Matière condensée topologique

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Théorie de la matière topologique au LPS












- *Isolants topologiques*
- *Graphène et semi-conducteurs bi-dimensionnels*
- *Semi-métaux de Dirac et de Weyl tri-dimensionnels*
- *Supraconductivité topologique*
- *Effets Hall quantiques*

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
- Weyl semimetals with smooth surfaces

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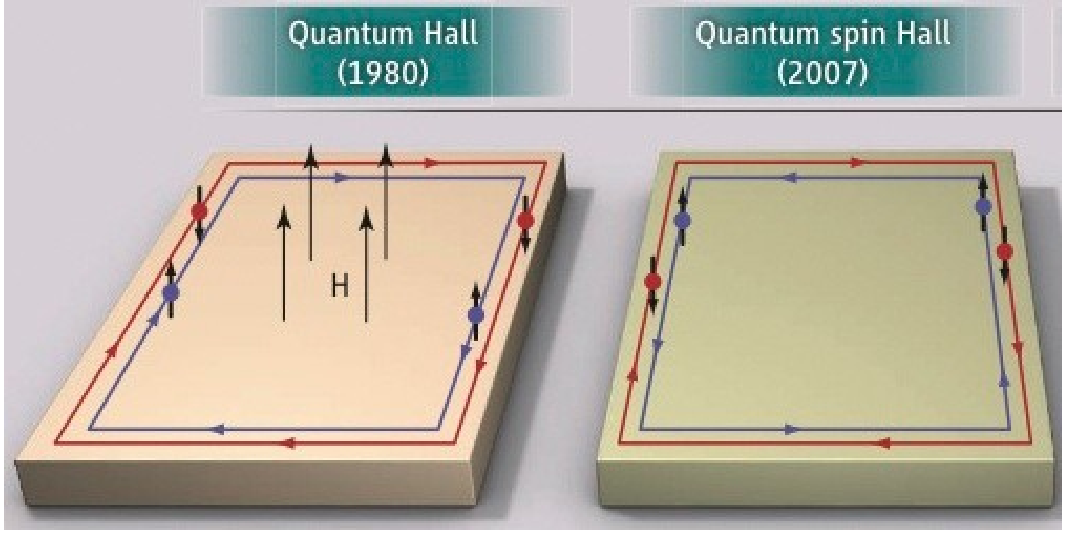
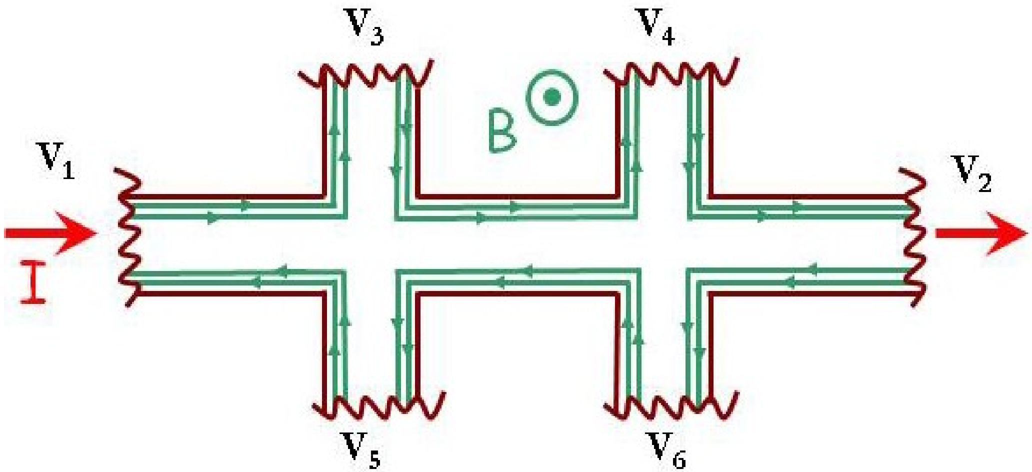
Topological insulators (1980→2007)



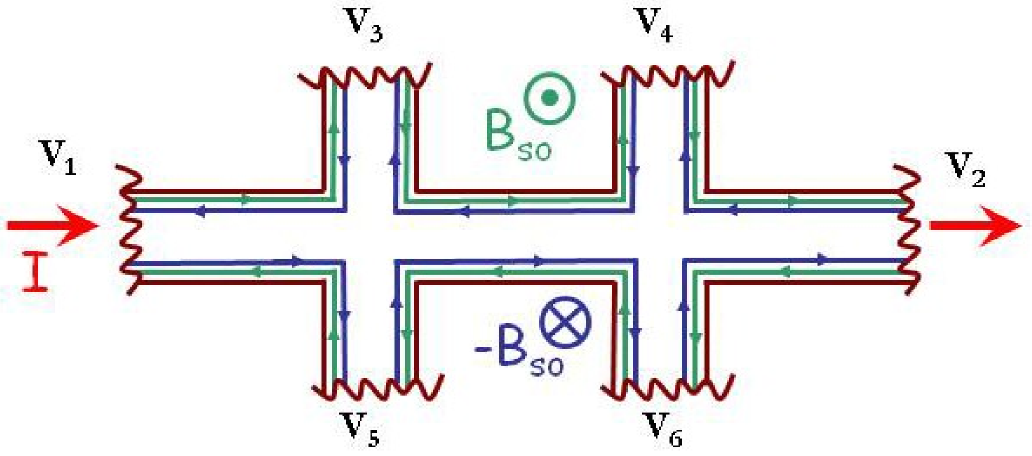
Science,766, ***318*** (2007),
Würzburg group

Topological insulator = Bulk insulator + Conducting edges (surfaces)

Quantum Hall effect



Quantum spin Hall effect



all states move in the same direction
(chiral edge states)

spin up and spin down states move in opposite directions
(helical edge states)

Information beyond the spectrum

$$H = \begin{pmatrix} \Delta & f(\mathbf{k})^* \\ f(\mathbf{k}) & -\Delta \end{pmatrix}$$

Wave functions (→ "spin"):

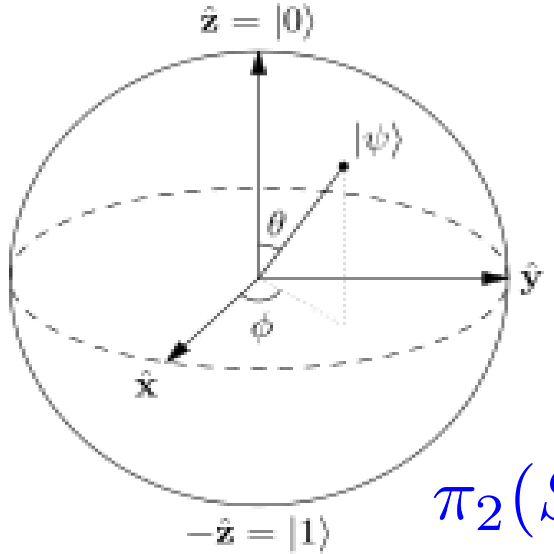
$$\psi_{+,\mathbf{k}} = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix} \qquad \psi_{-,\mathbf{k}} = \begin{pmatrix} -\sin\frac{\theta}{2} \\ e^{i\phi}\cos\frac{\theta}{2} \end{pmatrix}$$

with $\cos\theta = \frac{\Delta}{\sqrt{\Delta^2 + |f(\mathbf{k})|^2}}$ $\qquad \tan\phi = \frac{\mathrm{Im} f(\mathbf{k})}{\mathrm{Re} f(\mathbf{k})}$

→ topological invariant: number of Bloch sphere coverings

$$\psi_\pm : \qquad \mathbf{k} \in \mathcal{T}^2 \qquad \rightarrow$$

(Brillouin zone)



$\sim \mathcal{S}^2$

$\pi_2(S^2) = Z$

(Bloch sphere)

→ gap must change sign to have $n \neq 0$ ***("gap inversion") !!***

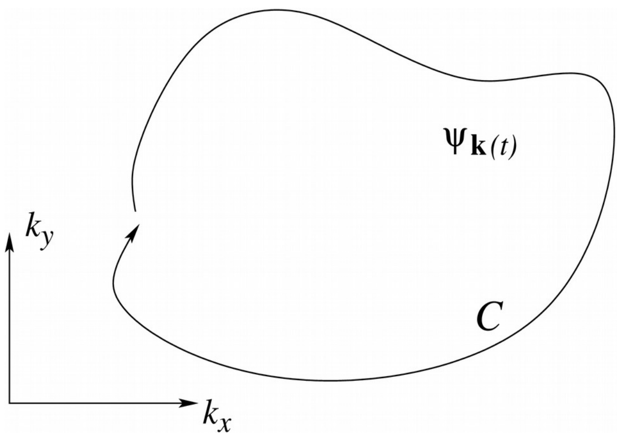
Mathematical formulation (→ Berry)

Geometric (Berry) phase (~ magnetic flux):

$$\gamma_C = \int_C d\mathbf{k} \cdot \mathcal{A}_\lambda(\mathbf{k})$$

$$\psi_\lambda(t) = e^{-iEt/\hbar} e^{-i\gamma_C} \psi_{\lambda,\mathbf{k}(t)}$$

$\lambda = \pm$: band index



Berry connection (~ vector potential):

$$\mathcal{A}_\lambda(\mathbf{k}) = i\psi^\dagger_{\lambda,\mathbf{k}} \nabla_\mathbf{k} \psi_{\lambda,\mathbf{k}}$$

Berry curvature (~ magnetic field):

$$\mathcal{B}_{\lambda,\mathbf{k}} = \nabla_\mathbf{k} \times \mathcal{A}_\lambda(\mathbf{k})$$

Chern number (topological invariant):

$$C_\lambda = \frac{1}{2\pi} \int_{BZ} d^2k \mathcal{B}_{\lambda,\mathbf{k}}$$

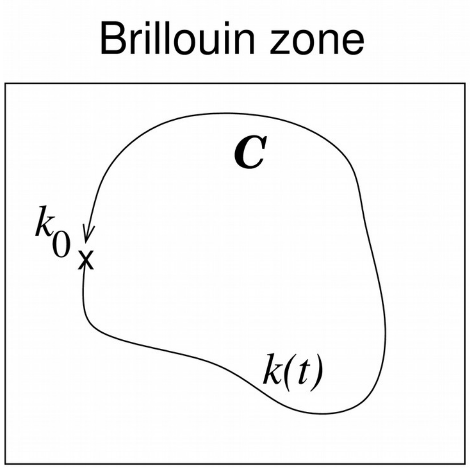
integer

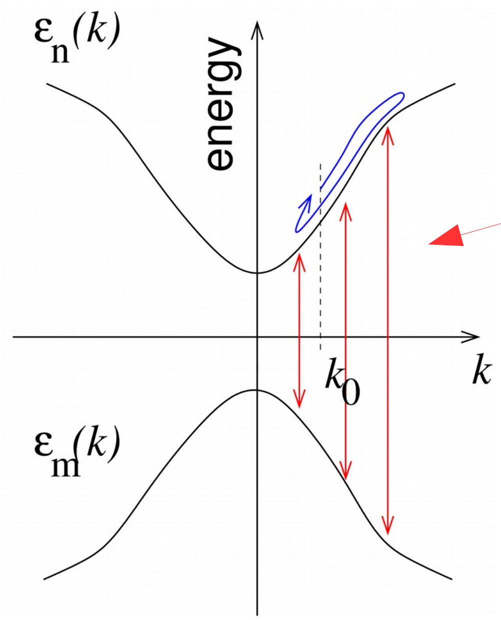
Berry curvature – some properties

$$\mathcal{B}_n^\sigma(\mathbf{k}) = i\epsilon^{\sigma\mu\nu} \sum_{m\neq n} \frac{\langle u_n|\partial_{k_\mu} H(\mathbf{k})|u_m\rangle\langle u_m|\partial_{k_\nu} H(\mathbf{k})|u_n\rangle}{[E_n(\mathbf{k}) - E_m(\mathbf{k})]^2}$$

→ link to perturbation theory :

$$|u_n(\mathbf{k}+d\mathbf{k})\rangle = |u_n(\mathbf{k})\rangle + \sum_{m\neq n} |u_m(\mathbf{k})\rangle \frac{\langle u_m(\mathbf{k})|d\mathbf{k}\cdot\nabla_{\mathbf{k}} H|u_n(\mathbf{k})\rangle}{E_n(\mathbf{k}) - E_m(\mathbf{k})}$$





