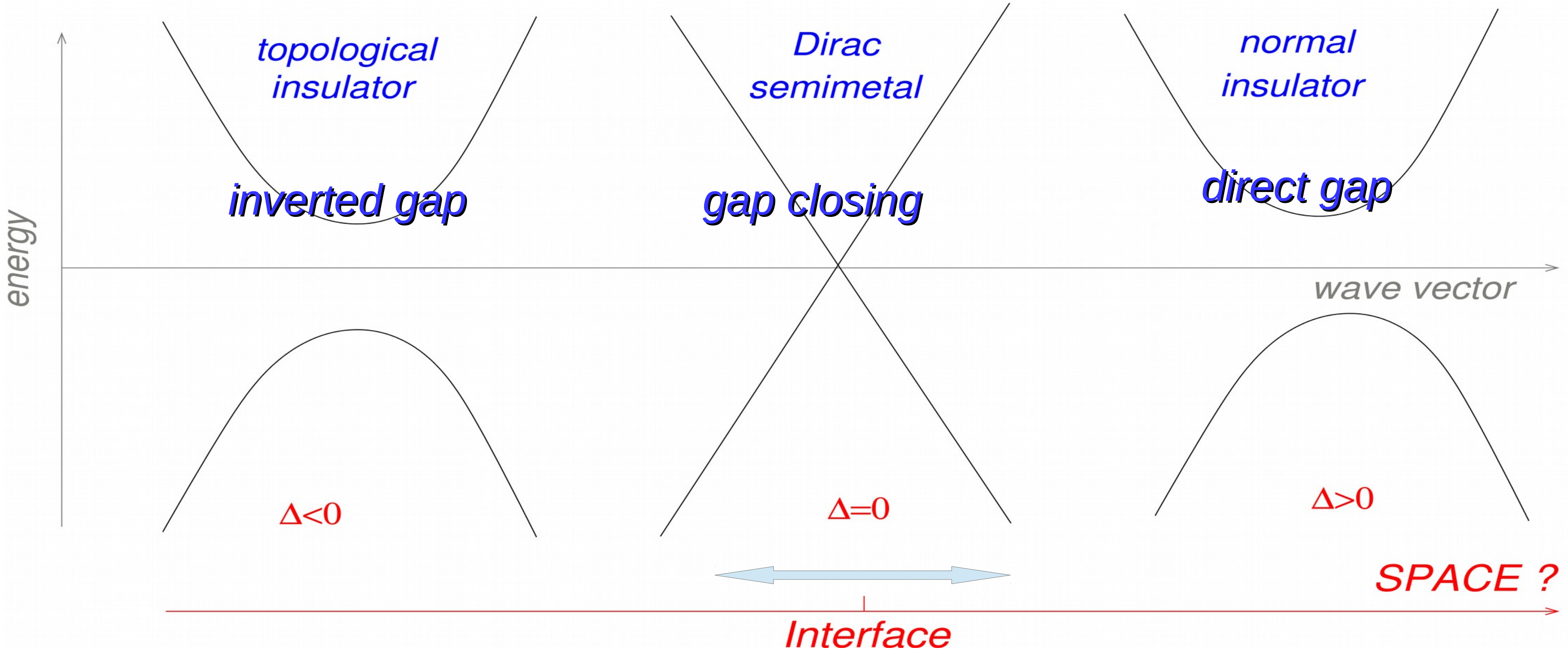
Mark Oliver Goerbig

Sergueï Tchoumakov, Xin Lu (PhD thesis)

Collaborators: M. Civelli (LPS), D. Carpentier & V. Jouffrey (ENS-Lyon) ;

Experiments: Plaçais group (ENS-Paris) ; Molenkamp group (Würzburg)

Reminder: simplified 2D model of a smooth interface (*topological heterojunction*)



$$H = \begin{pmatrix} \Delta \frac{x}{\ell} & \hbar v(q_x - i q_y) \\ \hbar v(q_x + i q_y) & -\Delta \frac{x}{\ell} \end{pmatrix}$$

Sign change in an interface of size ℓ

Simplified 2D model of a smooth interface (*topological heterojunction*)

→ Hamiltonian of massive Dirac fermions in a magnetic field

$$H = \begin{pmatrix} \hbar v q_y & \sqrt{2}\hbar \frac{v}{\ell_S}\hat{a} \\ \sqrt{2}\hbar \frac{v}{\ell_S}\hat{a}^\dagger & -\hbar v q_y \end{pmatrix}$$

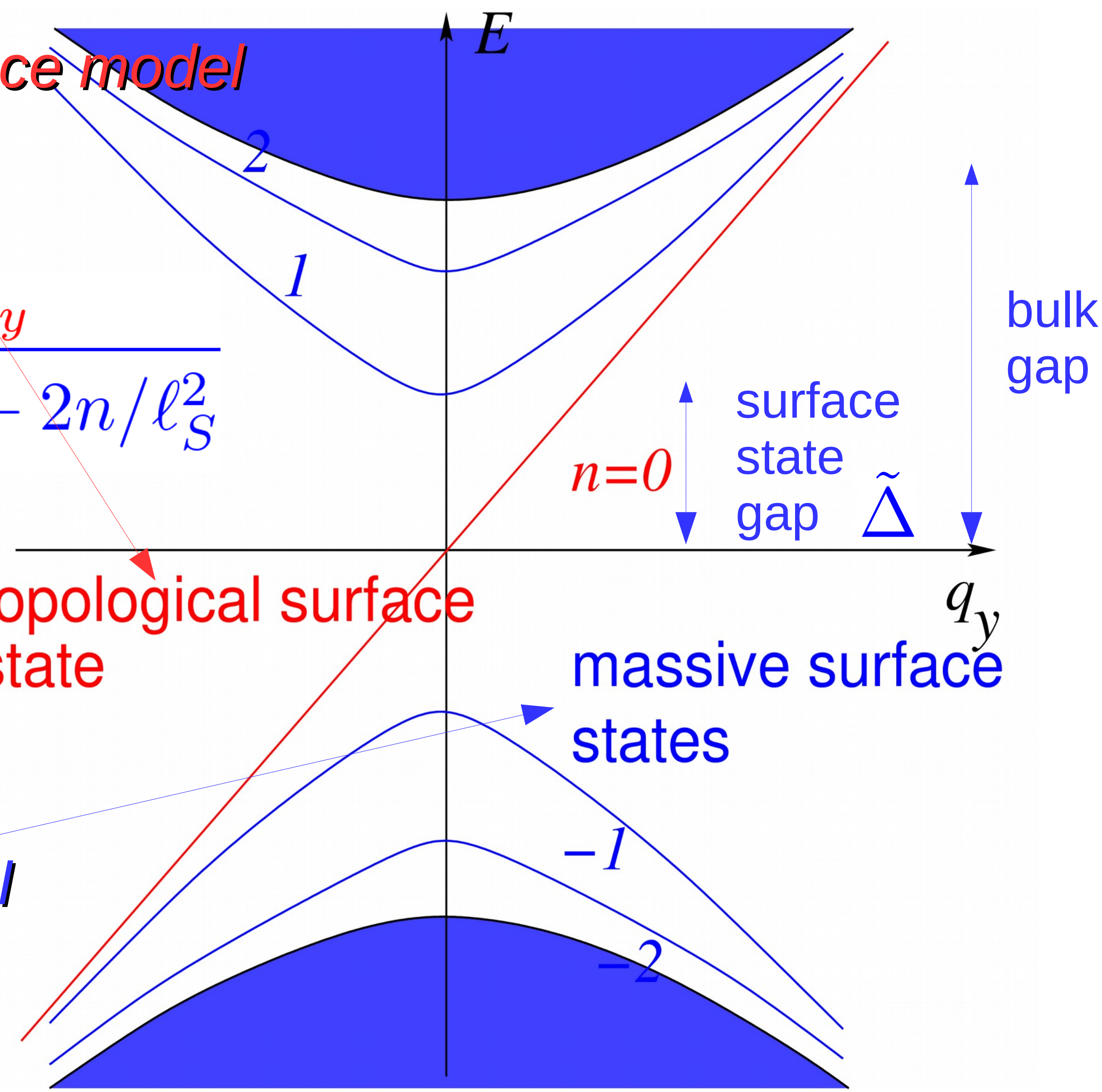
surface states ~ Landau levels

$$\begin{aligned} E_{n=0} &= \hbar v q_y \\ E_{\lambda,n\neq 0} &= \lambda \hbar v \sqrt{q_y^2 + 2n/\ell_S^2} \end{aligned}$$

Surface (edge) states

independent of surface model

$$E_{n=0} = \hbar v q_y$$
$$E_{\lambda,n\neq 0} = \lambda \hbar v \sqrt{q_y^2 + 2n/\ell_S^2}$$



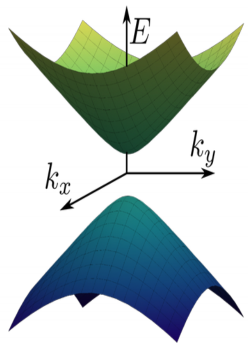
depends on surface model

$$\tilde{\Delta} = \sqrt{2}\hbar v/\sqrt{\ell \xi}$$

number of visible VP states : $N \sim \ell/\xi$

Surface states in 3D materials

- *e.g.* PbTe/SnTe and HgTe/CdTe interfaces : gap switches sign



Complication in 3D: 4x4 Hamiltonian

$$\ell_S^2 = \ell\xi = \ell\frac{\hbar v_F}{\Delta}$$

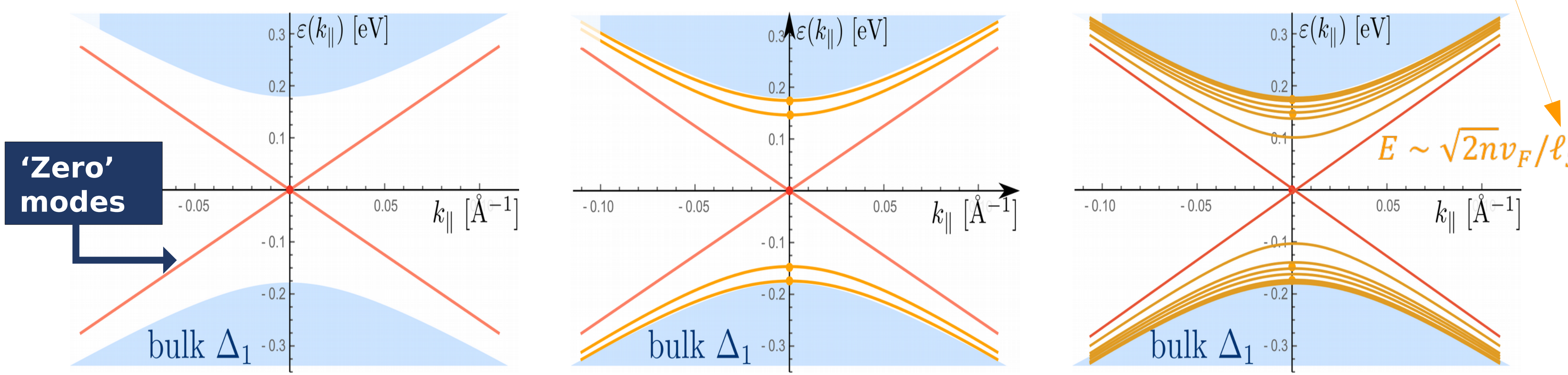
$$H = v_F(k_z \mathbb{1} \otimes \tau_y + (k_y\,\sigma_x - k_x\sigma_y) \otimes \tau_x) + \Delta(z)\,\mathbb{1} \otimes \tau_z$$

here: $$\Delta(z) = \Delta \tanh(z/\ell)$$

+ *numerical k.p calculations (→ ENS Lyon)*

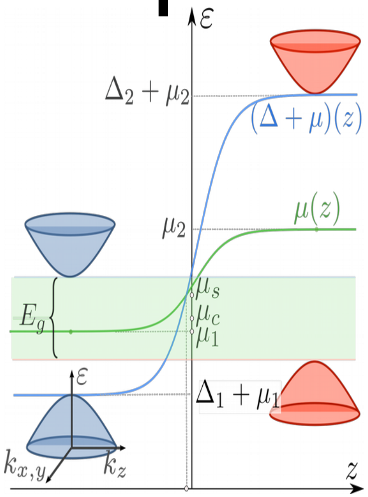
ℓ/ξ

abrupt | intermediate | very smooth



S. Tchoumakov et al., PRB 96, 201302 (2017)
Volkov and Pankratov, JETP Lett. 42, 4 (1985)

Special relativity in surface states

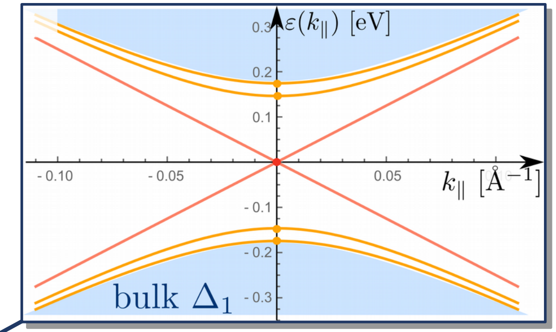


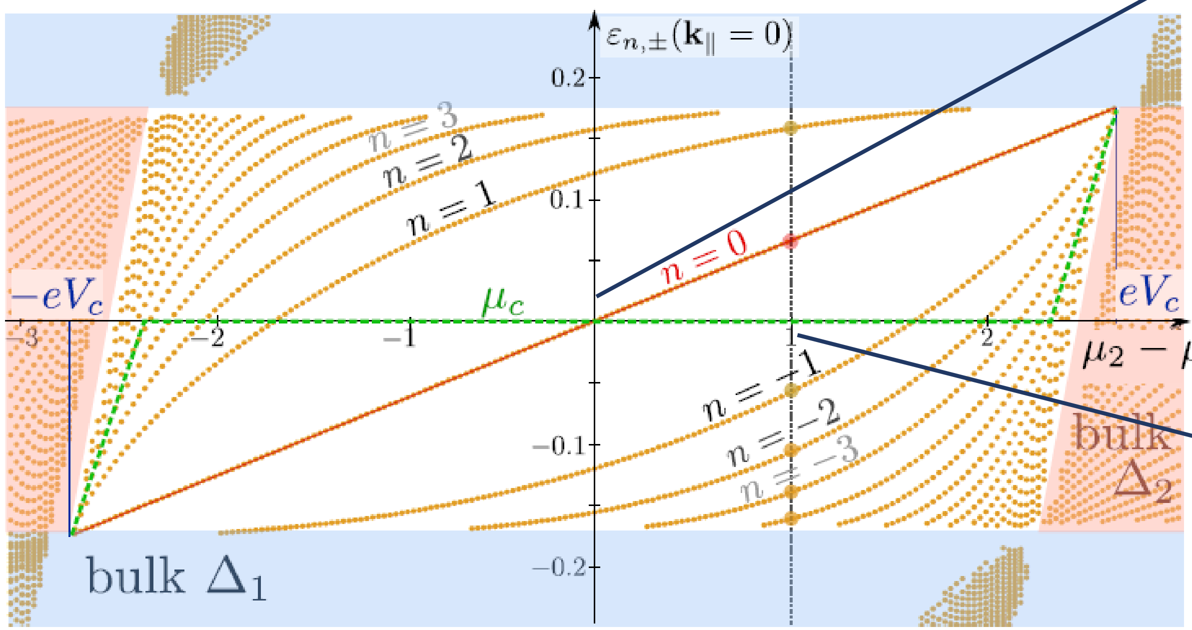
$$H = \mathbf{V(z)}\,\mathbb{1} + v_F(k_x\,\mathbb{1}\otimes\tau_y + (k_y\,\sigma_x - k_x\sigma_y)\otimes\tau_x) + \mathbf{\Delta(z)}\,\mathbb{1}\otimes\tau_z$$