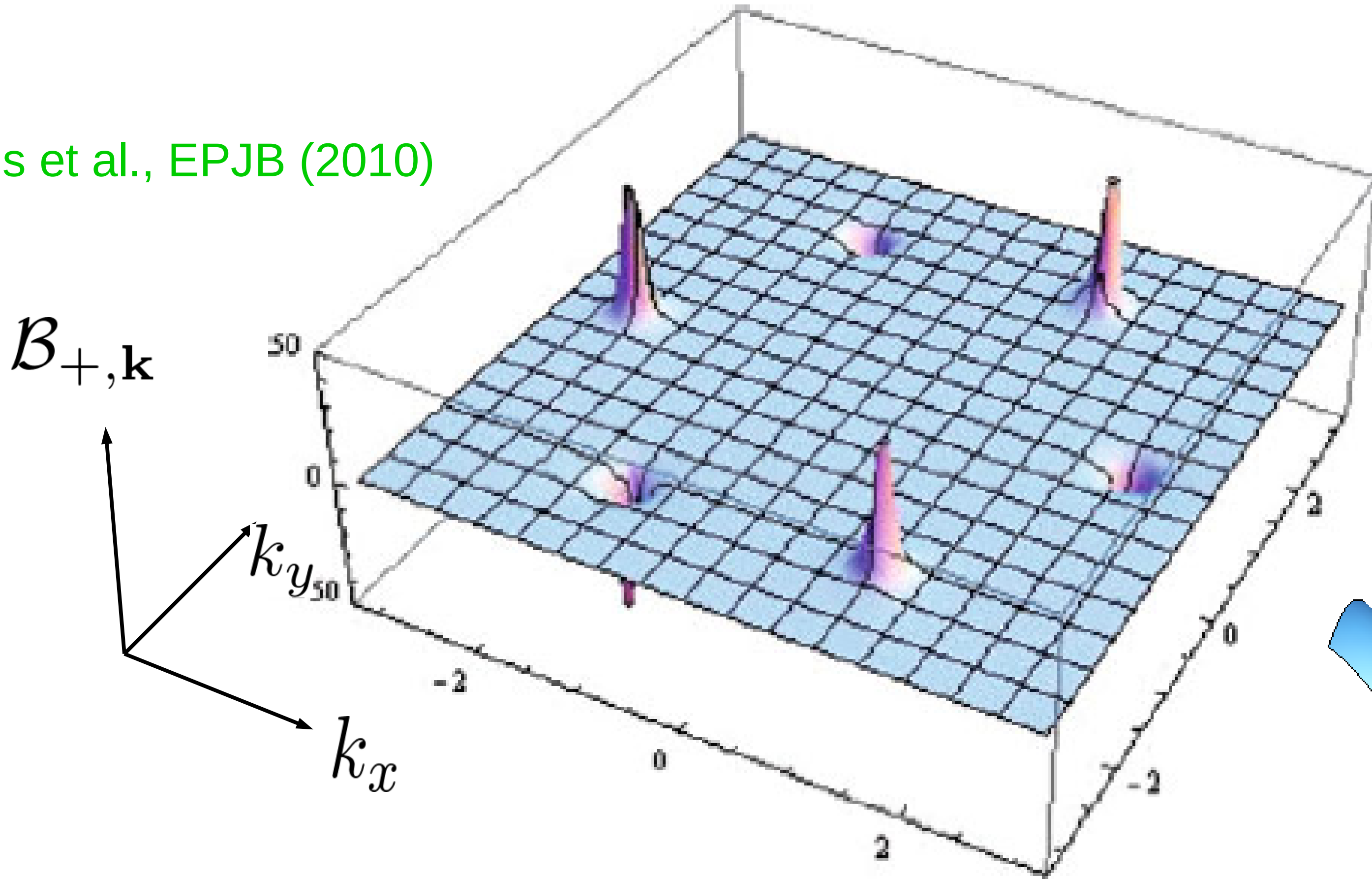
virtual transitions

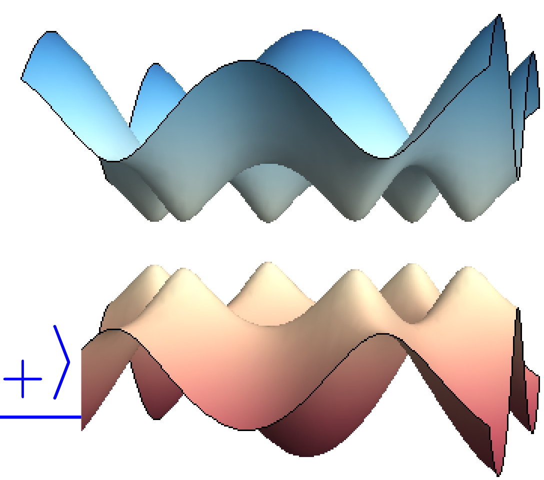
sum rule:

$$\sum_n \mathcal{B}_n^\sigma(\mathbf{k}) = 0$$

Berry curvature for insulating graphene

Fuchs et al., EPJB (2010)





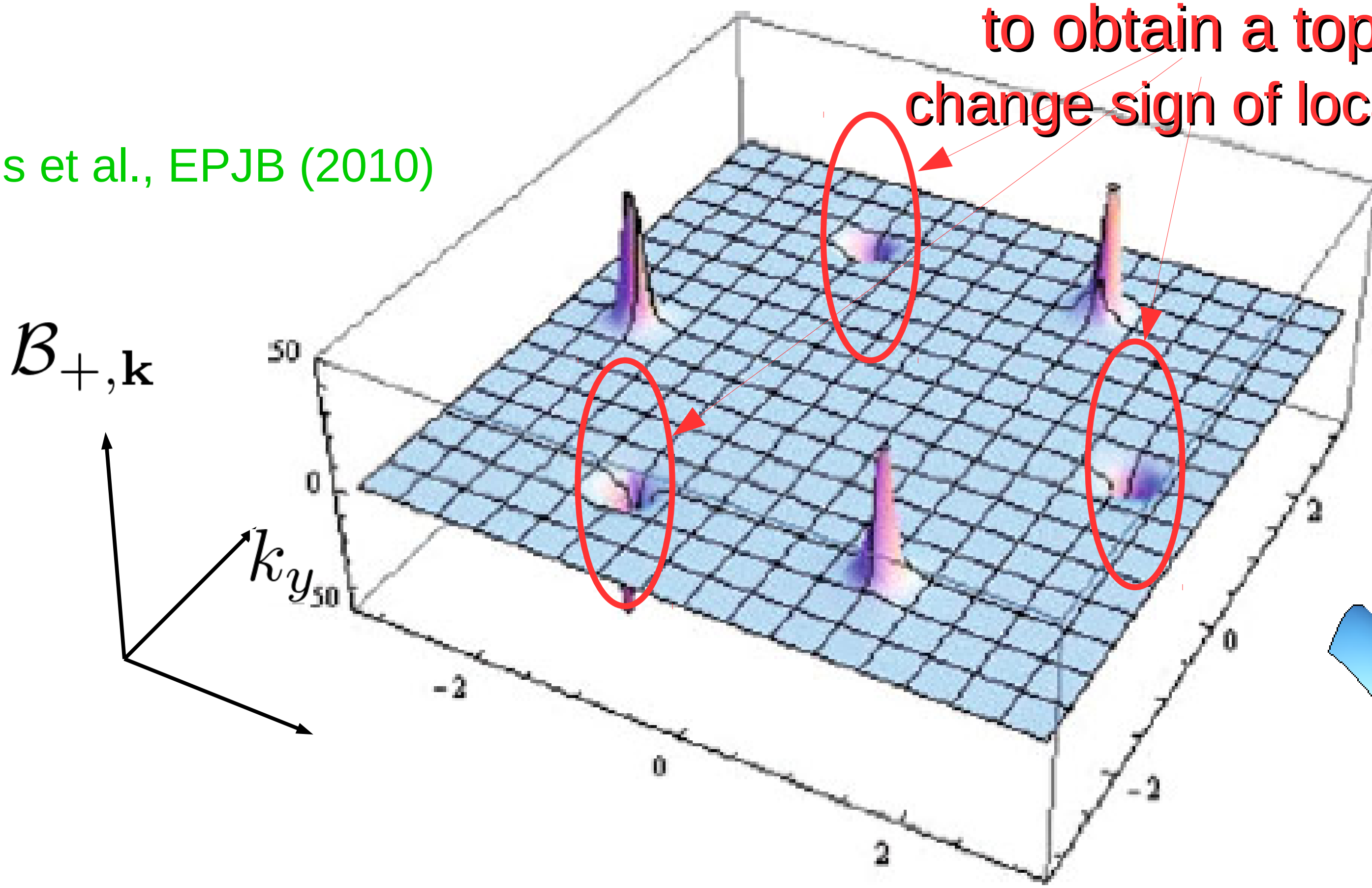
$$\mathcal{B}^{\sigma}_{+}(\mathbf{k}) = i\epsilon^{\sigma\mu\nu}\frac{\langle u_+|\partial_{k_\mu}H(\mathbf{k})|u_-\rangle\langle u_-|\partial_{k_\nu}H(\mathbf{k})|u_+\rangle}{[E_+(\mathbf{k})-E_-(\mathbf{k})]^2}$$

Berry curvature concentrated around Dirac points

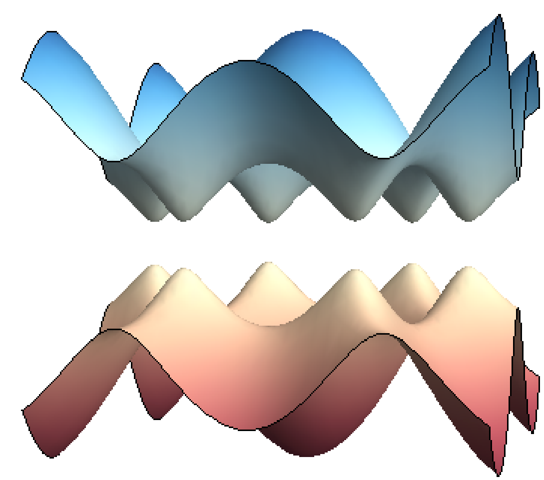
Berry curvature for insulating graphene

Fuchs et al., EPJB (2010)

to obtain a topological insulator
change sign of local Berry curvature !



→ local gap inversion



$C_\lambda = 0$ *Since curvature is antisymmetric*

Berry curvature concentrated around Dirac points

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Berry phase of a single Dirac point

Continuum Hamiltonian : $H_D = \begin{pmatrix} \sigma\Delta & \hbar v q e^{-i\xi\phi} \\ \hbar v q e^{i\xi\phi} & -\sigma\Delta \end{pmatrix}$

$\xi = \pm :$ *valley index (K and K')*

Berry connection: $\mathcal{A}_{\sigma,\lambda,\xi}(\mathbf{q}) = -\lambda\sigma \sin^2\frac{\theta}{2}\xi\nabla_{\mathbf{q}}\phi$

Berry curvature: $\mathcal{B}_{\sigma,\lambda,\xi}(\mathbf{q}) = -\frac{\lambda\sigma\xi}{2}\frac{\hbar^2 v^2\Delta}{(\Delta^2+\hbar^2 v^2 q^2)^{3/2}}$

→ Berry phase:

$$\Gamma_{|q|} = -\pi\lambda\sigma\xi\left(1-\frac{\Delta}{\sqrt{\Delta^2+\hbar^2 v^2 q^2}}\right) \to -\pi\lambda\sigma\xi$$

→ *Chern number:*

$$C_{\lambda,\xi} = -\frac{1}{2}\lambda\sigma\xi \quad ???$$

“Half Chern number”

- Calculation in continuum limit

  → non-compact space (2D plane)

  → Dirac points arise necessarily in pairs !

  [Nielssen and Ninomiya (1983)]

- Each (massive) Dirac point contributes $\pm 1/2$ to the total Chern number

  → in order to obtain a non-zero Chern number (per band), ***one needs an inverted gap***

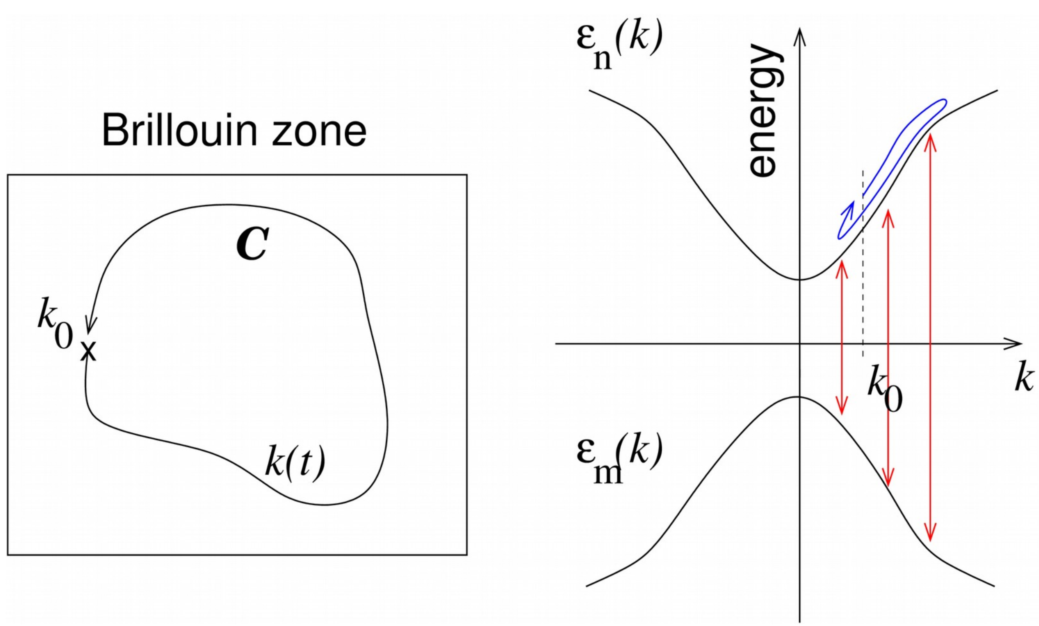
$$\sigma \to \sigma(\xi) = \sigma \xi$$

Berry curvature of a massive Dirac fermion → correlations

$$\mathcal{B}_{\sigma,\lambda,\xi}(\mathbf{q}) = -\frac{\lambda\sigma\xi}{2}\frac{\hbar^2 v^2 \Delta}{(\Delta^2 + \hbar^2 v^2 q^2)^{3/2}} \quad \stackrel{\mathbf{q}\to 0}{\longrightarrow} \quad -\frac{\lambda\sigma\xi}{2}\ell_C^2$$

$$\ell_C = \frac{\hbar v}{\Delta} = \frac{\hbar}{m_D v}$$: effective Compton length

→ "minimal" length scale



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→ Berry curvature corrections in exciton spectra of 2D TMDC

Zhou et al., PRL (2015)
Srivastava & Imamoglu, PRL (2015)
Trushin, MOG, Belzig, PRL (2018)
Hishri, Jaziri, MOG, arXiv (2018)

→ Stability of matter, breakdown effects for

$$\alpha^* > 1$$

→ “minimal” length scale

→ important for ***correlations***

$$\ell_C = \alpha^* a_B^*$$

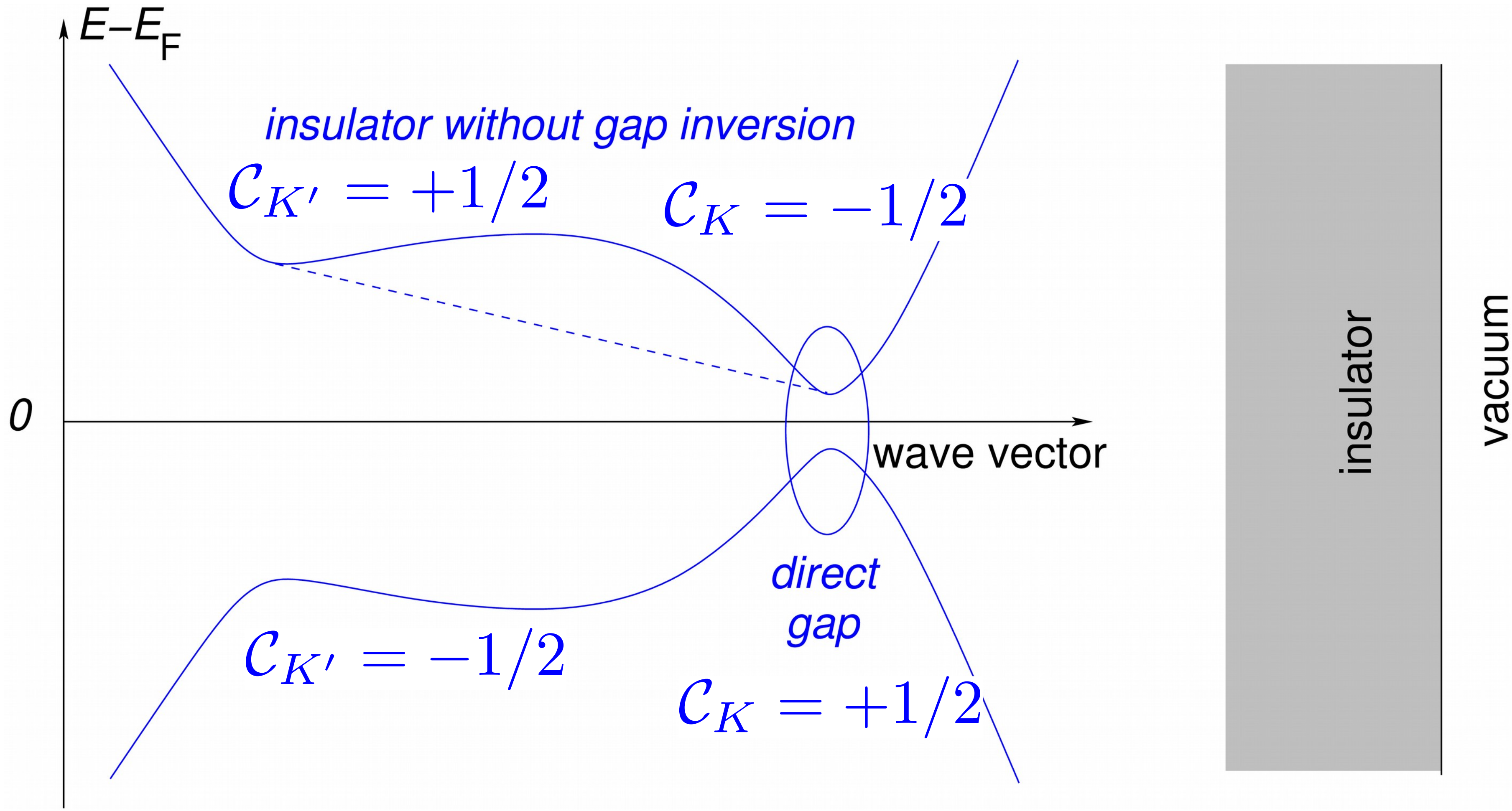
$$\alpha^* = \frac{e^2}{\hbar \epsilon v}$$

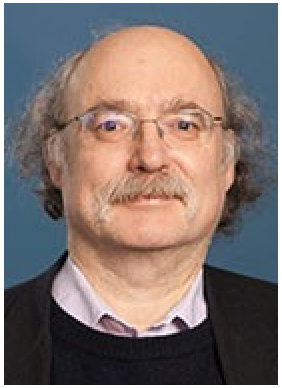
effective fine-structure constant

$$a_B^* = \frac{\hbar^2 \epsilon}{m_D e^2}$$

effective Bohr radius

Haldane model (broken time-reversal symmetry, 1988)

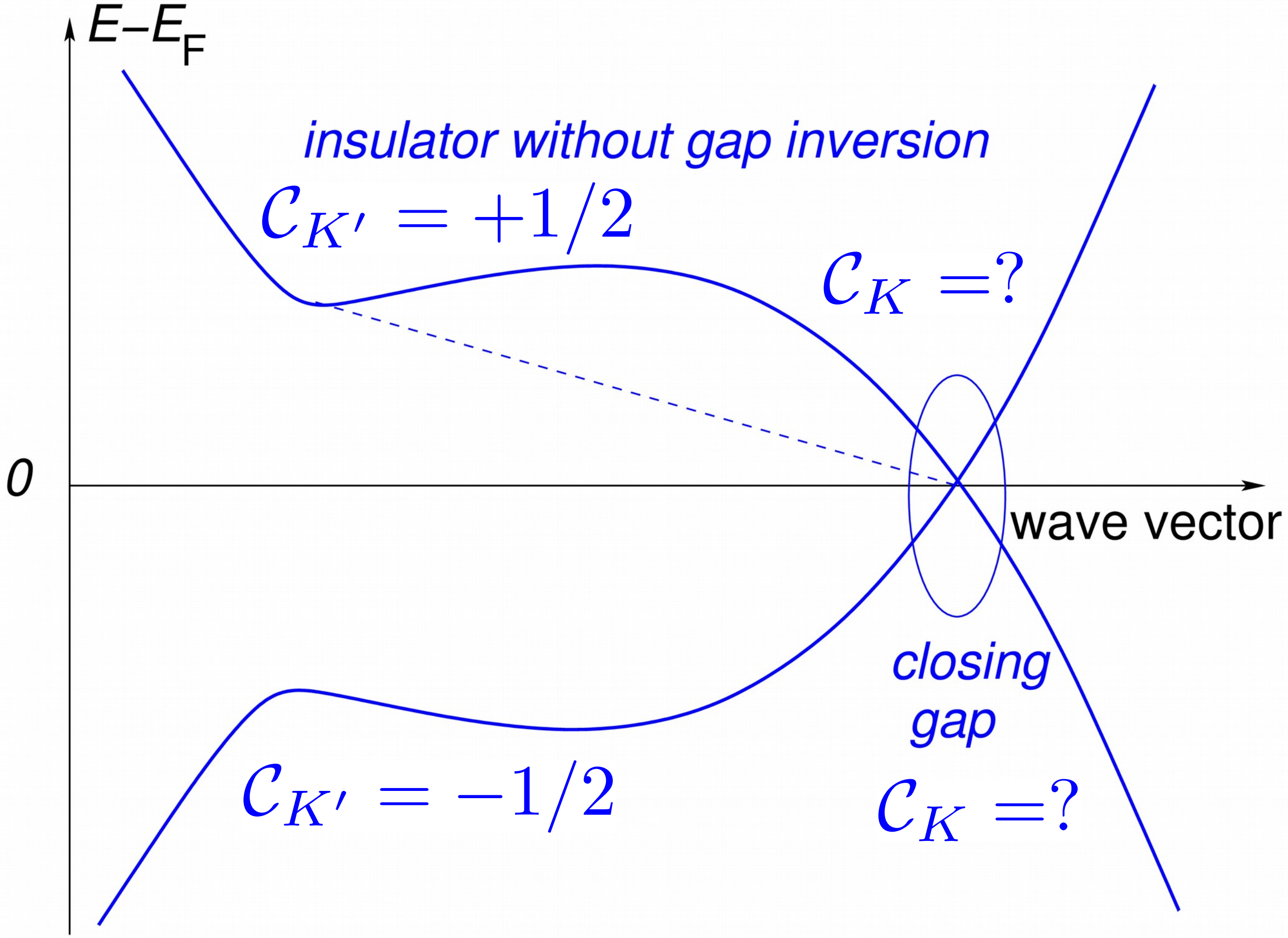


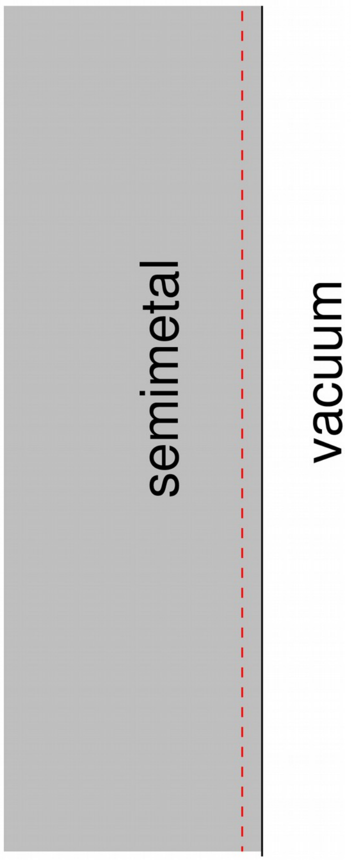


Broken TR symmetry : $E(\mathbf{k}) \neq E(-\mathbf{k})$

modify Dirac points independently from one another

Haldane model (broken time-reversal symmetry, 1988)





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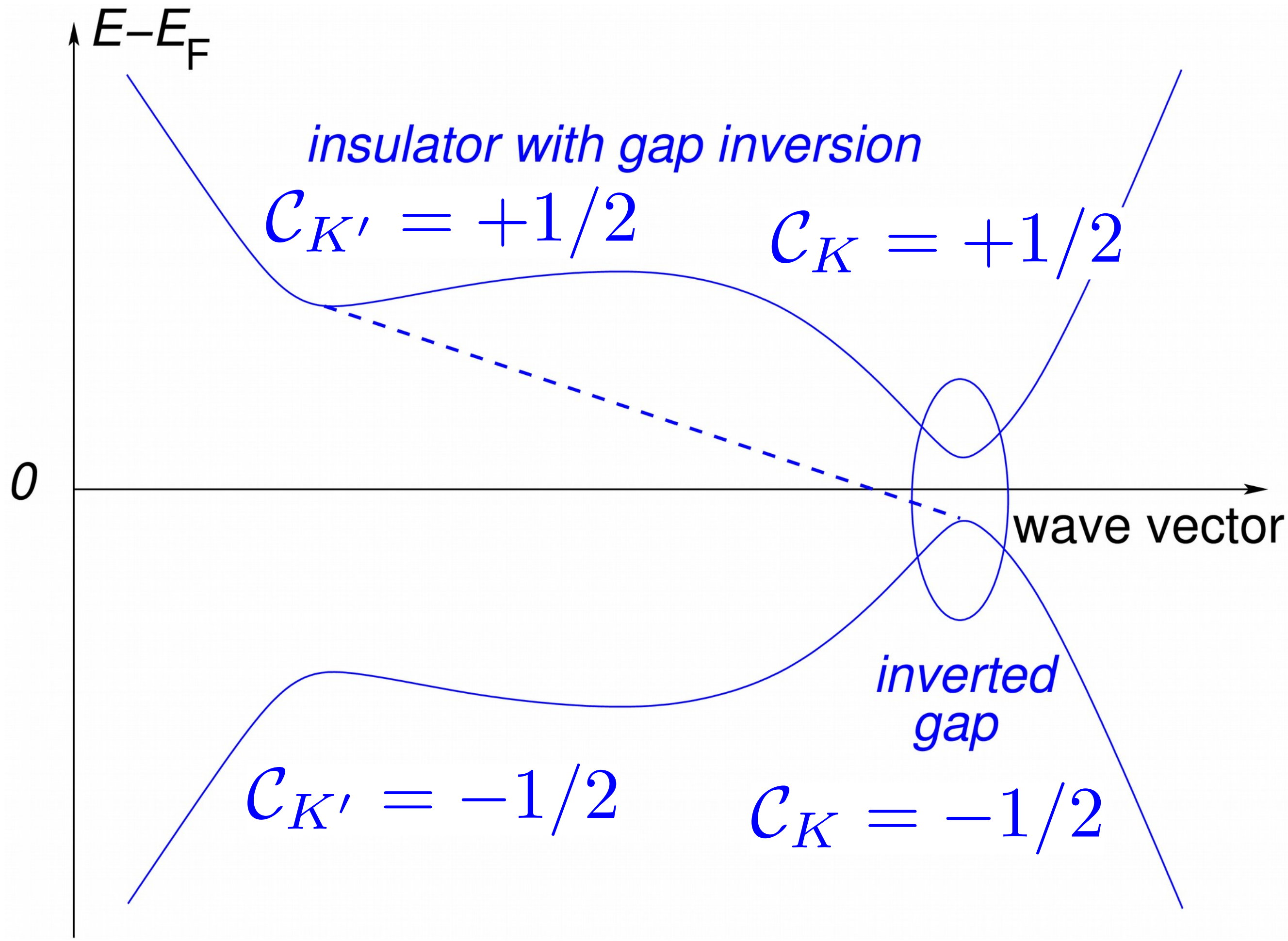
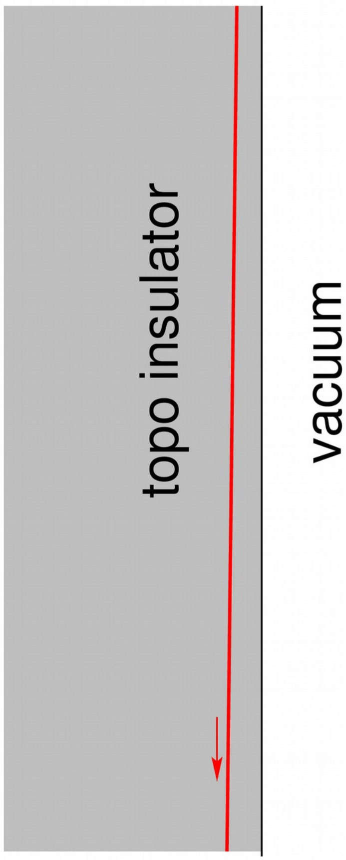