Lorentz boost : $\beta = -\frac{\mu_2-\mu_1}{\Delta_2-\Delta_1}$

Electric field: $E \rightarrow E' = 0$

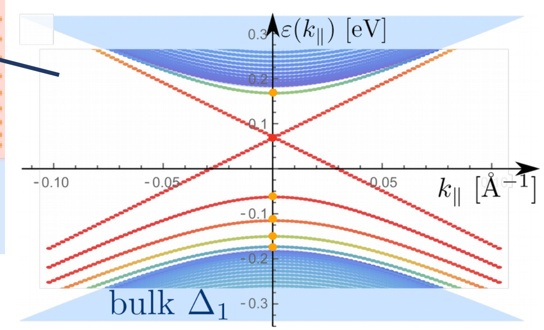
Magnetic field: $B \rightarrow B\sqrt{1-\beta^2}$





$$\Delta_n' \approx (1-\beta^2)^{3/4}\Delta_n$$

$$\mu_s' = -\beta\Delta_1$$

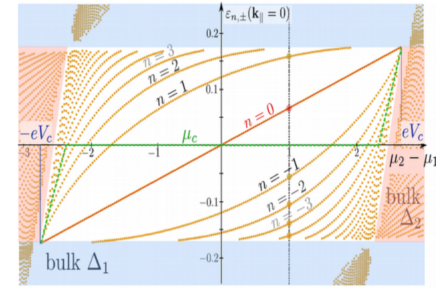


S. Tchoumakov, V. Jouffrey et al., PRB 96, 201302 (2017)

Outline

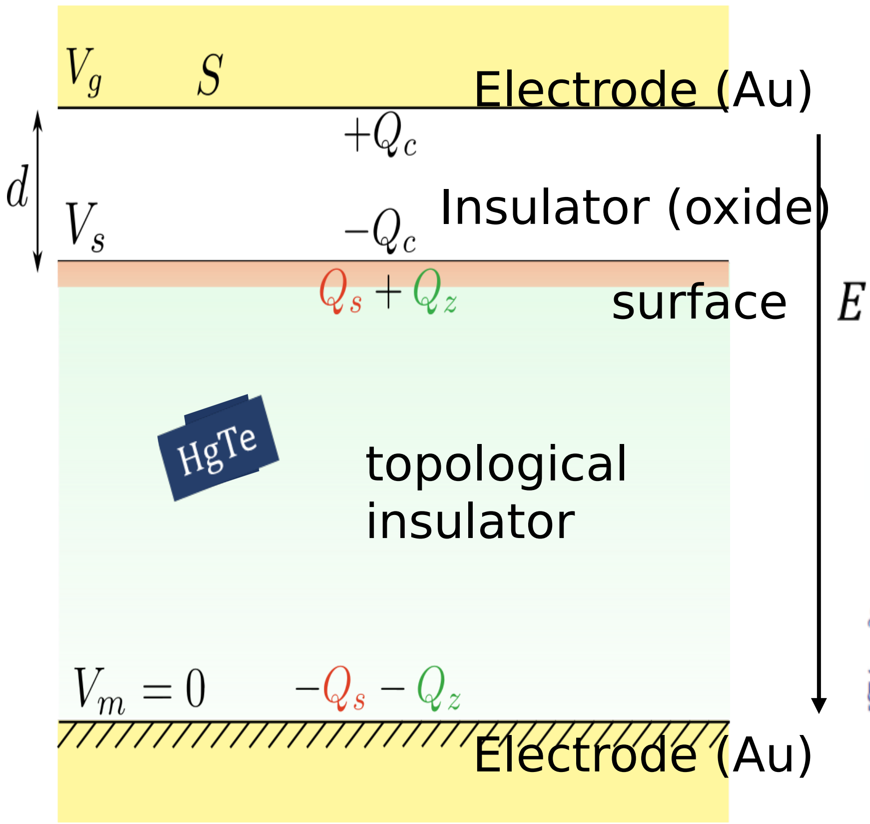
- Introduction to Berry curvature and bulk-edge correspondence
- Dirac fermions and “half Chern numbers”
- 2D Model of a smooth interface – from chiral to massive *relativistic* interface states
- First experimental evidence
- Weyl semimetals with smooth surfaces
- Possible identification of surface states beyond the chiral ones in (magneto-)optical spectroscopy

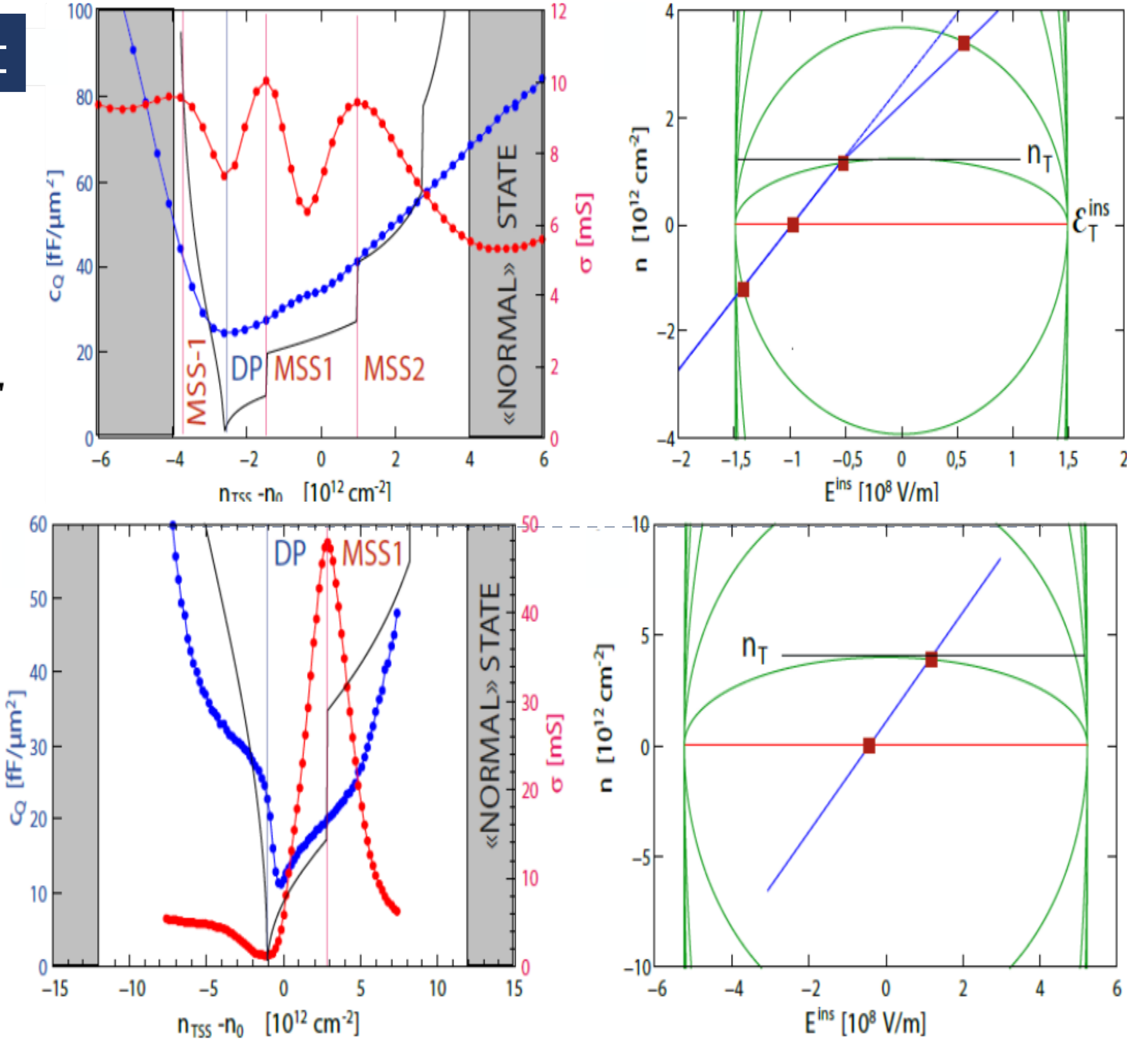
Experimental evidence



- Electrical resistance and capacitance of HgTe

Qualitative agreement



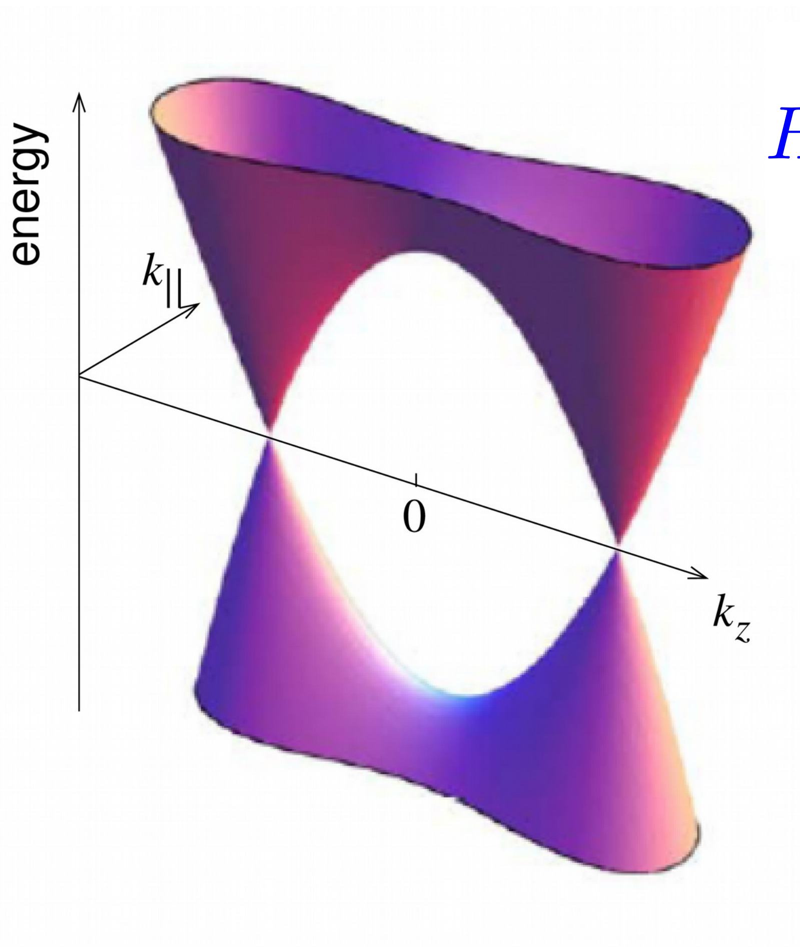


A. Inhofer *et al.*, PRB 96, 195104 (2017)

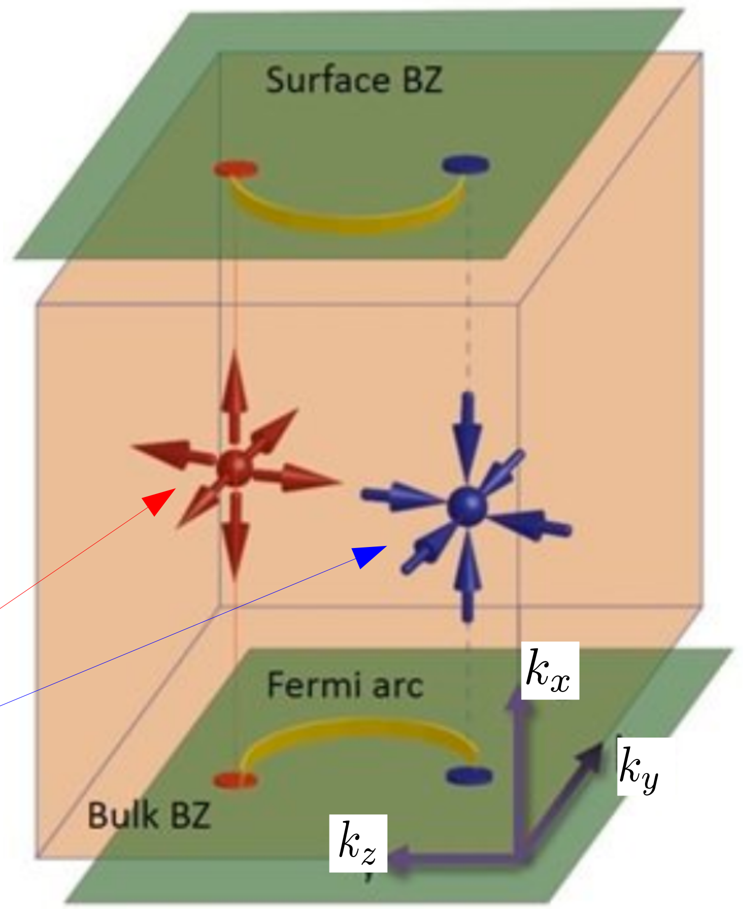
Outline

- Introduction to Berry curvature and bulk-edge correspondence
- Dirac fermions and “half Chern numbers”
- 2D Model of a smooth interface – from chiral to massive *relativistic* interface states
- First experimental evidence
- Weyl semimetals with smooth surfaces
- Possible identification of surface states beyond the chiral ones in (magneto-)optical spectroscopy

Weyl semimetals – “3D graphene”

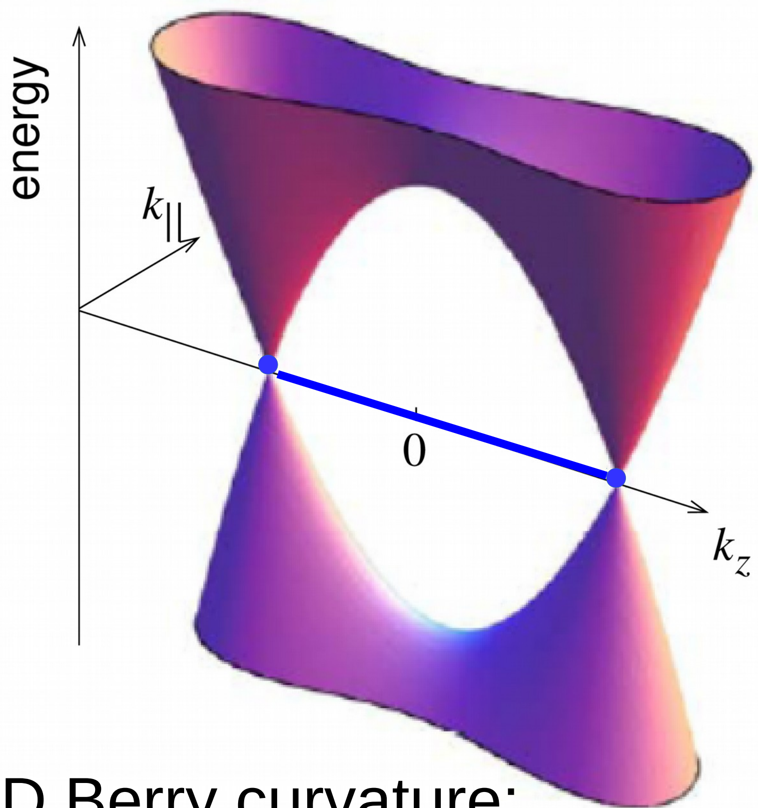


$$H = \begin{pmatrix} \Delta - \frac{\hbar^2 k_z^2}{2m_0} & \hbar v(k_x - i k_y) \\ \hbar v(k_x + i k_y) & -\Delta + \frac{\hbar^2 k_z^2}{2m_0} \end{pmatrix}$$