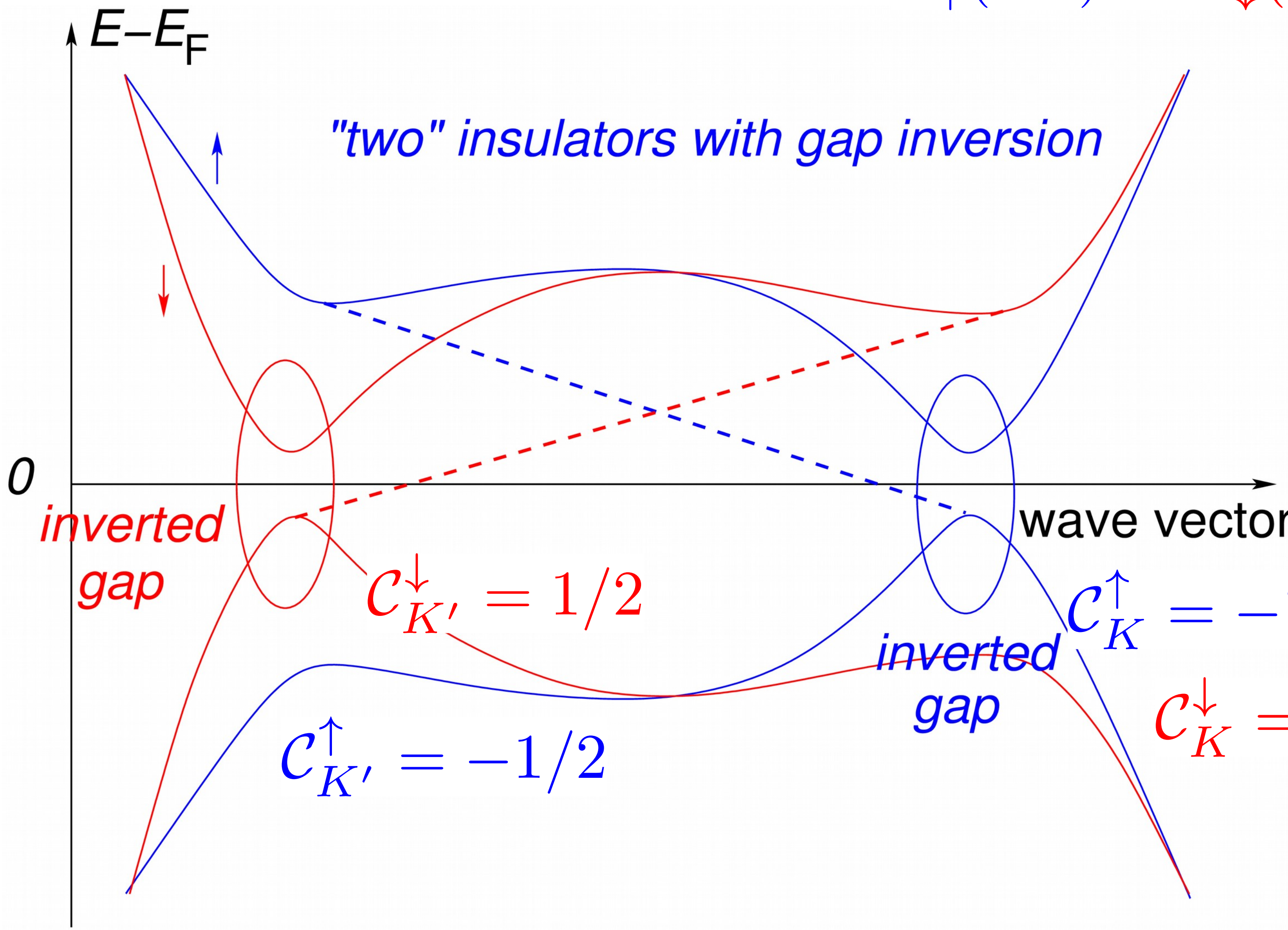
Broken TR symmetry : $E(\mathbf{k}) \neq E(-\mathbf{k})$

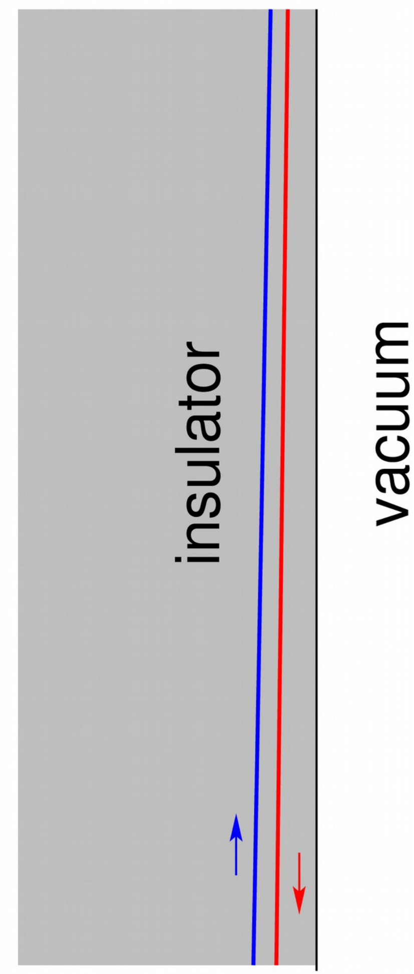
Change in total Chern number: $\Delta C = \Delta\mathcal{C}_K = \pm 1$

Kane-Mele model (2005) → TR symmetry respected

profit from spin !

$E_{\uparrow}(-\mathbf{k}) = E_{\downarrow}(\mathbf{k})$





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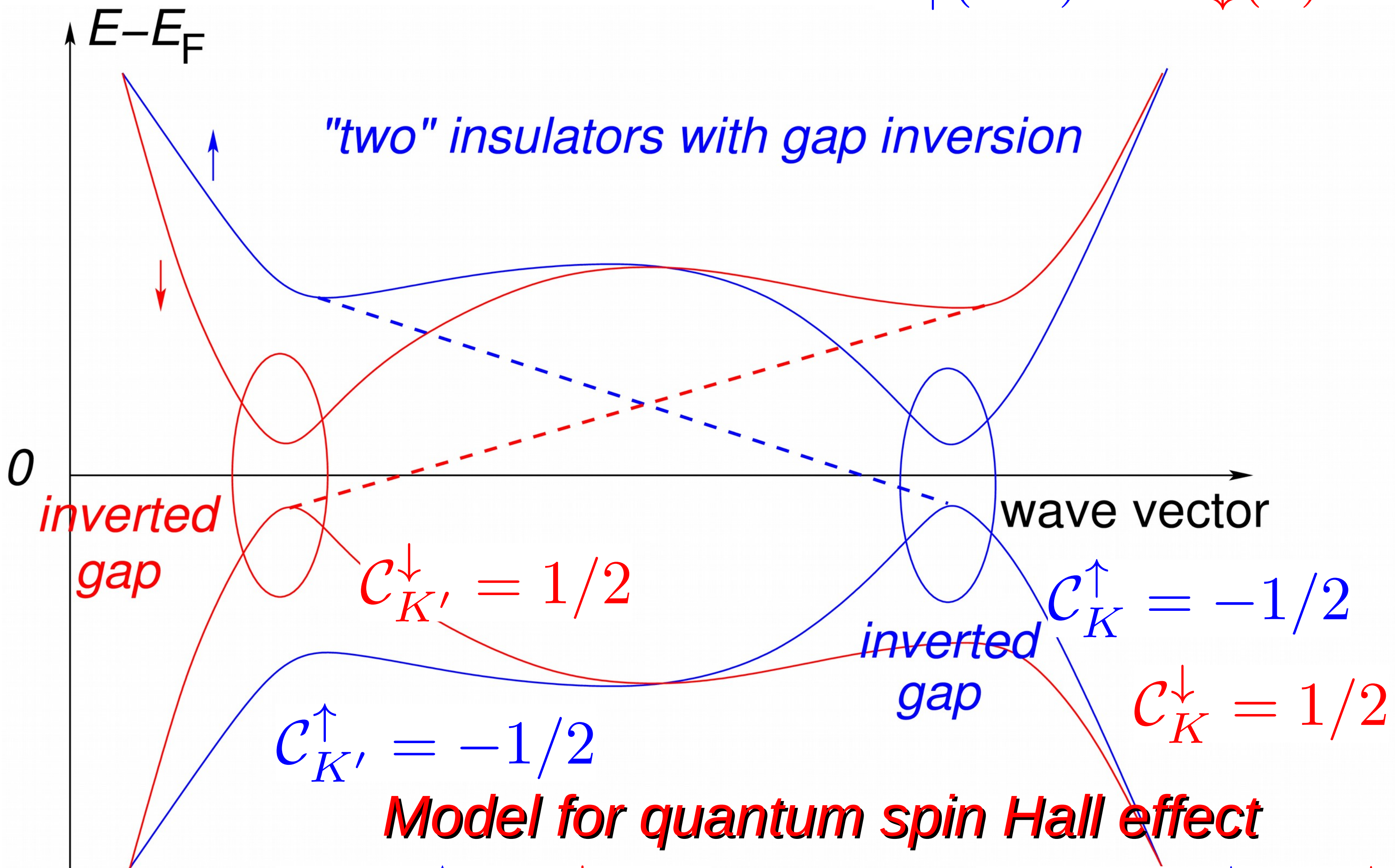

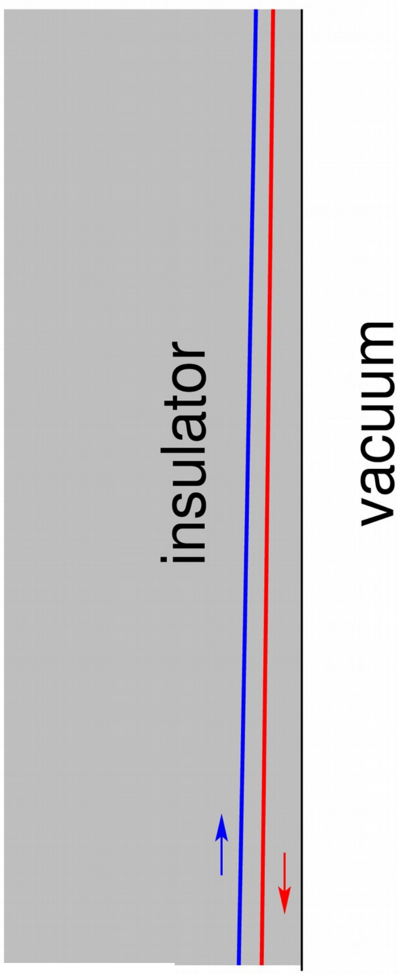

Model for quantum spin Hall effect

$\mathcal{C} = \mathcal{C}^{\uparrow} + \mathcal{C}^{\downarrow} = 0$ **but** $\mathcal{C}_{\mathrm{spin}} = \mathcal{C}^{\uparrow} - \mathcal{C}^{\downarrow} = -2$