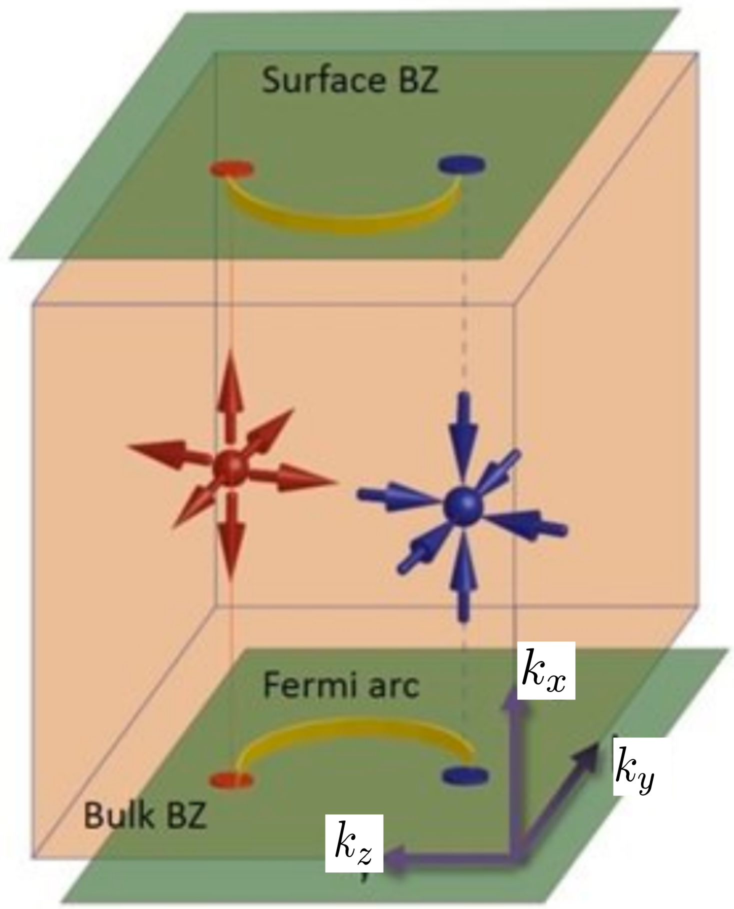
Dirac monopoles
(in wave function)

Weyl semimetals – “3D graphene”



$$H = \begin{pmatrix} \Delta - \frac{\hbar^2 k_z^2}{2m_0} & \hbar v(k_x - ik_y) \\ \hbar v(k_x + ik_y) & -\Delta + \frac{\hbar^2 k_z^2}{2m_0} \end{pmatrix}$$

Δ_{k_z}



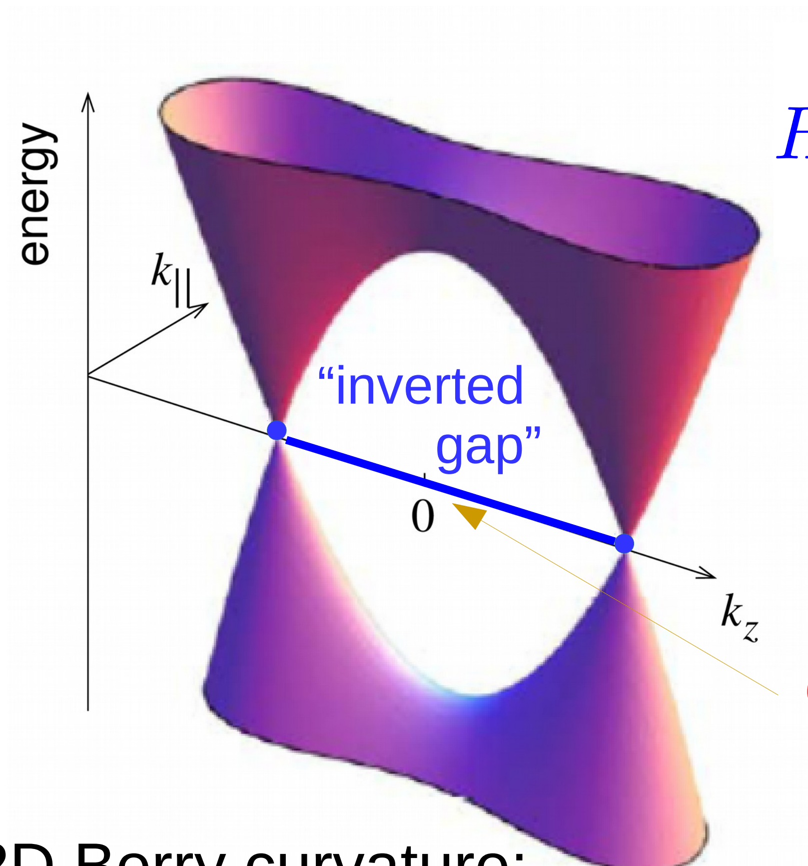
2D Berry curvature:

$$\mathcal{B}_{\lambda,k_z}(k_\parallel) = -\frac{\lambda}{2}\frac{\hbar^2 v^2 \Delta_{k_z}}{(\Delta_{k_z}^2 + \hbar^2 v^2 k_\parallel^2)^{3/2}}$$

“half Chern number”:

$$C_\lambda(k_z) = -\frac{1}{2}\lambda\,\mathrm{sgn}(\Delta_{k_z})$$

Weyl semimetals – “3D graphene”

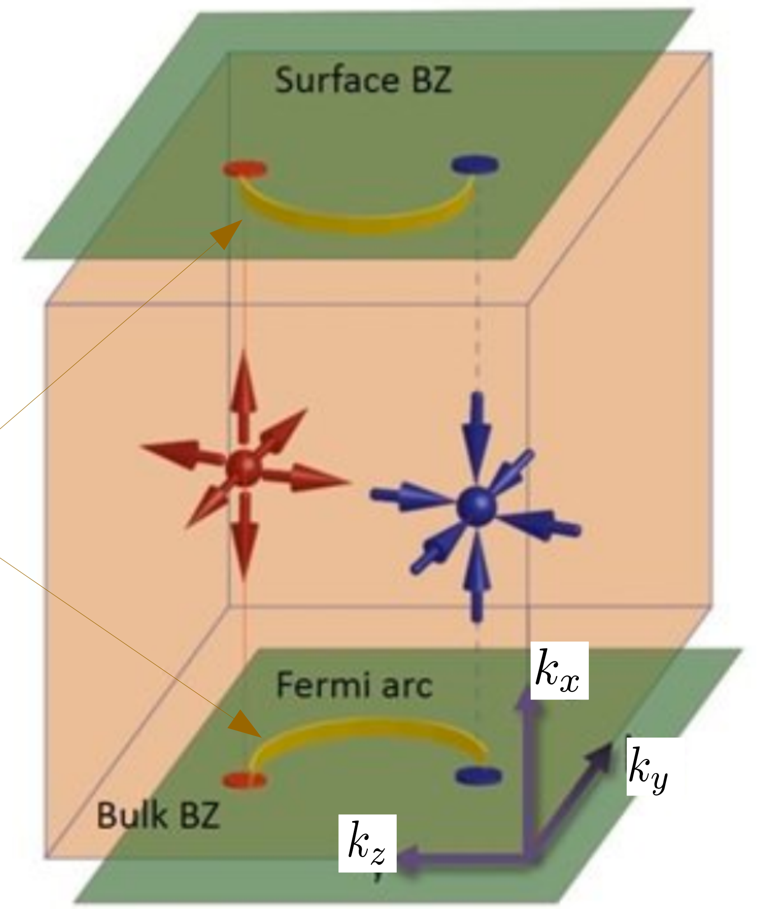


$$H = \begin{pmatrix} \Delta - \frac{\hbar^2 k_z^2}{2m_0} & \hbar v(k_x - ik_y) \\ \hbar v(k_x + ik_y) & -\Delta + \frac{\hbar^2 k_z^2}{2m_0} \end{pmatrix}$$

Δ_{k_z}

edge states

$\epsilon_{0,k_z}(k_y)$



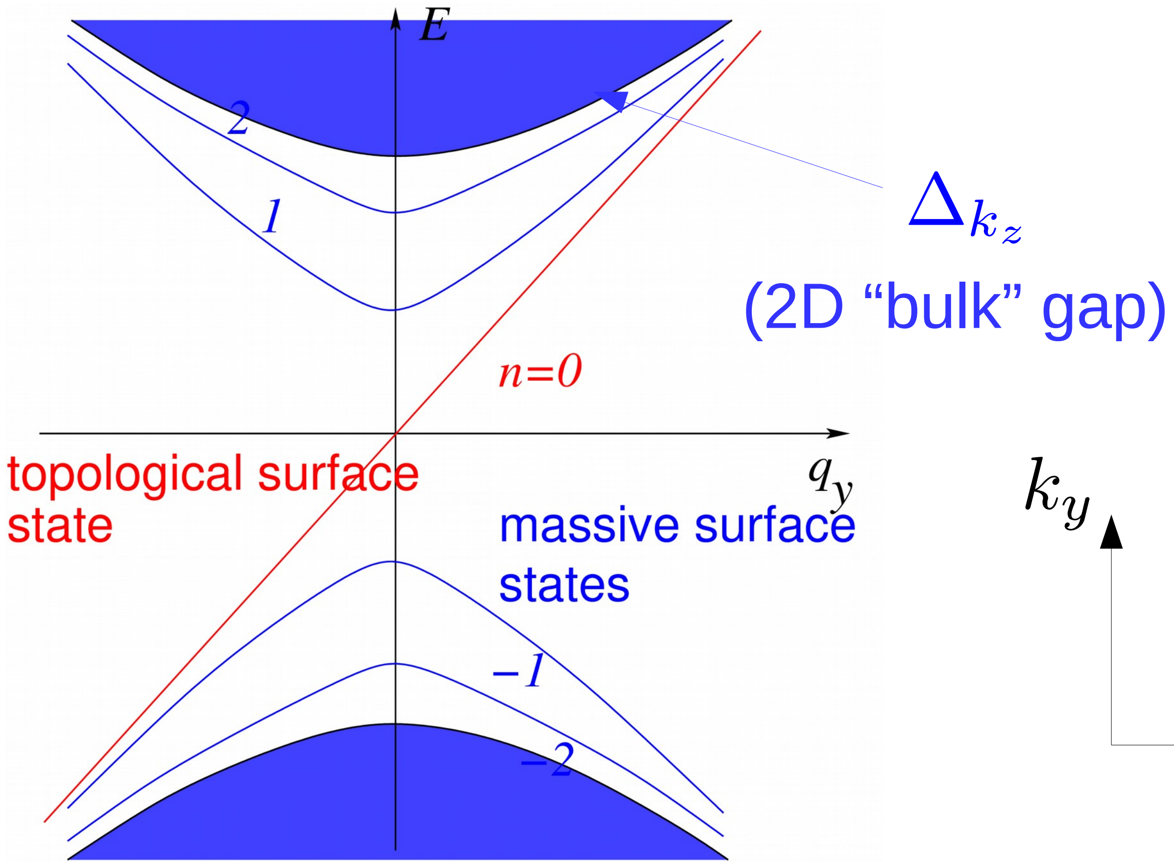
2D Berry curvature:

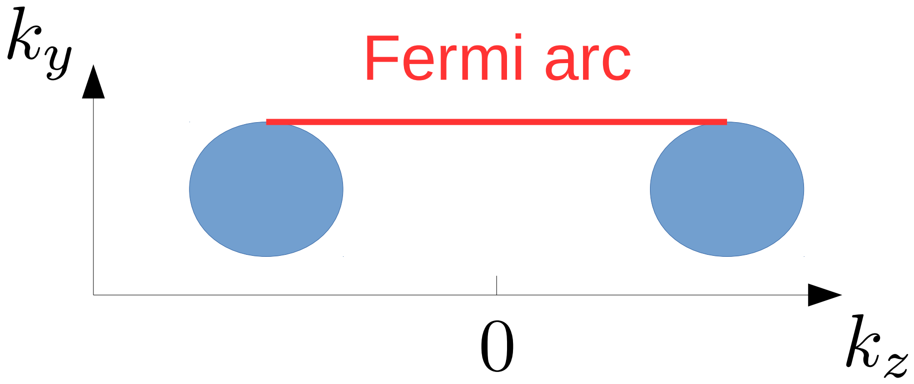
$$\mathcal{B}_{\lambda,k_z}(k_{\parallel}) = -\frac{\lambda}{2}\frac{\hbar^2 v^2 \Delta_{k_z}}{(\Delta_{k_z}^2 + \hbar^2 v^2 k_{\parallel}^2)^{3/2}}$$

“half Chern number”:

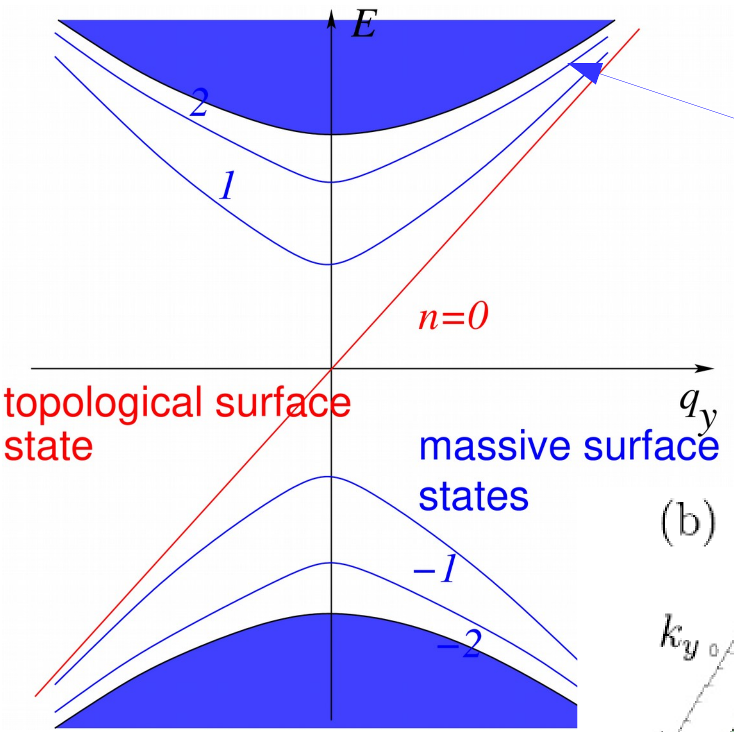
$$C_\lambda(k_z) = -\frac{1}{2}\lambda\,\mathrm{sgn}(\Delta_{k_z})$$

Fermi arc as a collection of 1D edge channels



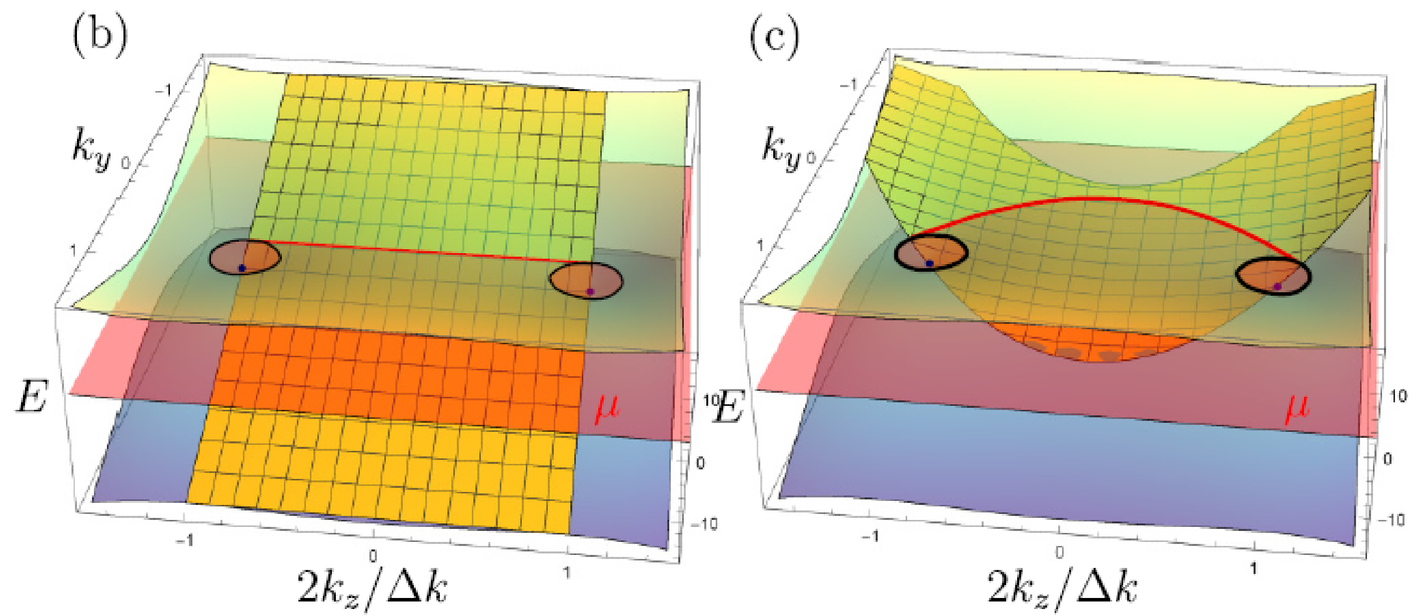


Fermi arc as a collection of 1D edge channels



Δ_{k_z}

(2D “bulk” gap)



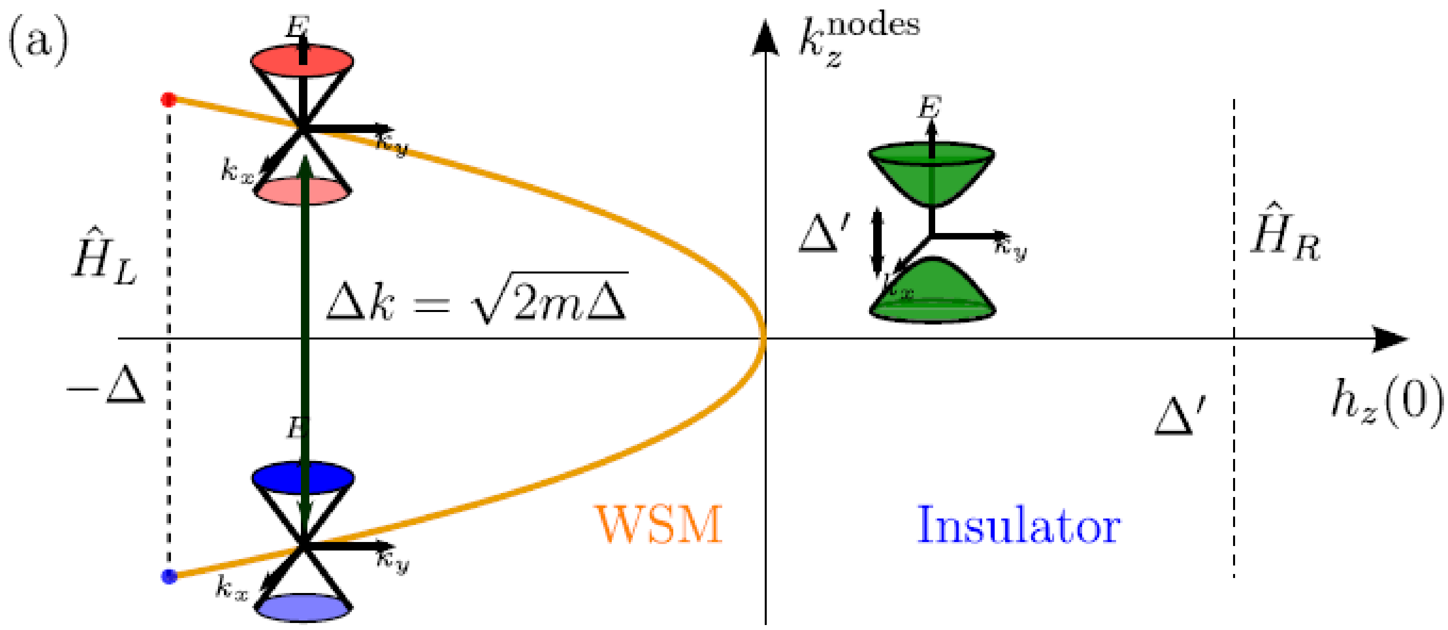
Tchoumakov, Civelli & MOG, PRB (2017)

Fermi arc in a smooth interface → TI

Effective interface model for Weyl node merging:

$$\Delta \to \Delta(x) = \Delta - \Delta' \frac{x}{\ell}$$

$$H = \begin{pmatrix} \Delta(x) - \frac{\hbar^2 k_z^2}{2m_0} & \hbar v(k_x - i k_y) \\ \hbar v(k_x + i k_y) & -\Delta(x) + \frac{\hbar^2 k_z^2}{2m_0} \end{pmatrix}$$



Fermi arc in a smooth interface → TI

Effective interface model for Weyl node merging:

$$\Delta \to \Delta(x) = \Delta - \Delta' \frac{x}{\ell}$$

change of "quantization axis" (unitary trafo)

$$\sigma_z \to -\sigma_y, \qquad \sigma_y \to \sigma_z$$

$$H = \begin{pmatrix} \hbar v k_y & \sqrt{2}\hbar \frac{v}{\ell_S} a \\ \sqrt{2}\hbar \frac{v}{\ell_S} a^\dagger & \hbar v k_y \end{pmatrix}$$

ladder operators:

$$a = \frac{\ell_S}{\sqrt{2}} \left[k_x + i \frac{x - x_0}{\ell_S^2} \right] \quad \text{and} \quad a^\dagger = \frac{\ell_S}{\sqrt{2}} \left[k_x - i \frac{x - x_0}{\ell_S^2} \right]$$

with $[a, a^\dagger] = 1$

Tchoumakov, Civelli & MOG, PRB (2017)
Grushin et al., PRX (2016)

Fermi arc in a smooth interface → TI

Effective interface model for Weyl node merging:

$$\Delta \to \Delta(x) = \Delta - \Delta' \frac{x}{\ell}$$

change of “quantization axis” (unitary trafo)

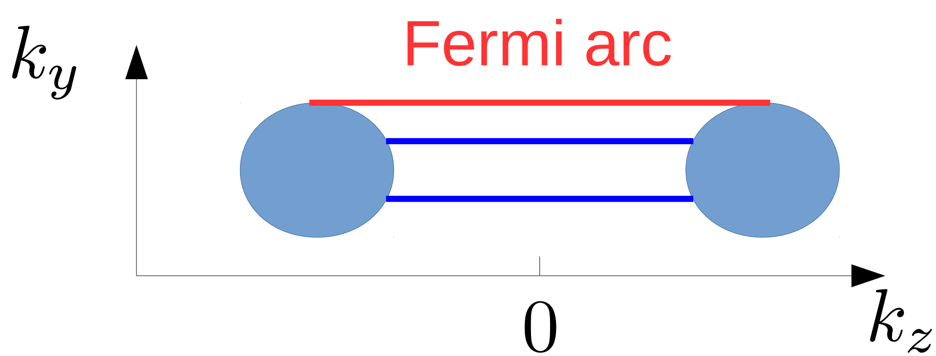
$$\sigma_z \to -\sigma_y, \qquad \sigma_y \to \sigma_z$$

$$H = \begin{pmatrix} \hbar v k_y & \sqrt{2}\hbar \frac{v}{\ell_S} a \\ \sqrt{2}\hbar \frac{v}{\ell_S} a^\dagger & \hbar v k_y \end{pmatrix}$$

“Landau levels”:

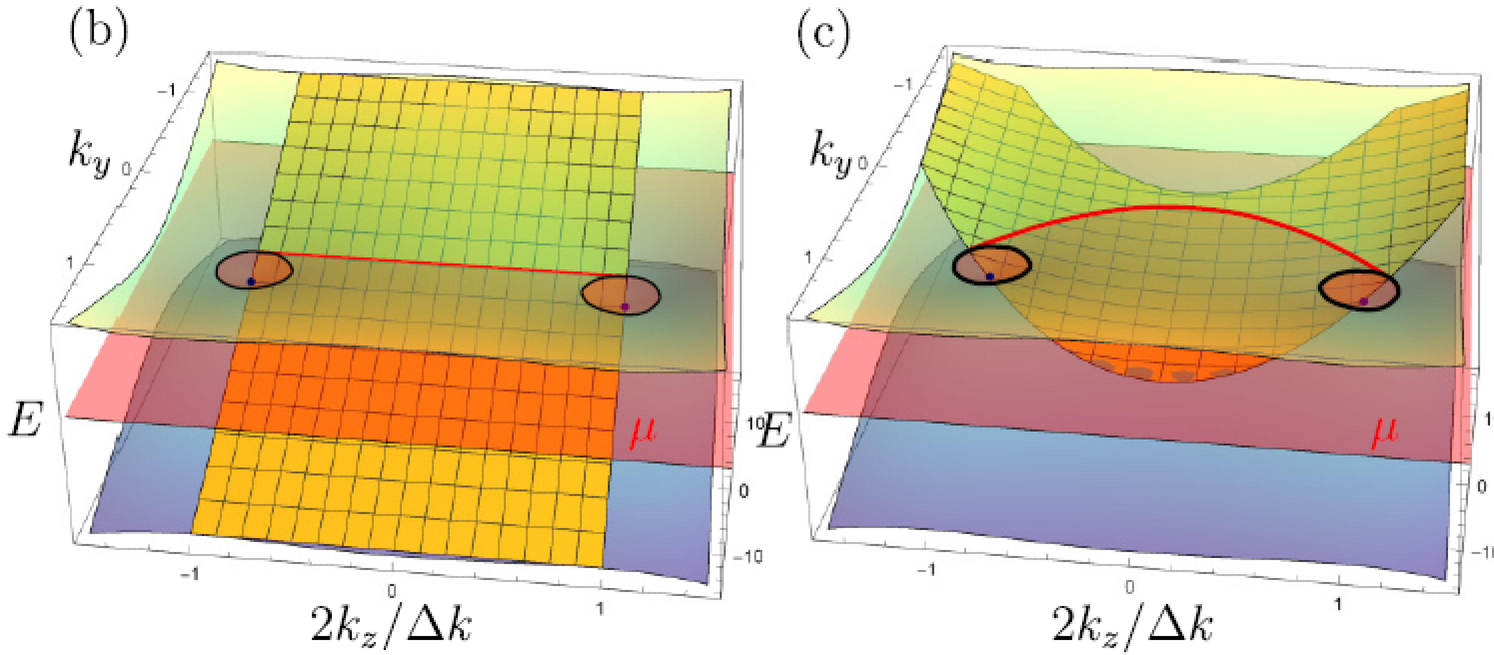
$$E_{n=0}(k_y) = \hbar v k_y$$ ← *Fermi arc*

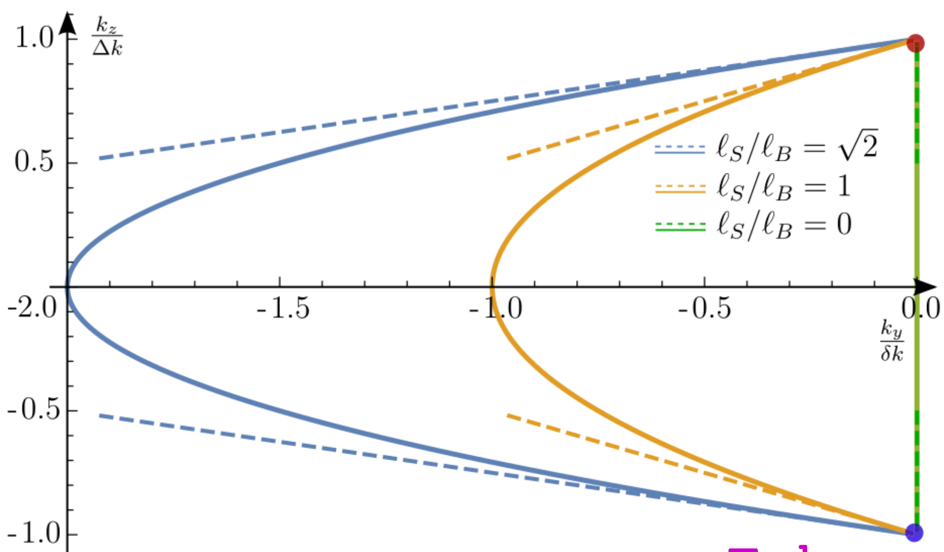
$$E_{\lambda, n\neq 0}(k_y) = \lambda \hbar v \sqrt{k_y^2 + 2n/\ell_S^2}$$ ← *massive VP states*



Tchoumakov, Civelli & MOG, PRB (2017)

Dispersing Fermi arcs



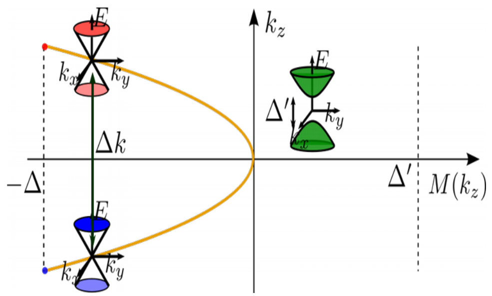


dispersion of Fermi arcs in k_z

→ magnetic field in interface (conspires with confinement)

Tchoumakov, Civelli & MOG, PRB (2017)

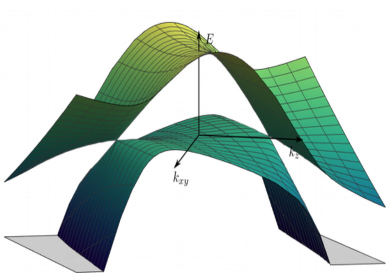
Surface states of tilted Weyl nodes



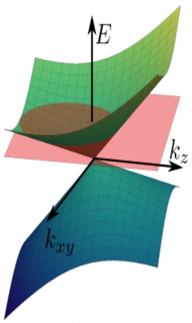
electric

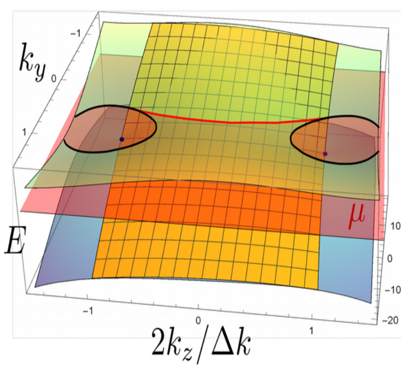
$$H = t_z(x)\left(\frac{k_z^2}{2m} - \Delta(x)\right) + \frac{v_F k_z}{\Delta k}\left(t_x k_x + t_y(x) k_y\right) + v_F\left(k_x \sigma_x + k_y \sigma_y\right) + \left[\frac{k_z^2}{2m} - \Delta(x)\right]\sigma_z$$