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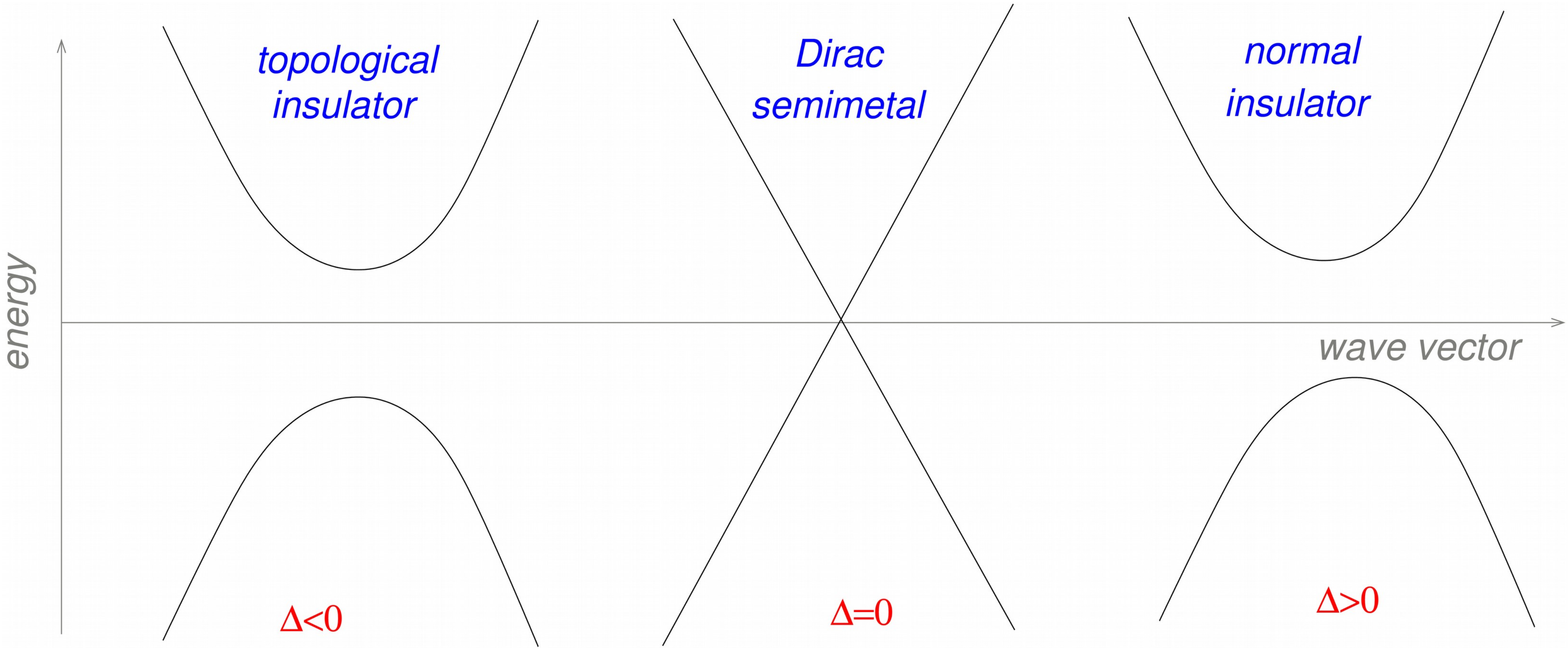
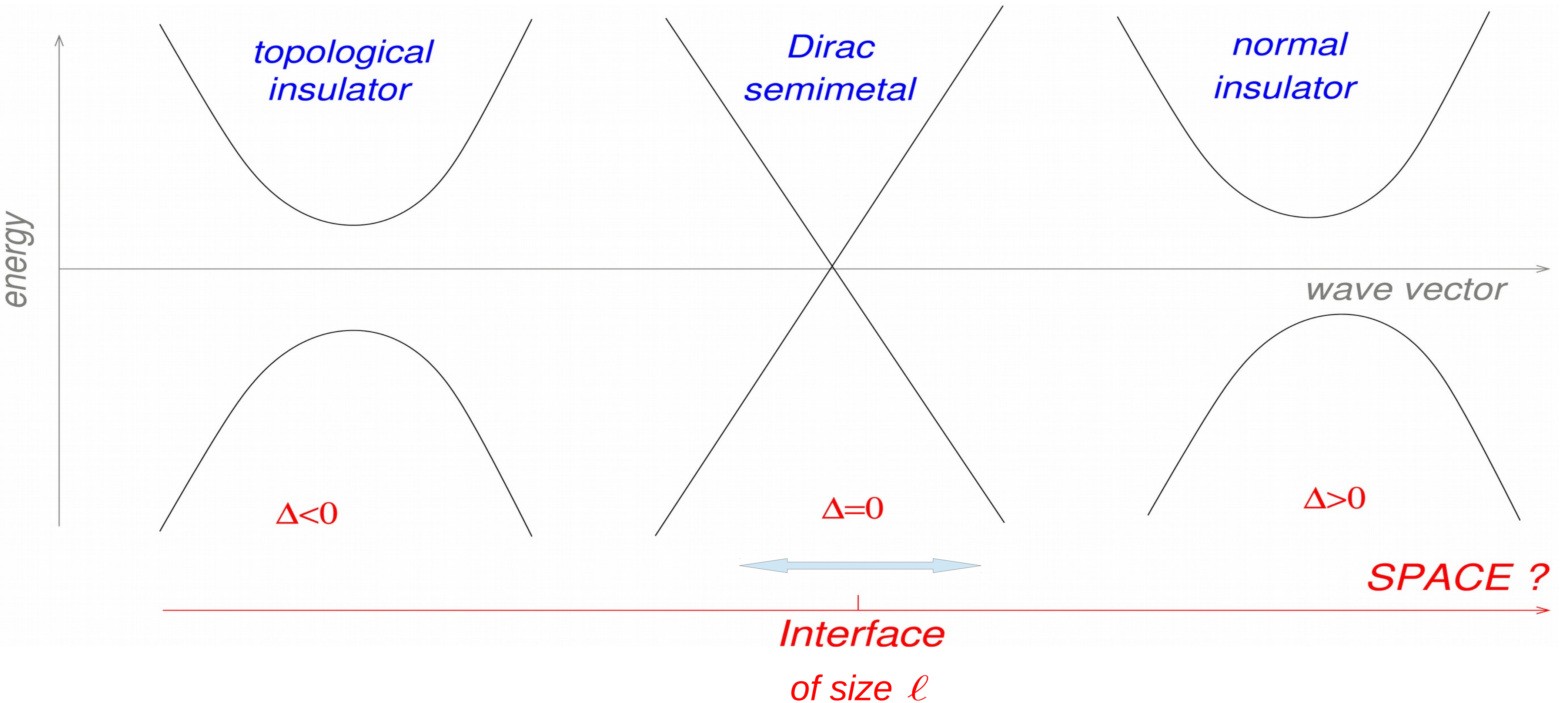
How can we use this to describe an interface ?



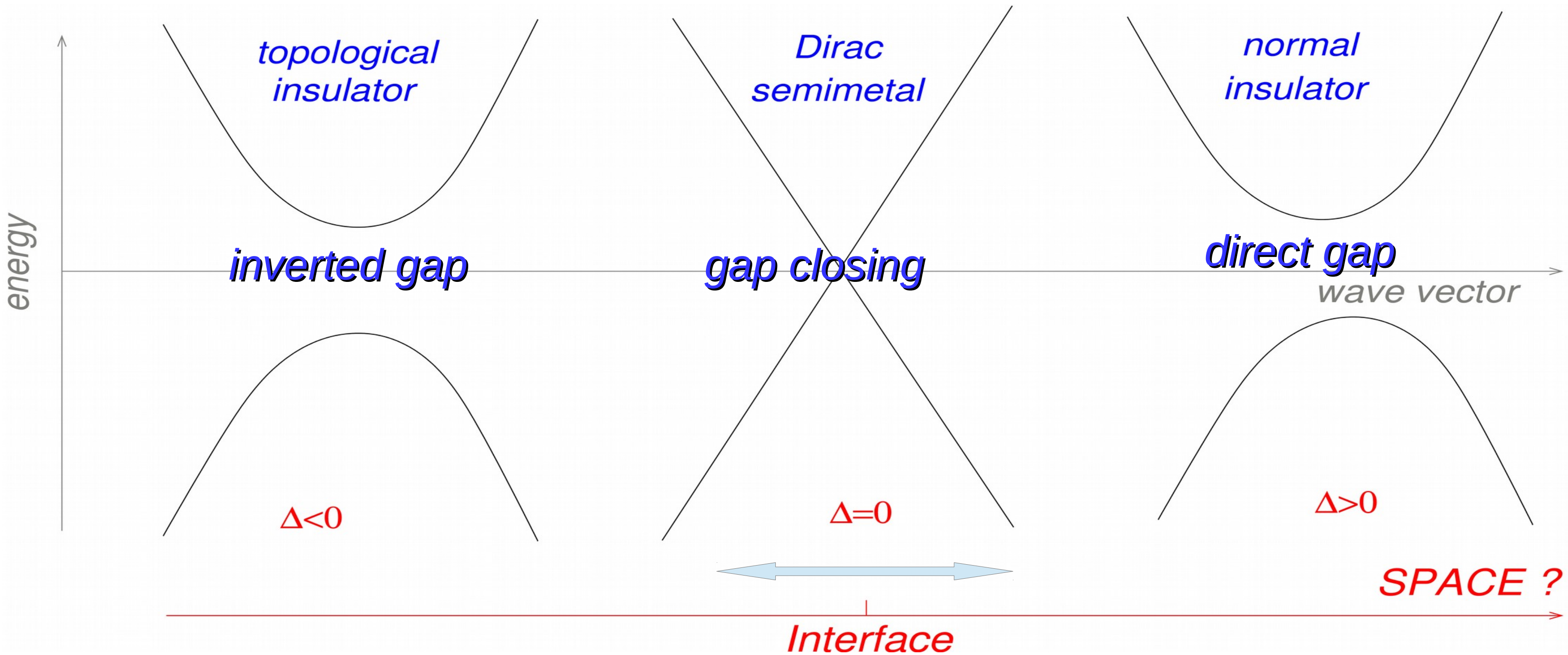
in parameter space

How can we use this to describe an interface ?



$$\Delta \quad \rightarrow \quad \Delta \frac{x}{\ell}$$

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*)

Change of “quantization axis” (unitary trafo)

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

$$H = \hbar \begin{pmatrix} v q_y & v(q_x + i\frac{x}{\ell_S^2}) \\ v(q_x - i\frac{x}{\ell_S^2}) & -v q_y \end{pmatrix}$$

With characteristic (~”magnetic”) length: $\ell_S = \sqrt{\ell \hbar v/\Delta} = \sqrt{\ell \xi}$

(intrinsic length: $\xi = \hbar v/\Delta$)

solution via ladder operators of harmonic oscillator:

$$\hat{a} = \frac{\ell_S}{\sqrt{2}}(q_x + ix/\ell_S^2) \qquad \hat{a}^\dagger = \frac{\ell_S}{\sqrt{2}}(q_x - ix/\ell_S^2) \qquad [\hat{a}, \hat{a}^\dagger] = 1$$

Tchoumakov et al., PRB (2017)

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

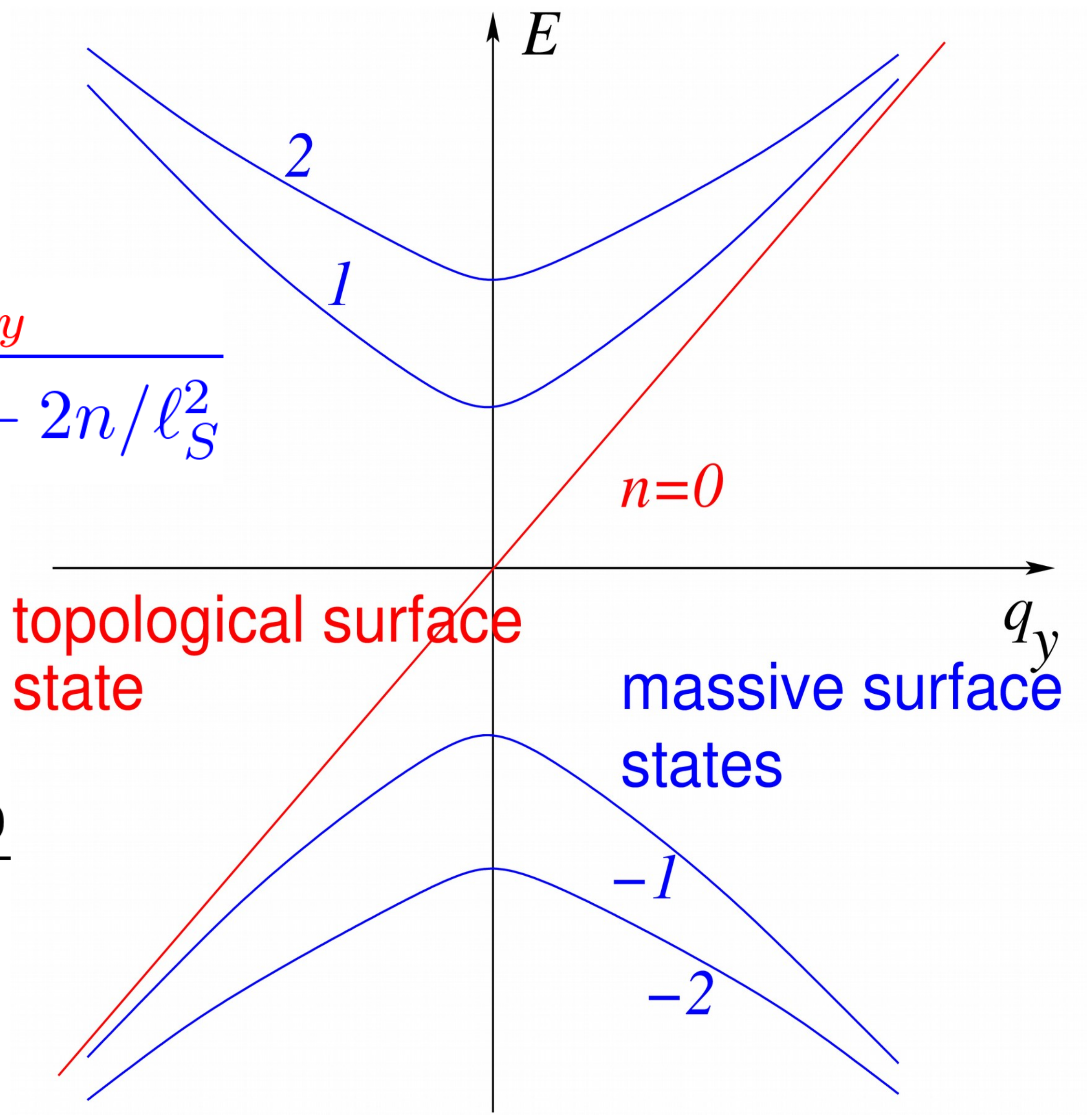
$$\begin{aligned} E_{n=0} &= v q_y \\ E_{\lambda, n\neq 0} &= \lambda v \sqrt{q_y^2 + 2n/\ell_S^2} \end{aligned}$$

Surface (edge) states

$$E_{n=0} = vq_y$$

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

chirality : sign of $\dfrac{\partial E_0}{\partial q_y}$

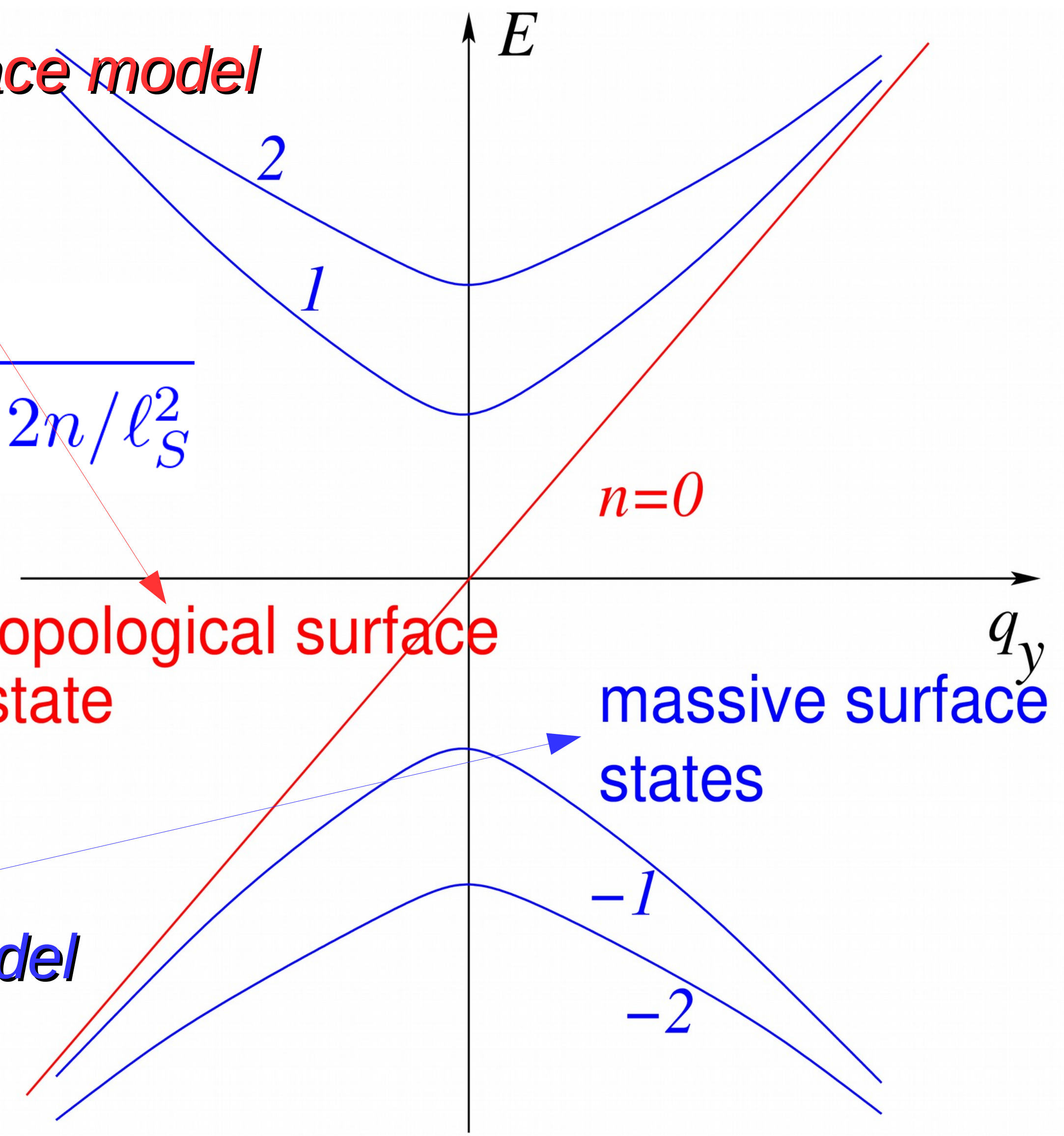


Surface (edge) states

independent of surface model

$$E_{n=0} = vq_y$$

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



depends on surface model

Surface (edge) states

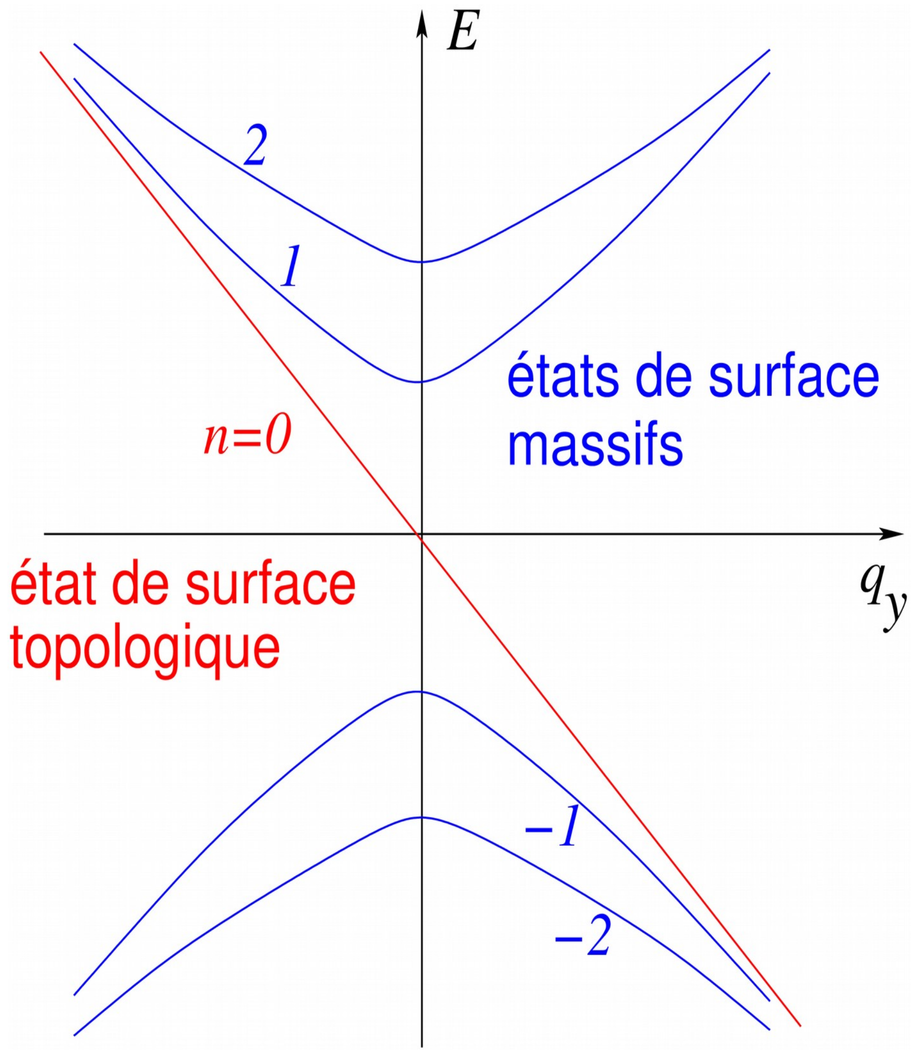
- How to change sign of chirality:

→ changing the valley (for helical edge states with spin)

$$\xi \to -\xi$$

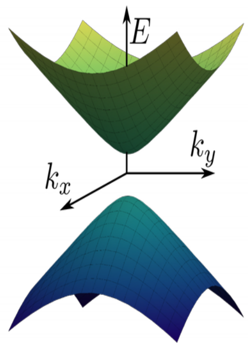
→ changing the edge (~ flipping orientation of “magnetic field”)

$$\ell \to -\ell$$



Surface states in 3D materials

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



Complication in 3D: 4x4 Hamiltonian

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

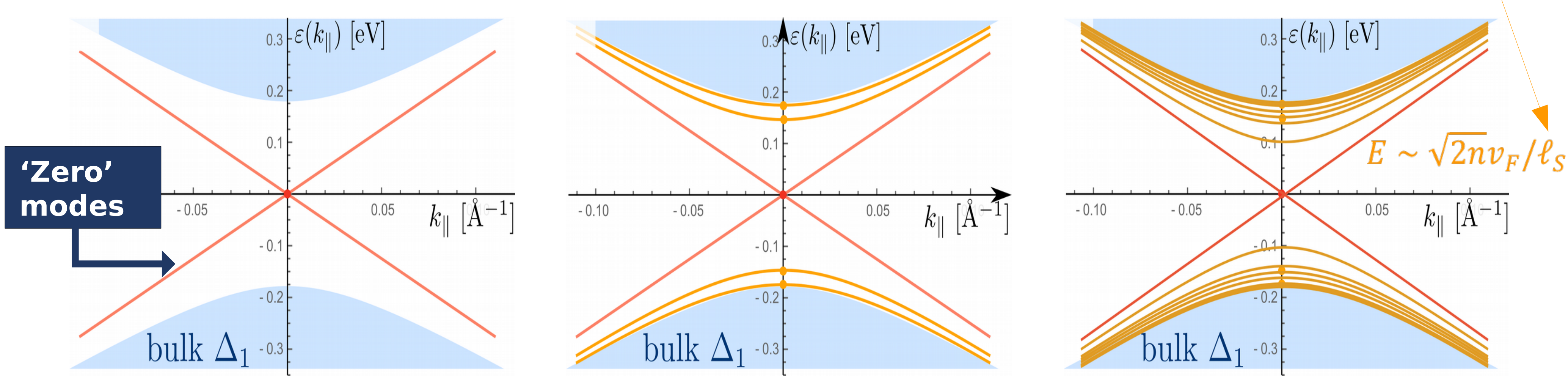
$$H = v_F(k_z \mathbb{1} \otimes \tau_y + (k_y\,\sigma_x - k_x\sigma_y) \otimes \tau_x) + \Delta(z)\, \mathbb{1} \otimes \tau_z$$

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

<u>*+ numerical k.p calculations (→ ENS Lyon)*</u>

ℓ/ξ

abrupt — intermediate — very smooth



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

Conclusions

- Surface states of topological materials with smooth interfaces ~ Landau bands of Dirac fermions
- Topologically protected surface state ~ chiral n=0 Landau band
- Additional massive Landau bands ($n \neq 0$)
- *Intriguing relativistic effects*
- *Experimental evidence in HgTe samples*

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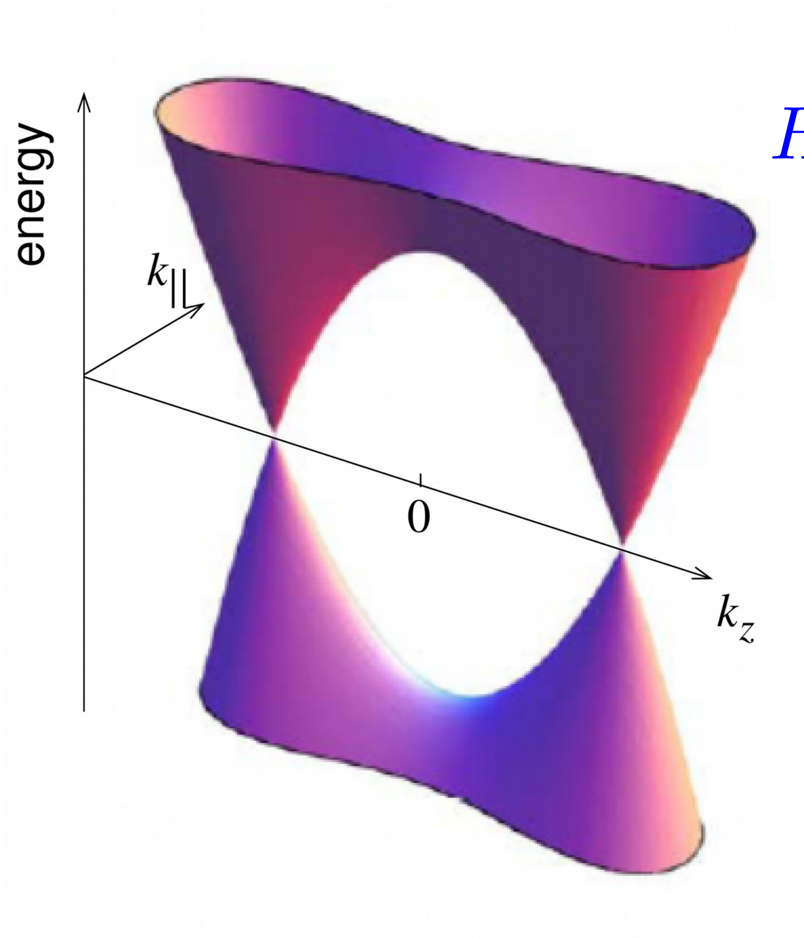
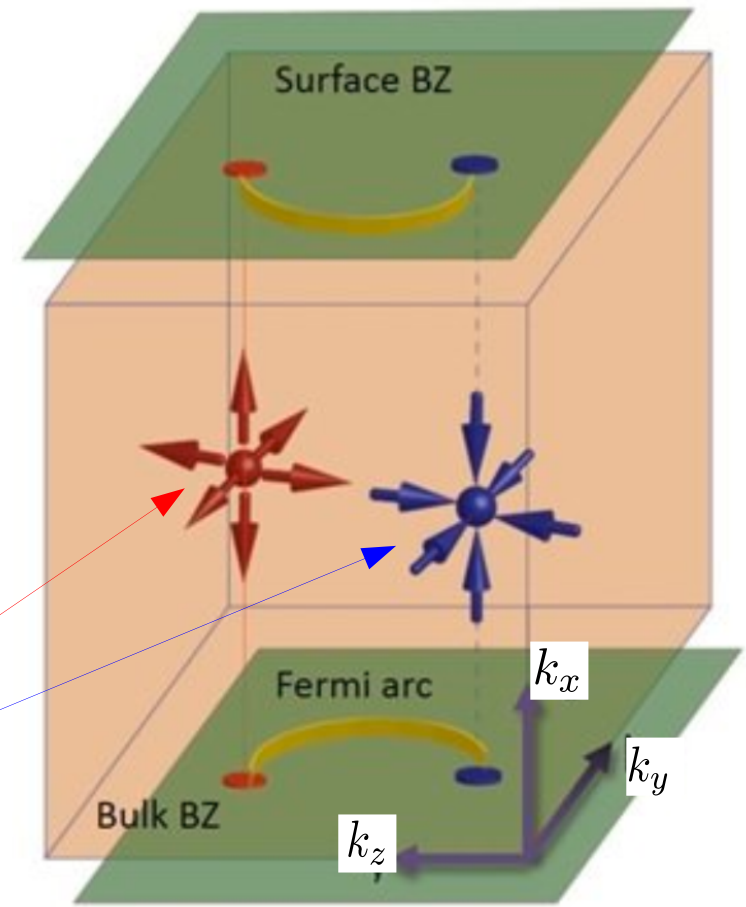
Weyl semimetals – "3D graphene"