magnetic

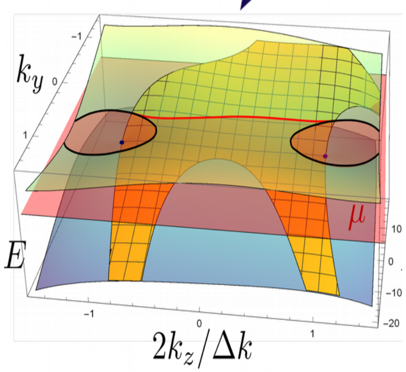


- Type-I Weyl semimetals



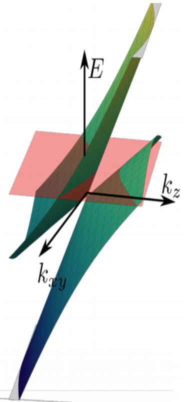


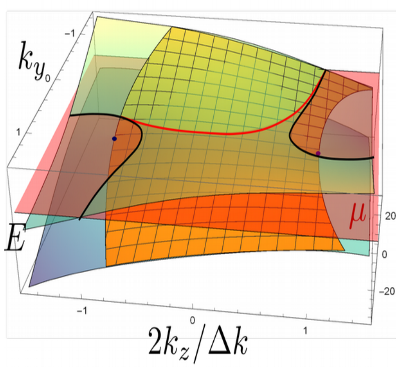
$\Delta' \gg \Delta$



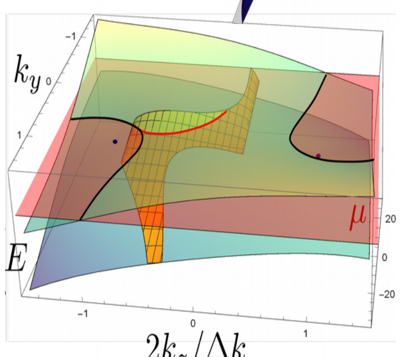
$\Delta' \sim \Delta$

- Type-II Weyl semimetals





$\Delta' \gg \Delta$



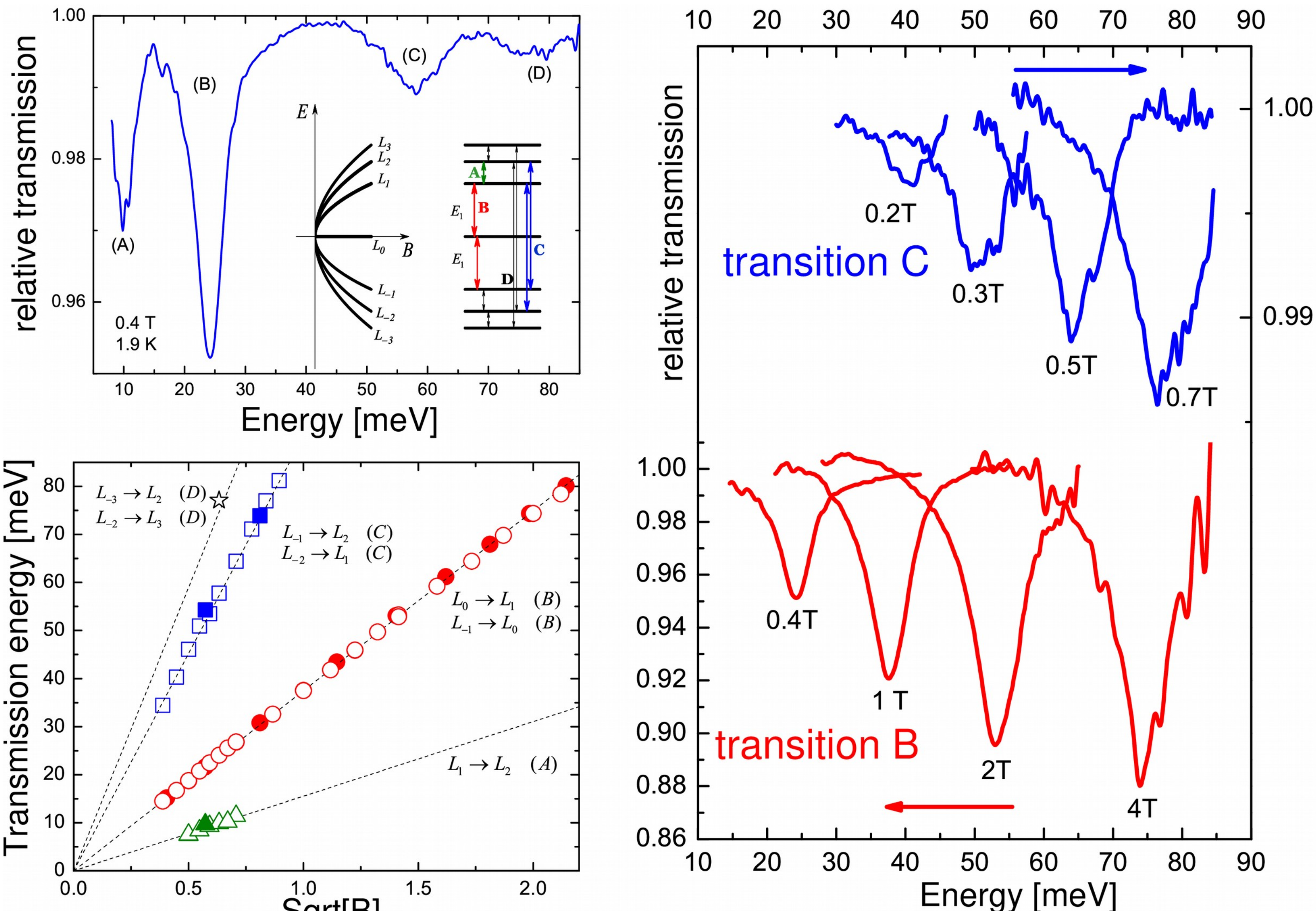
$\Delta' \sim \Delta$

S. Tchoumakov, M. Civelli and M.O. Goerbig, Phys. Rev. B **95**, 125306 (2017)

Outline

- Introduction to Berry curvature and bulk-edge correspondence
- Dirac fermions and “half Chern numbers”
- 2D Model of a smooth interface – from chiral to massive *relativistic* interface states
- First experimental evidence
- Weyl semimetals with smooth surfaces
- Possible identification of surface states beyond the chiral ones in (magneto-)optical spectroscopy

Magneto-optics in the study of relativistic materials (→ graphene)



Grenoble high–field group: Sadowski et al., PRL 97, 266405 (2007)

selection rules:

$$\lambda, n \to \lambda, n \pm 1$$

Magneto-optics in the study of relativistic materials

Optical conductivity (in a magnetic field):

Pauli principle

$$\sigma_{ij}(\omega) = i\hbar e^2 \sum_{\substack{m,n\in\mathbb{N}\\ \lambda,\lambda'}} \int_{-\infty}^{+\infty} \frac{d^d k}{(2\pi)^d} \frac{f_D(E_{\lambda,n}) - f_D(E_{\lambda',m})}{E_{\lambda',m} - E_{\lambda,n} - \hbar\omega + i\delta} \frac{\langle \psi_m^{\lambda'} | \hat{v}_i | \psi_n^{\lambda} \rangle \langle \psi_m^{\lambda'} | \hat{v}_j | \psi_n^{\lambda} \rangle^*}{E_{\lambda',m} - E_{\lambda,n}}$$

matrix elements encode selection rules for light polarisation i,j

(joint) density of states → shape of absorption lines

Magneto-optics in the study of relativistic materials

Optical conductivity (in a magnetic field):

$$\sigma_{ij}(\omega) = i\hbar e^2 \sum_{\substack{m,n\in\mathbb{N}\\ \lambda,\lambda'}} \int_{-\infty}^{+\infty} \frac{d^d k}{(2\pi)^d} \frac{f_D(E_{\lambda,n}) - f_D(E_{\lambda',m})}{E_{\lambda',m} - E_{\lambda,n} - \hbar\omega + i\delta} \frac{\langle \psi_m^{\lambda'} | \hat{v}_i | \psi_n^{\lambda} \rangle \langle \psi_m^{\lambda'} | \hat{v}_j | \psi_n^{\lambda} \rangle^*}{E_{\lambda',m} - E_{\lambda,n}}$$

thumb rule:

(effective dimensionality + band dispersion)

$$\sigma_{i,j}(\omega) \sim \frac{\mathrm{jDOS}}{\omega} \times \mathrm{sel.\ rules}$$

Magneto-optics in the study of relativistic materials

$$\sigma_{i,j}(\omega) \sim \frac{\text{jDOS}}{\omega} \times \text{sel. rules}$$

Example: bulk Landau levels (massive Dirac fermion) with $\mathbf{B} = B\mathbf{u}_z$

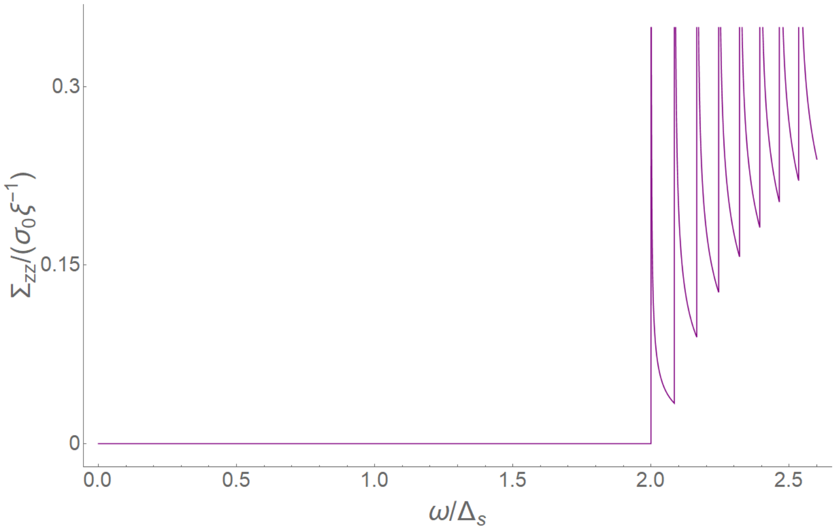
selection rules:

$$\lambda, n \to \lambda', n \pm 1 \quad \text{for} \quad \sigma_{xx},\ \sigma_{yy}$$
$$\lambda, n \to \lambda', n \quad \text{for} \quad \sigma_{zz}$$

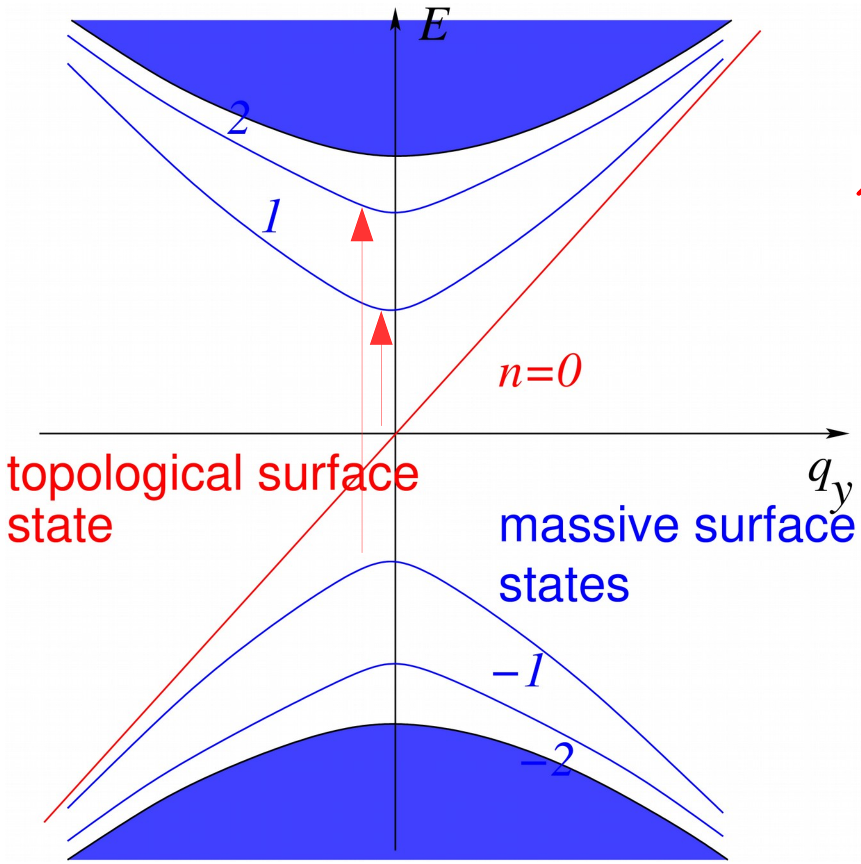
$$E_{\lambda,n}(k_z) = \lambda\sqrt{\Delta^2 + \hbar^2 v^2 (2n/l_B^2 + k_z^2)}$$

joint DOS :

$$\rho(\omega) \sim \frac{1}{\sqrt{\hbar\omega - \Delta_n}}\theta(\hbar\omega - \Delta_n)$$



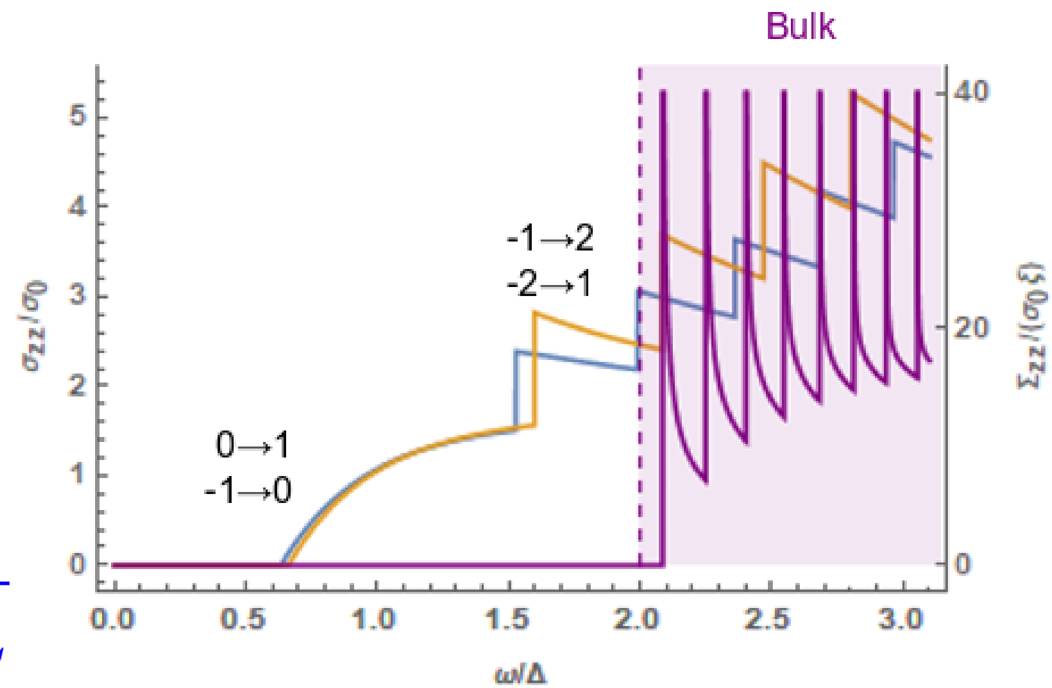
Magneto-optical signatures of surface states in 3D (no magnetic field) *[X. Lu, MOG, arXiv (2019)]*



selection rules:

$$\lambda, n \to \lambda', n \pm 1 \qquad \text{for} \qquad \sigma_{zz}$$

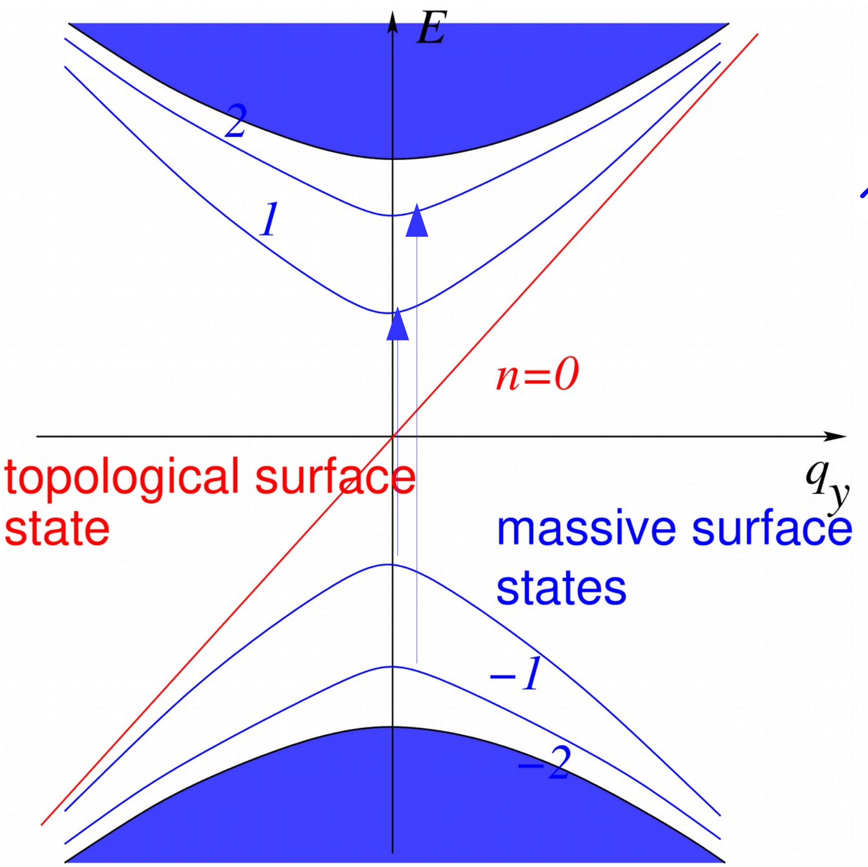
(polarisation perpendicular to surface)