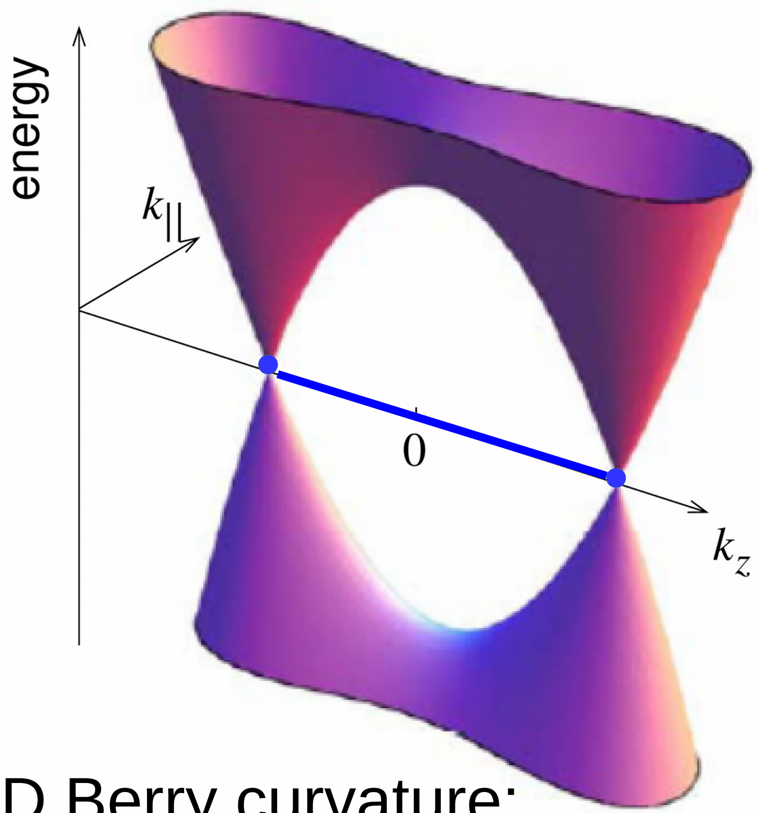


$$H = \begin{pmatrix} \Delta - \frac{\hbar^2 k_z^2}{2m_0} & \hbar v(k_x - ik_y) \\ \hbar v(k_x + ik_y) & -\Delta + \frac{\hbar^2 k_z^2}{2m_0} \end{pmatrix}$$



Dirac monopoles
(in wave function)

Weyl semimetals – "3D graphene"



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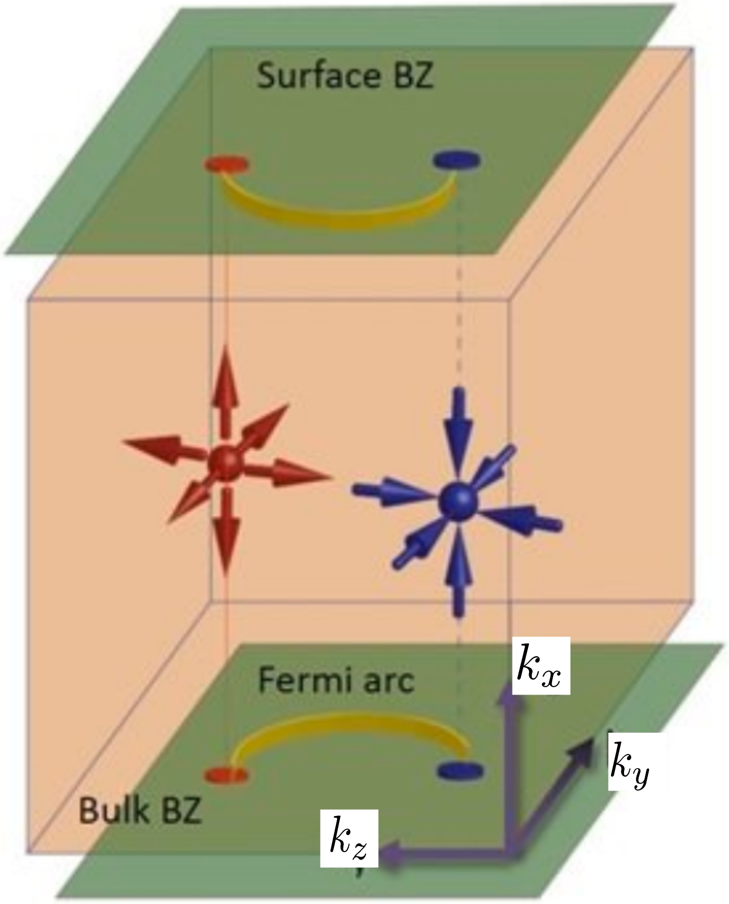
Δ_{k_z}



2D Berry curvature:

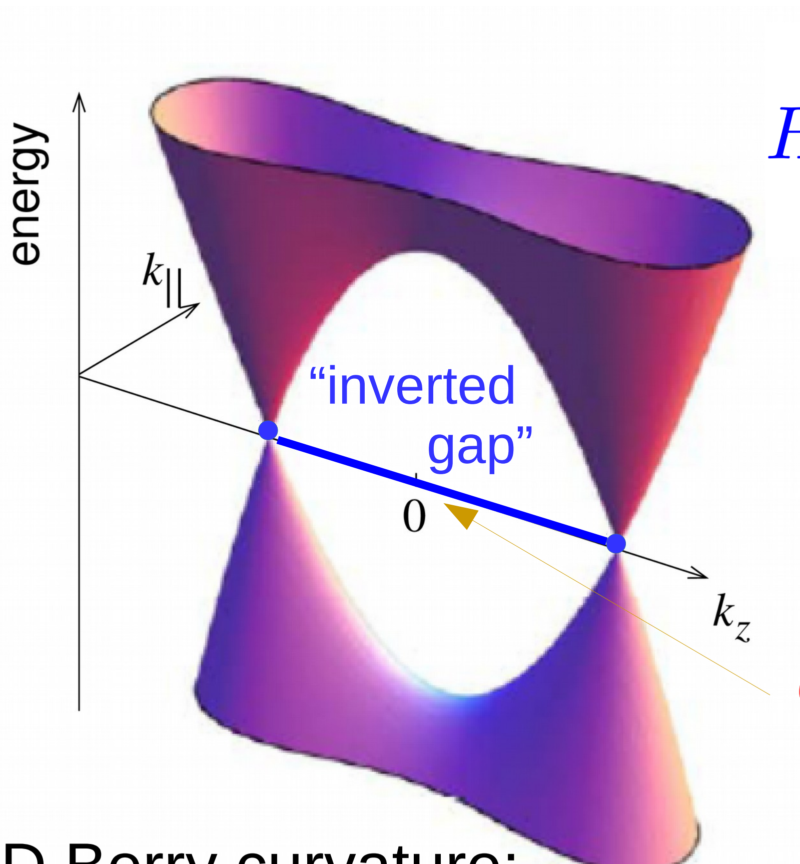
$$\mathcal{B}_{\lambda,k_z}(k_{\|}) = -\frac{\lambda}{2}\frac{\hbar^2 v^2 \Delta_{k_z}}{(\Delta_{k_z}^2 + \hbar^2 v^2 k_{\|}^2)^{3/2}}$$

"half Chern number":

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

Weyl semimetals – "3D graphene"

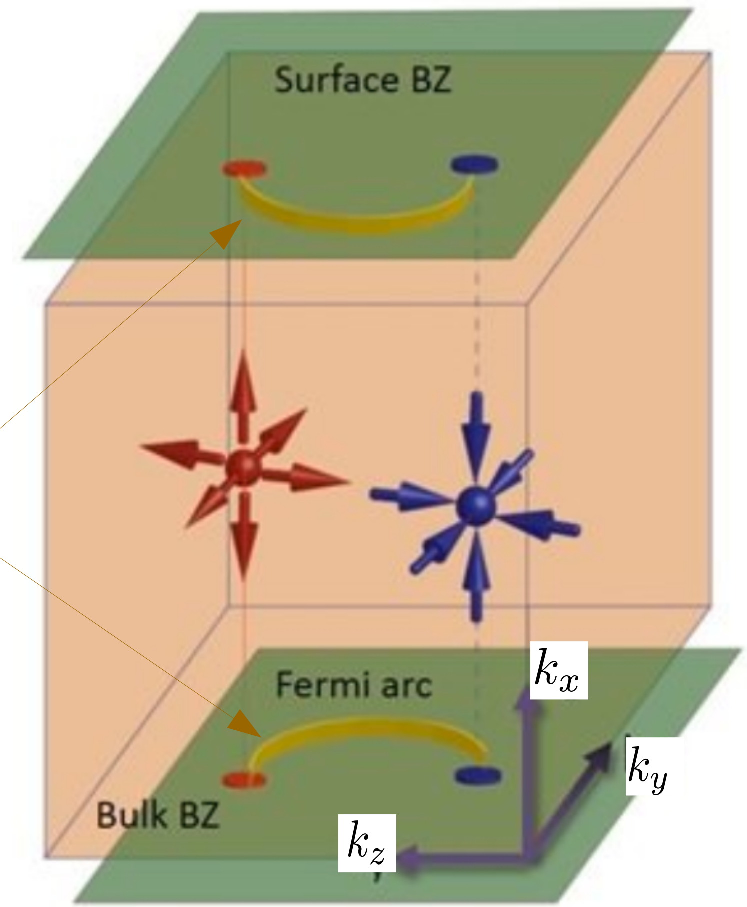
$$H = \begin{pmatrix} \Delta - \frac{\hbar^2 k_z^2}{2m_0} & \hbar v (k_x - i k_y) \\ \hbar v (k_x + i k_y) & -\Delta + \frac{\hbar^2 k_z^2}{2m_0} \end{pmatrix}$$



Δ_{k_z}

edge states

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



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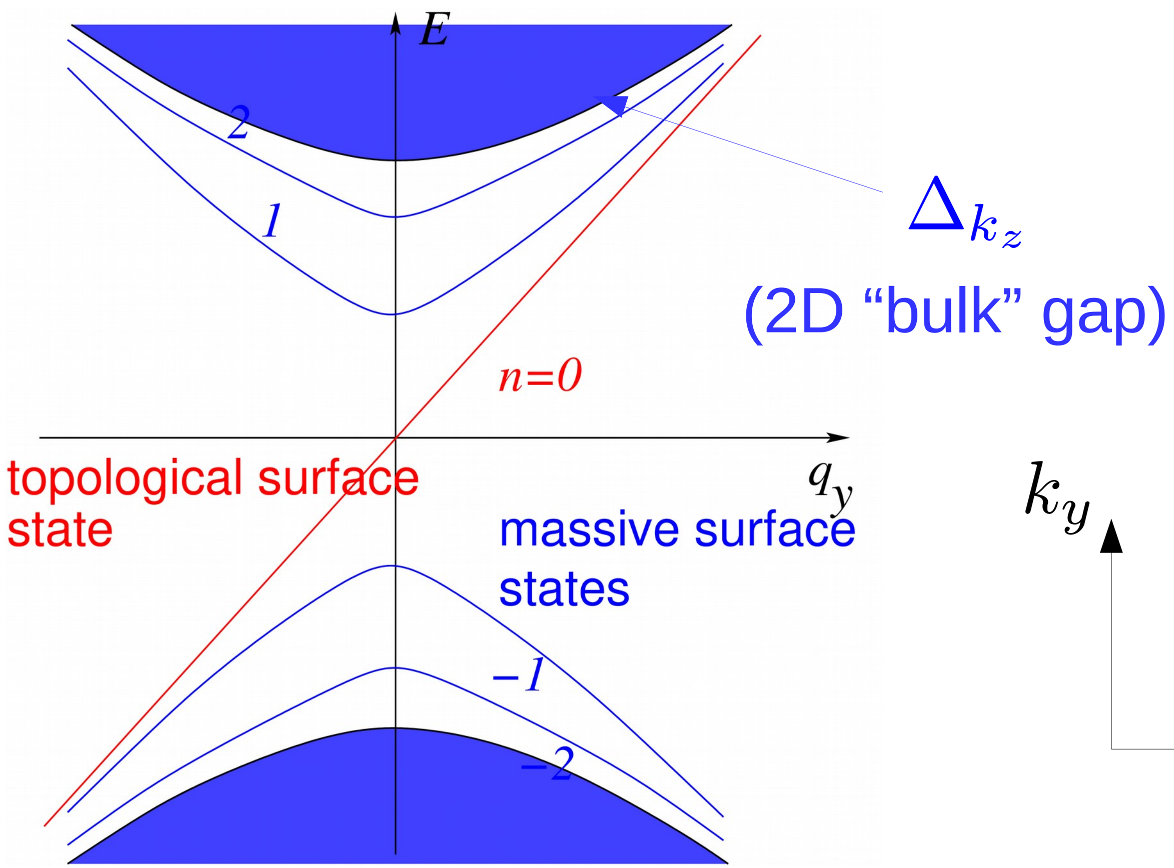
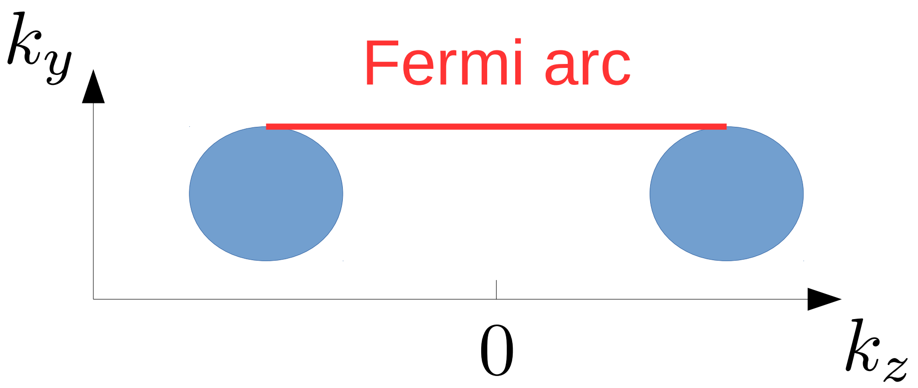
"half Chern number":