$$E_{n=0} = \hbar v q_{\|}$$

$$E_{\lambda, n\neq 0} = \lambda \hbar v \sqrt{q_{\|}^2 + 2n/\ell_S^2}$$

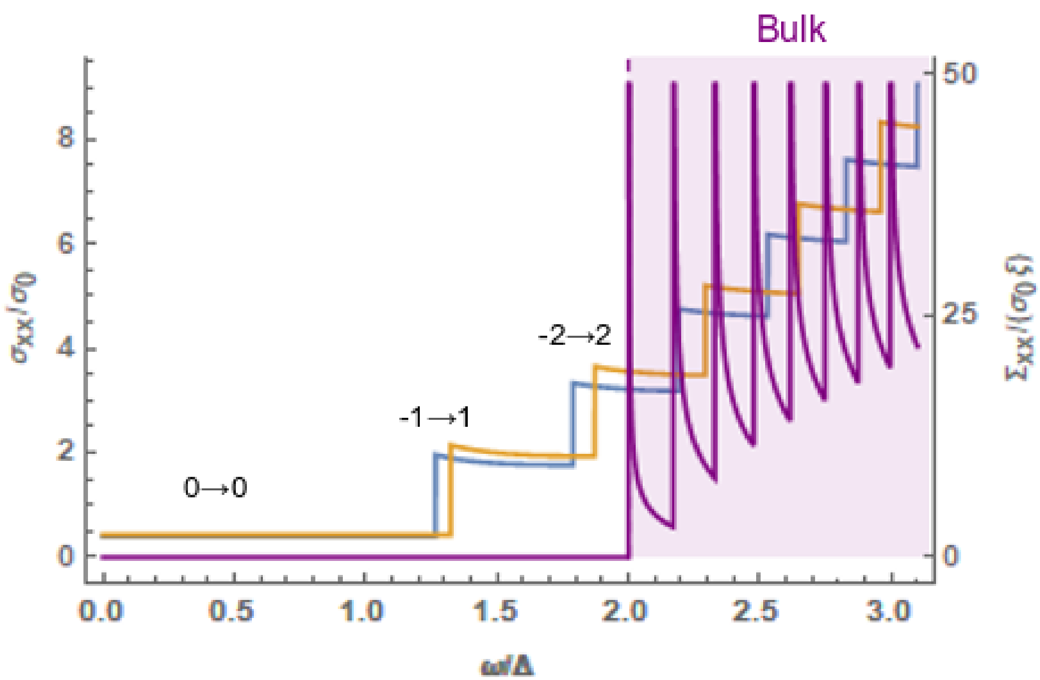
Magneto-optical signatures of surface states in 3D (no magnetic field) *[X. Lu, MOG, arXiv (2019)]*



selection rules:

$$\lambda, n \to \lambda', n \qquad \text{for} \qquad \sigma_{xx},\ \sigma_{yy}$$

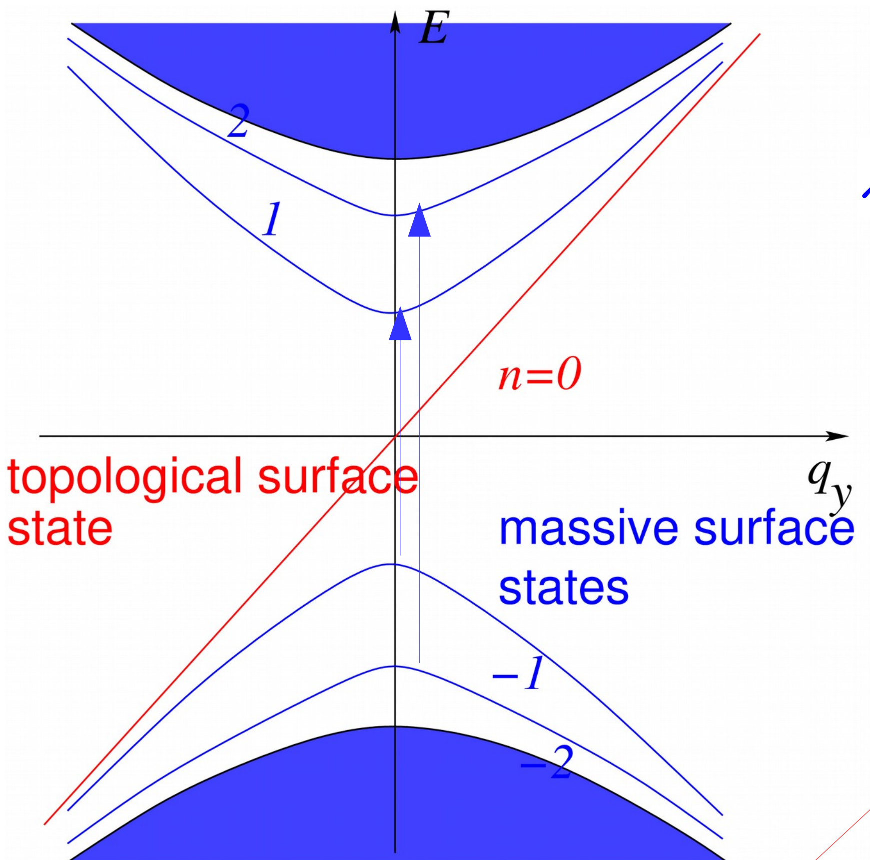
(polarisation in surface)



$$E_{n=0} = \hbar v q_{\|}$$

$$E_{\lambda,n\neq 0} = \lambda \hbar v \sqrt{q_{\|}^2 + 2n/\ell_S^2}$$

Magneto-optical signatures of surface states in 3D (no magnetic field) [X. Lu, MOG, arXiv (2019)]



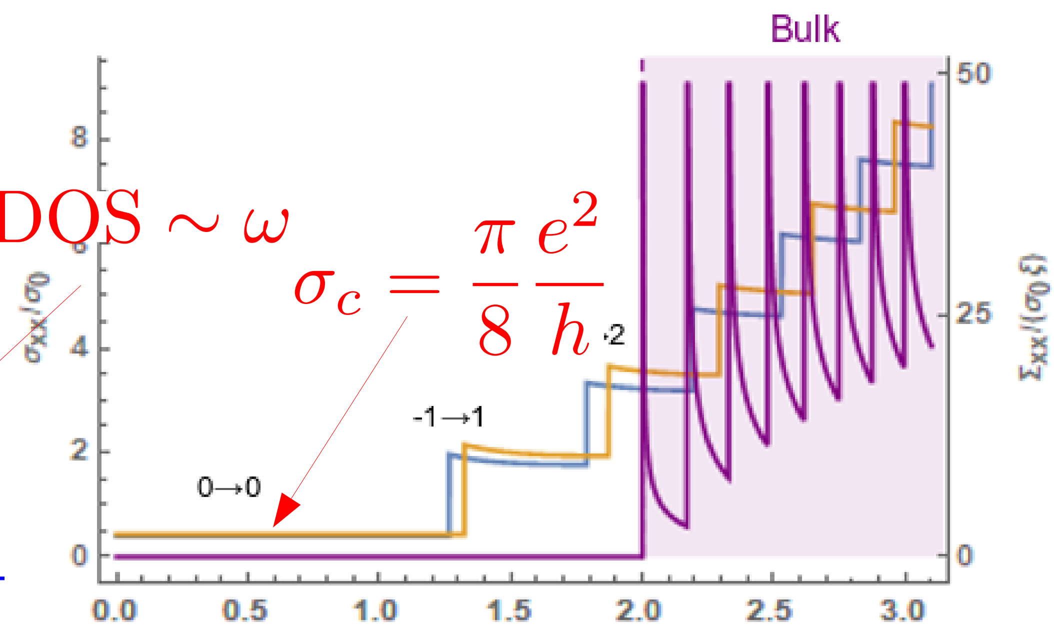
selection rules:

$$\lambda, n \to \lambda', n \qquad \text{for} \qquad \sigma_{xx},\ \sigma_{yy}$$

(polarisation in surface)

DOS $\sim \omega$

$$\sigma_c = \frac{\pi}{8}\frac{e^2}{h}$$



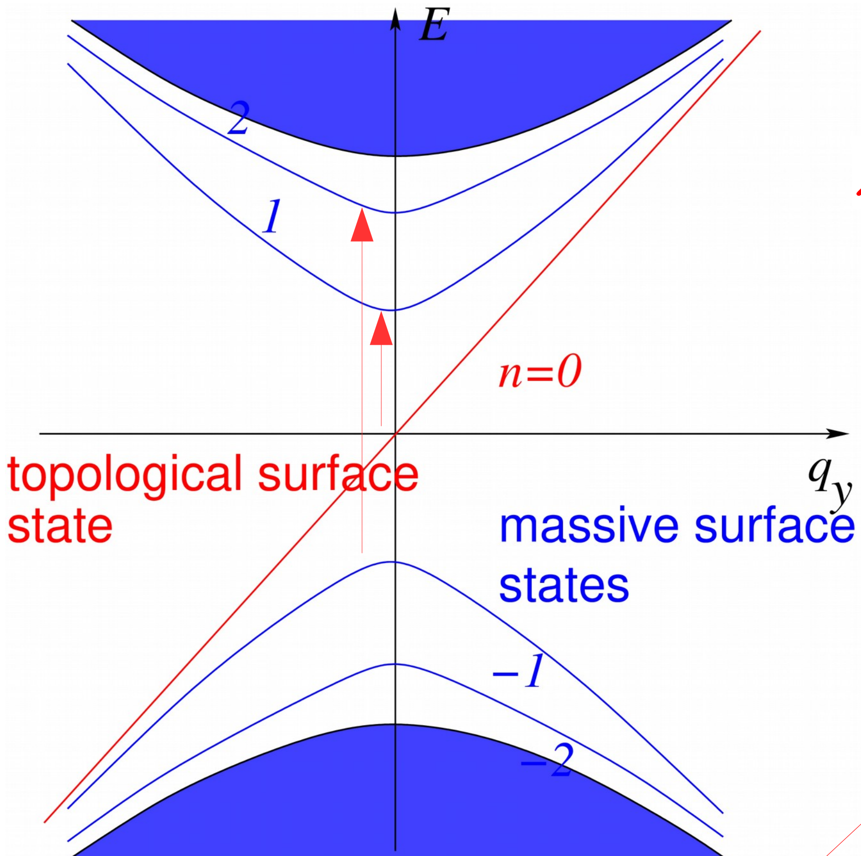
$$E_{n=0} = \hbar v q_{\|}$$

$$E_{\lambda,n\neq 0} = \lambda\hbar v\sqrt{q_{\|}^2 + 2n/\ell_S^2}$$

DOS $\sim \omega^0 = \text{const.}$

Magneto-optical signatures of surface states in 3D (no magnetic field)

[X. Lu, MOG, arXiv (2019)]

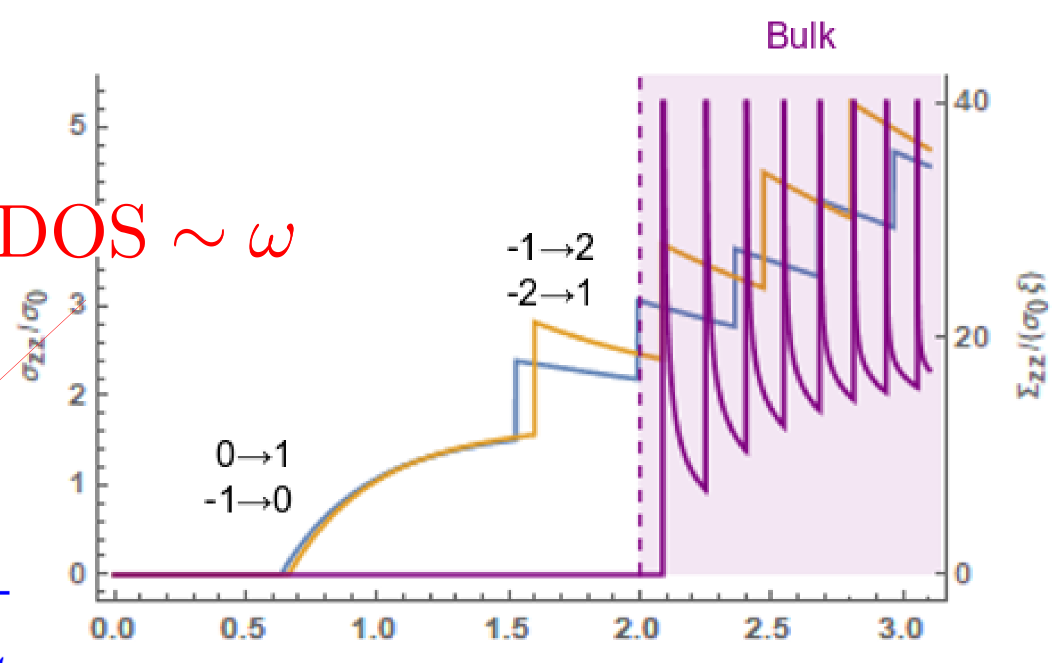


selection rules:

$$\lambda, n \to \lambda', n \pm 1 \qquad \text{for} \qquad \sigma_{zz}$$

(polarisation perpendicular to surface)

DOS $\sim \omega$

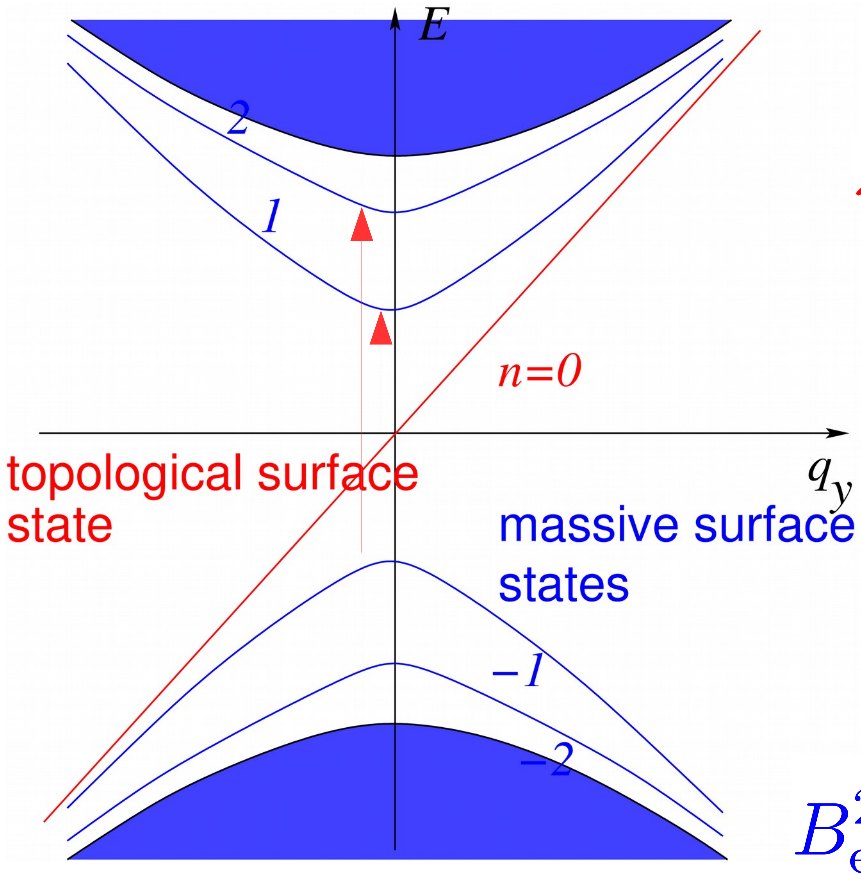


$$E_{n=0} = \hbar v q_{\parallel}$$

$$E_{\lambda,n\neq 0} = \lambda\hbar v\sqrt{q_{\parallel}^2 + 2n/\ell_S^2}$$

DOS $\sim \omega^0 = \text{const.}$

Magneto-optical signatures of surface states in 3D (magnetic field in surface) *[X. Lu, MOG, arXiv (2019)]*



selection rules:

$$\lambda, n \to \lambda', n \pm 1 \qquad \text{for} \qquad \sigma_{zz}$$

(polarisation perpendicular to surface)

→ *inplane magnetic field* $\mathbf{B}_\parallel = B\mathbf{u}_x$ conspires with confinement

→ increase of effective field :

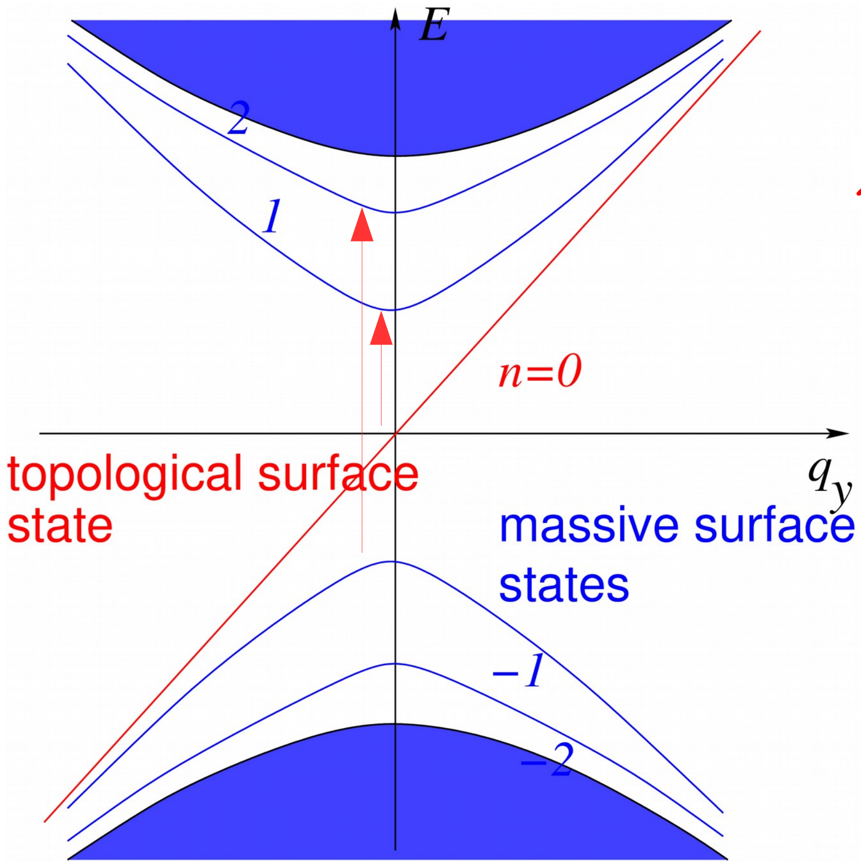
$$B_{\text{eff}}^2 = B_{\text{conf}}^2 + B_\parallel^2 \quad \Leftrightarrow \quad \frac{1}{\gamma^4} = \frac{1}{\ell_S^4} + \frac{1}{l_B^4}$$

$$E_{n=0} = \hbar v q_{\parallel,\theta}$$

$$E_{\lambda,n\neq 0} = \lambda\hbar v\sqrt{q_{\parallel,\theta}^2 + 2n/\gamma^2}$$

$$q_{\parallel,\theta}^2 = q_x^2 + q_y^2\frac{\gamma^4}{\ell_S^4}$$

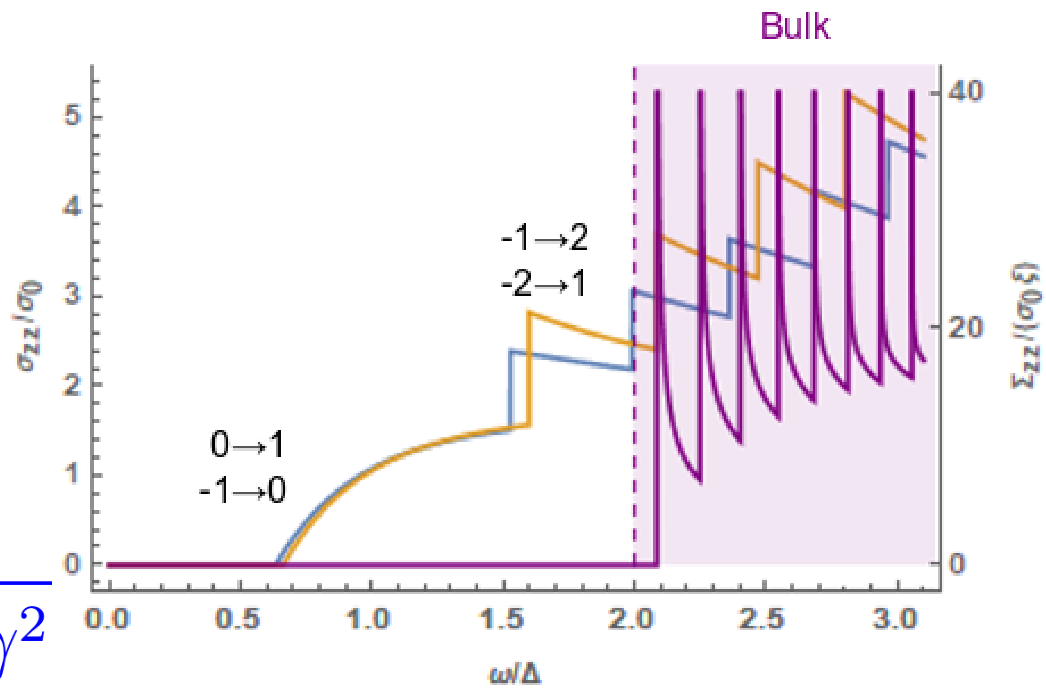
Magneto-optical signatures of surface states in 3D (magnetic field in surface) [X. Lu, MOG, arXiv (2019)]



selection rules:

$$\lambda, n \rightarrow \lambda', n \pm 1 \qquad \text{for} \qquad \sigma_{zz}$$

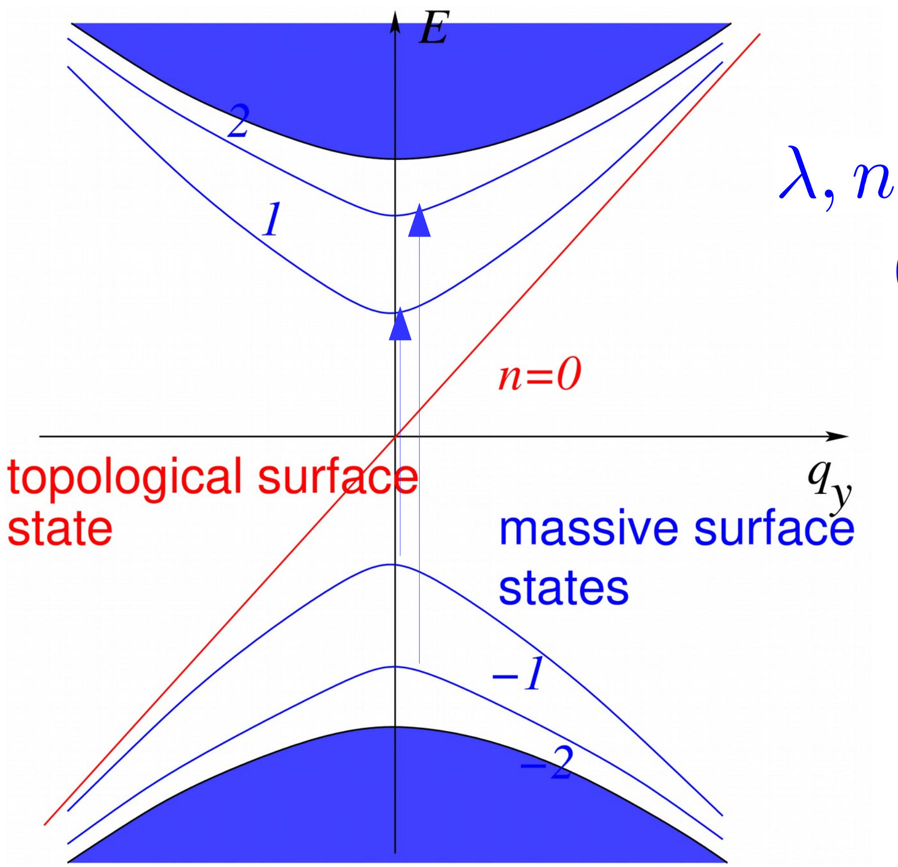
(polarisation perpendicular to surface)



$$E_{n=0} = \hbar v q_{\|,\theta}$$

$$E_{\lambda,n\neq 0} = \lambda \hbar v \sqrt{q_{\|,\theta}^2 + 2n/\gamma^2}$$

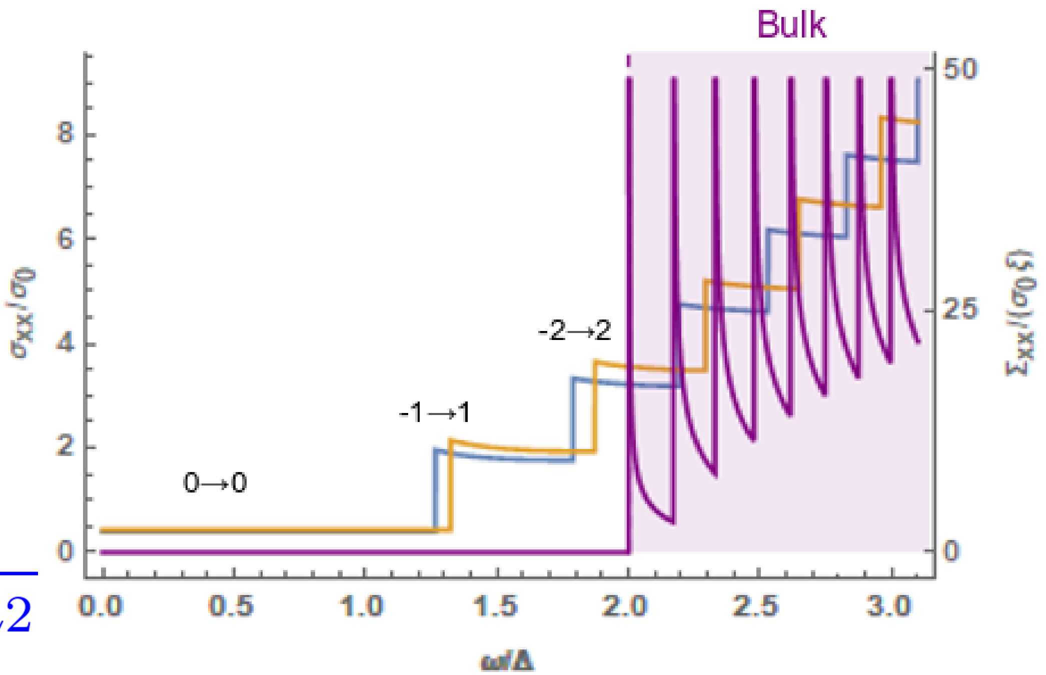
Magneto-optical signatures of surface states in 3D (magnetic field in surface) [X. Lu, MOG, arXiv (2019)]



selection rules:

$$\lambda, n \to \lambda', n \qquad \text{for} \qquad \sigma_{xx}$$

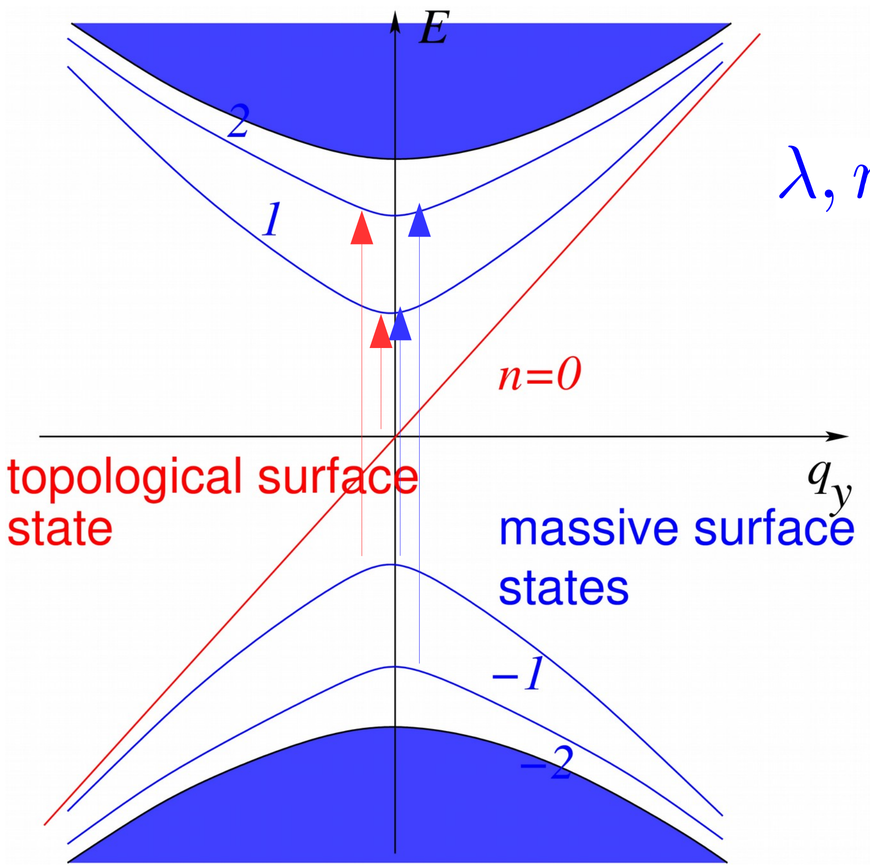
(polarisation in surface)



$$E_{n=0} = \hbar v q_{\|,\theta}$$

$$E_{\lambda,n\neq 0} = \lambda \hbar v \sqrt{q_{\|,\theta}^2 + 2n/\gamma^2}$$

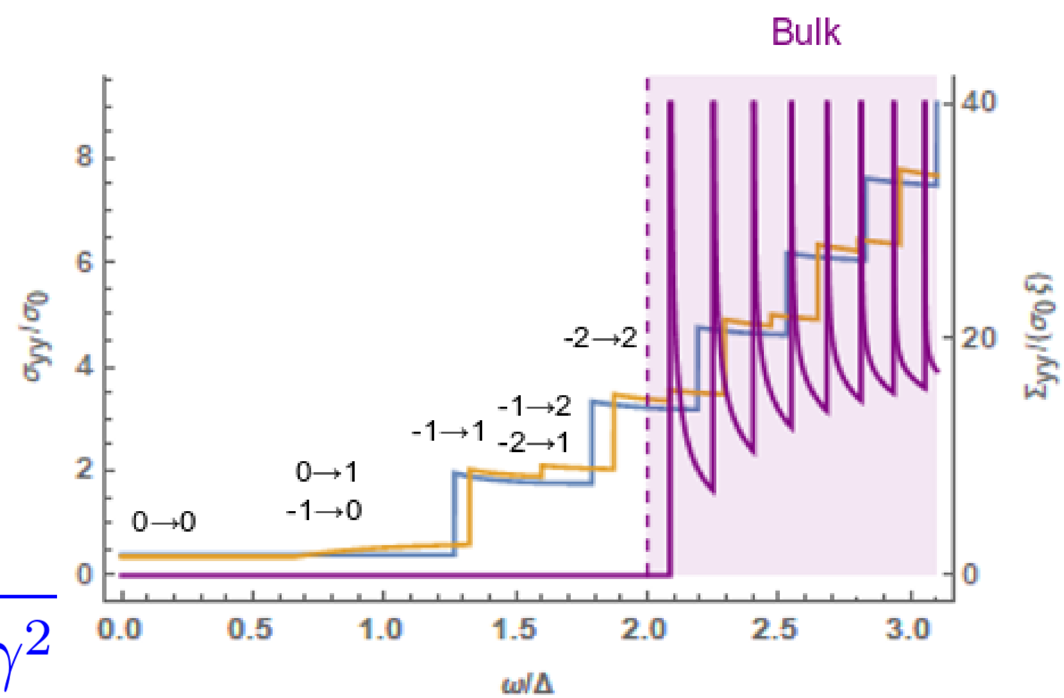
Magneto-optical signatures of surface states in 3D (magnetic field in surface) [X. Lu, MOG, arXiv (2019)]



selection rules:

$\lambda, n \to \lambda', n$ and $n \pm 1$ for σ_{yy}

(polarisation in surface)

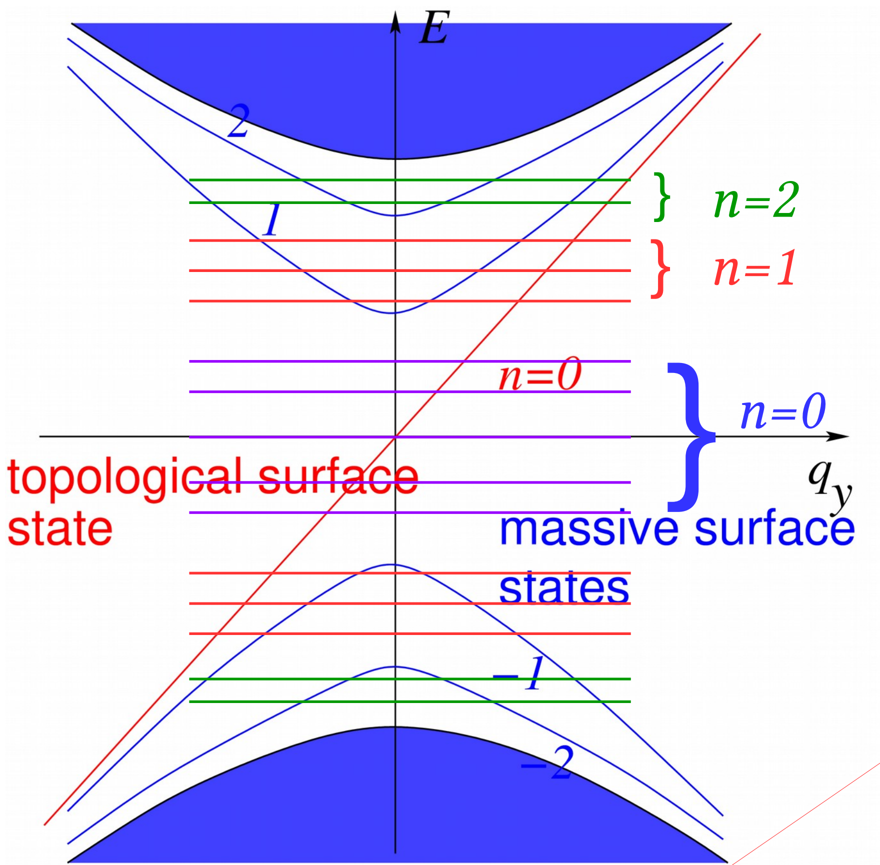


$$E_{n=0} = \hbar v q_{\parallel,\theta}$$

$$E_{\lambda,n\neq 0} = \lambda \hbar v \sqrt{q_{\parallel,\theta}^2 + 2n/\gamma^2}$$

Magneto-optical signatures of surface states in 3D (magnetic field perpendicular to surface)

[X. Lu, MOG, arXiv (2019)]

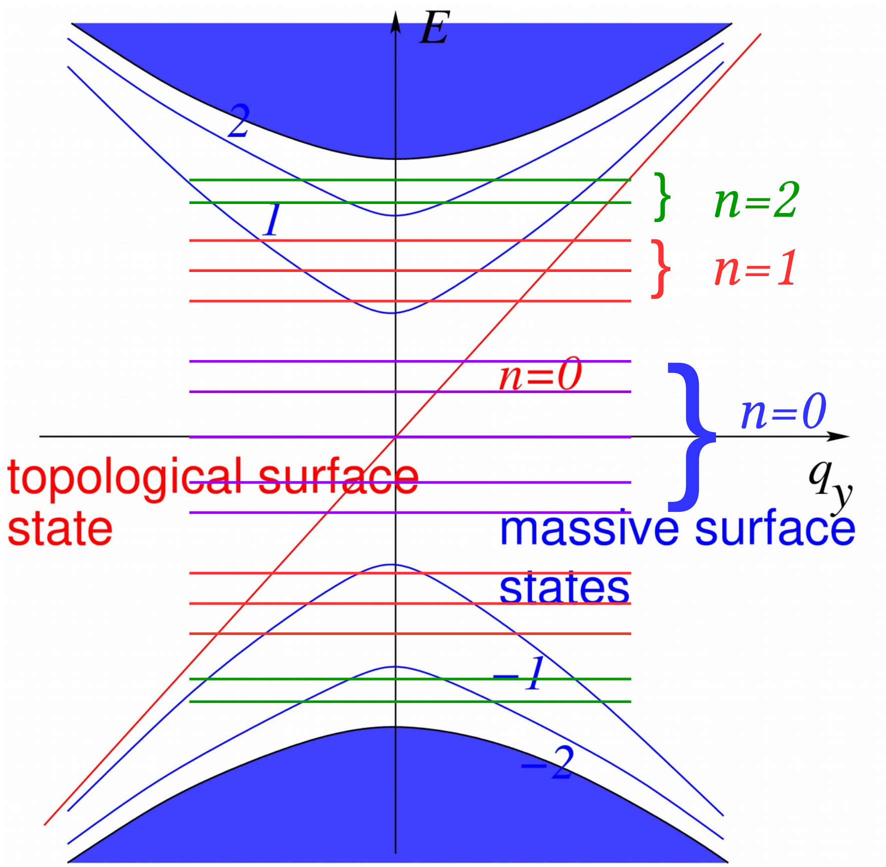


motion in surface gets quantised by $\mathbf{B} = B_\perp \mathbf{u}_z$

$$E_{\lambda,m,n} = \lambda \hbar v \sqrt{2m/l_B^2 + 2n/\ell_S^2}$$

Magneto-optical signatures of surface states in 3D (magnetic field perpendicular to surface)

[X. Lu, MOG, arXiv (2019)]

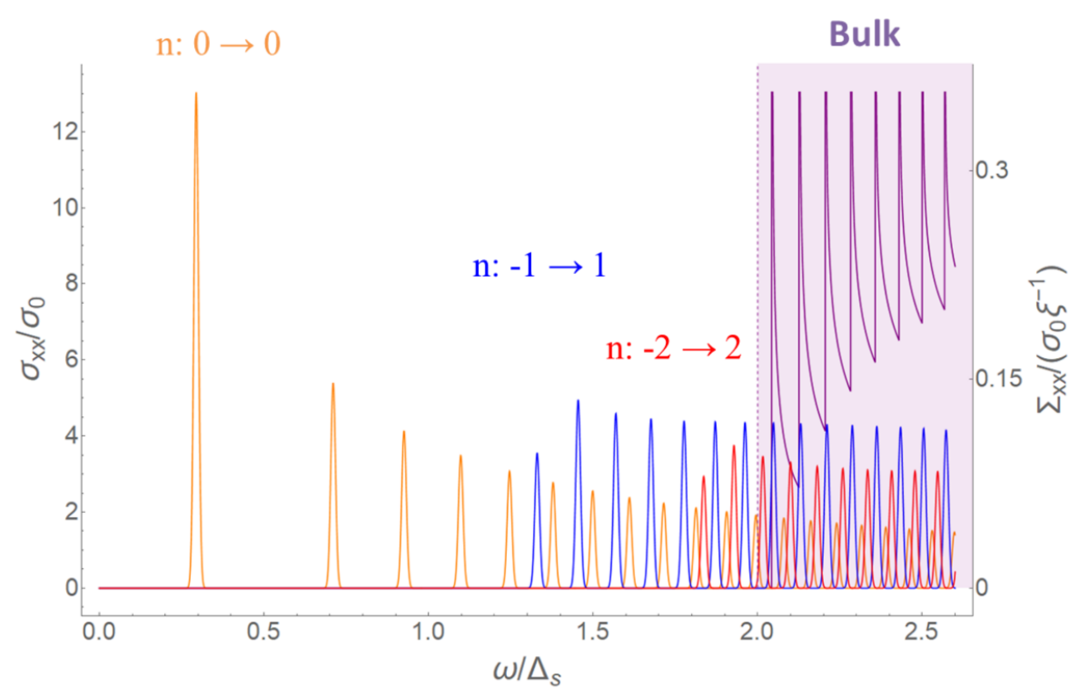


selection rules:

$$\lambda, n, m \to \lambda', n, m \pm 1$$

$$\text{for } \sigma_{xx} = \sigma_{yy}$$

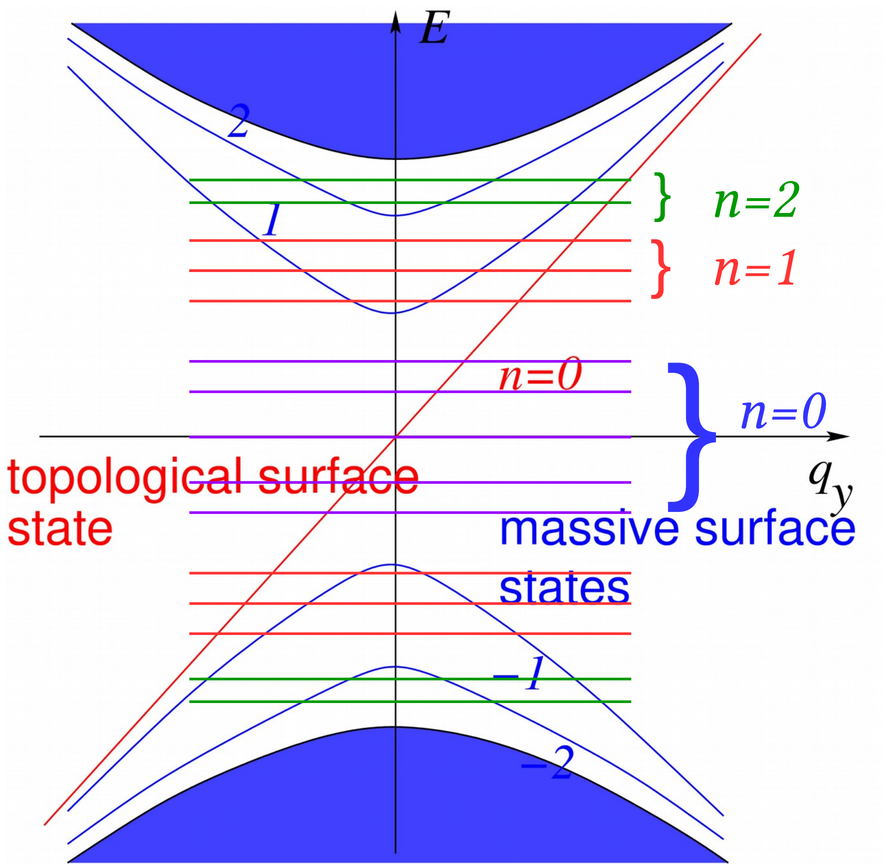
(polarisation in surface)



$$E_{\lambda,m,n} = \lambda\hbar v\sqrt{2m/l_B^2 + 2n/\ell_S^2}$$

Magneto-optical signatures of surface states in 3D (magnetic field perpendicular to surface)

[X. Lu, MOG, arXiv (2019)]

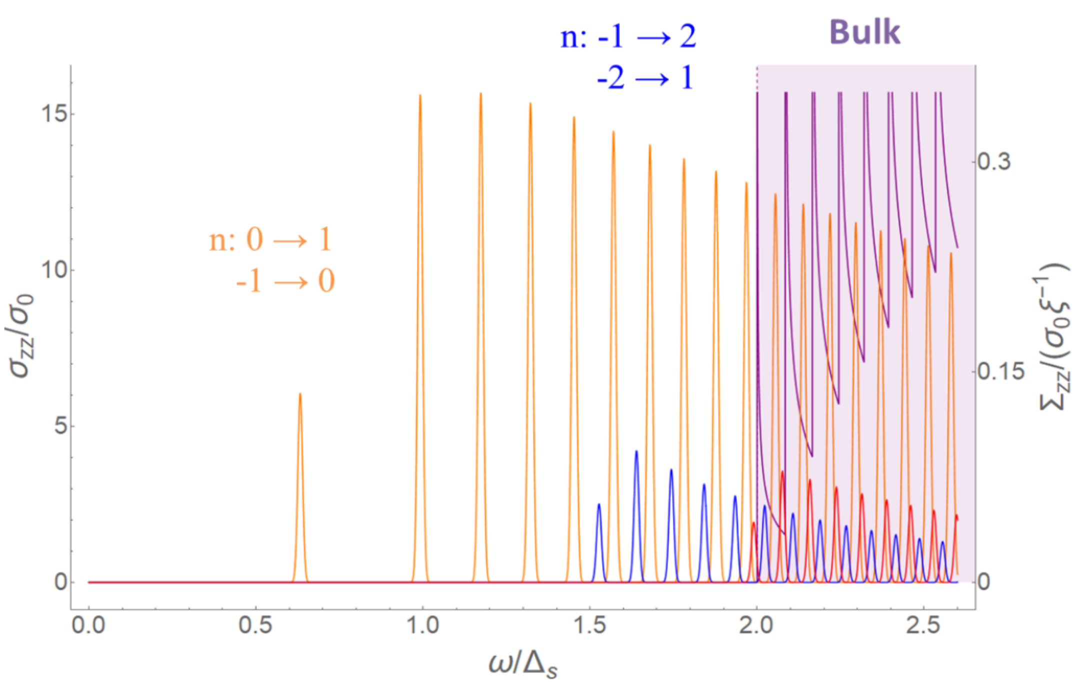


selection rules:

$$\lambda, n, m \to \lambda', n \pm 1, m$$

for σ_{zz}

(polarisation perpendicular to surface)



$$E_{\lambda,m,n} = \lambda \hbar v \sqrt{2m/l_B^2 + 2n/\ell_S^2}$$

Conclusions

- Surface states of *topological materials* with smooth interfaces ~ Landau bands of Dirac fermions (generic ! → *TI, WSM, topo. SC,...*)
- Topologically protected surface state ~ chiral n=0 Landau band
- Additional massive Landau bands ($n \neq 0$)

  → *Volkov-Pankratov states*
- Intriguing relativistic effects
- First experimental evidence in HgTe samples
- Clear signature expected in *magneto-optical spectroscopy*

  → for TI interfaces *[X. Lu & MOG, arXiv (2019)]*

  → for WSM interfaces *[D.K. Mukherjee & MOG, in prep.]*