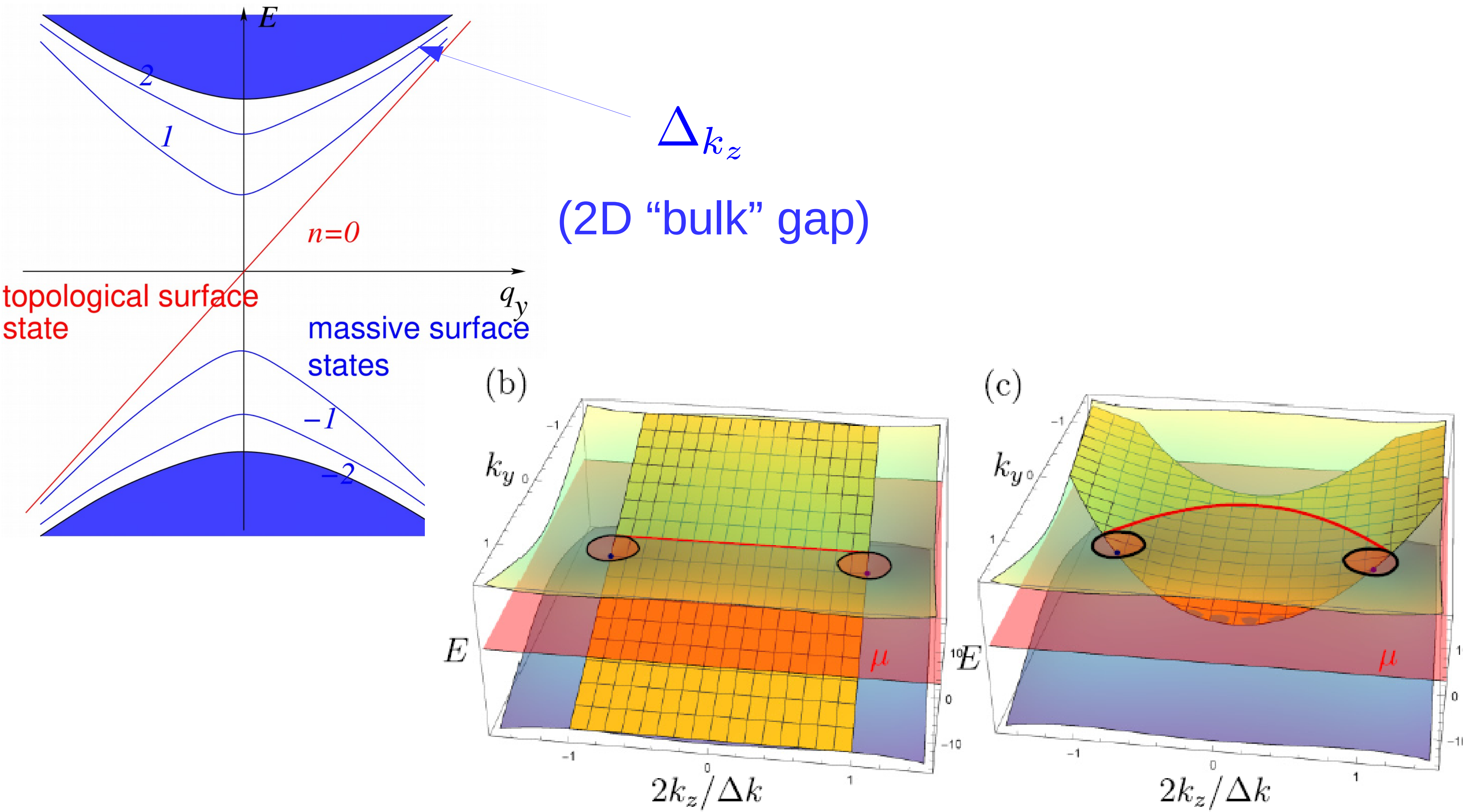
$$C_\lambda(k_z) = -\frac{1}{2} \lambda \, \mathrm{sgn}(\Delta_{k_z})$$

Fermi arc as a collection of 1D edge channels





Fermi arc as a collection of 1D edge channels



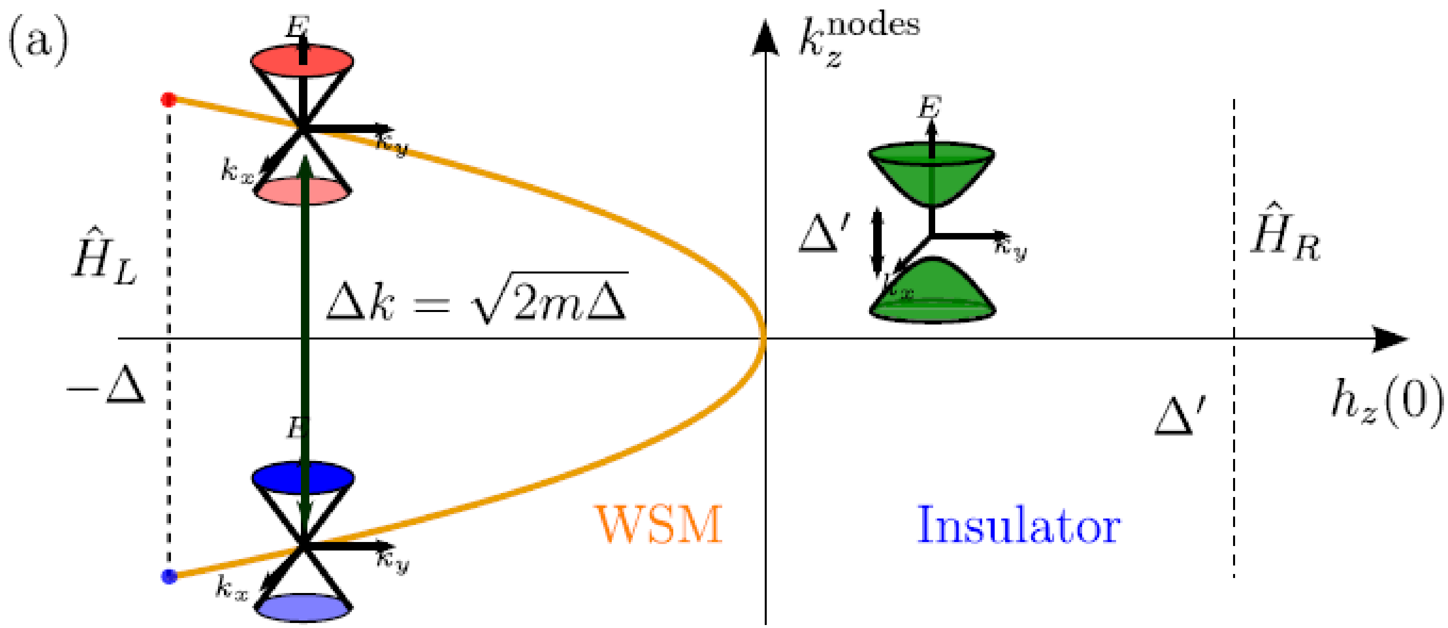
Tchoumakov, Civelli & MOG, PRB (2017)

Fermi arc in a smooth interface → TI

Effective interface model for Weyl node merging:

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

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



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:

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

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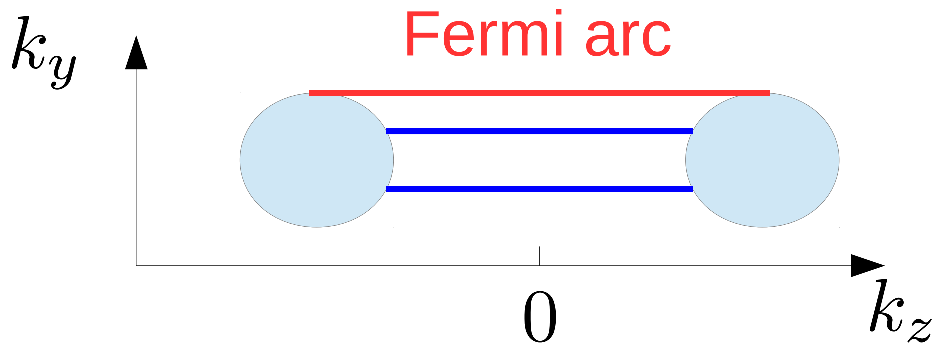
"Landau levels":

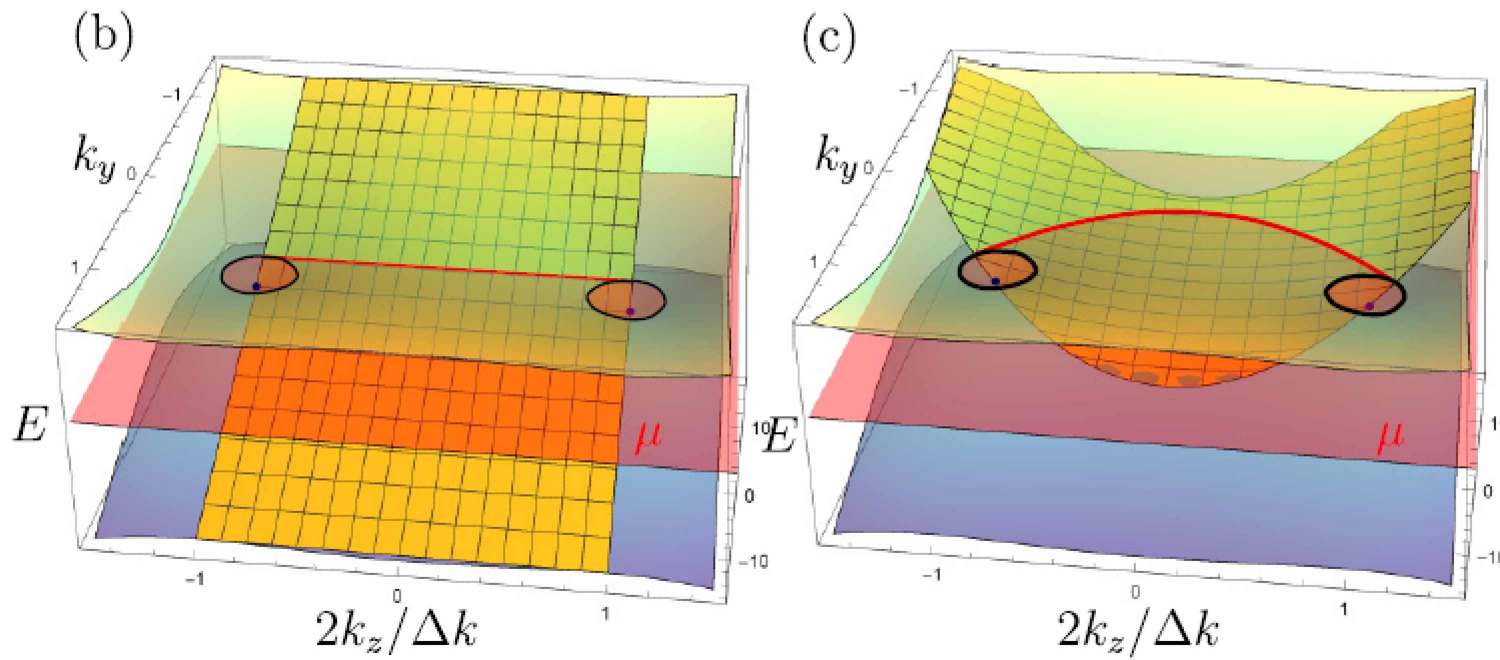
$$E_{n=0}(k_y) = \hbar v k_y$$ ← *Fermi arc*

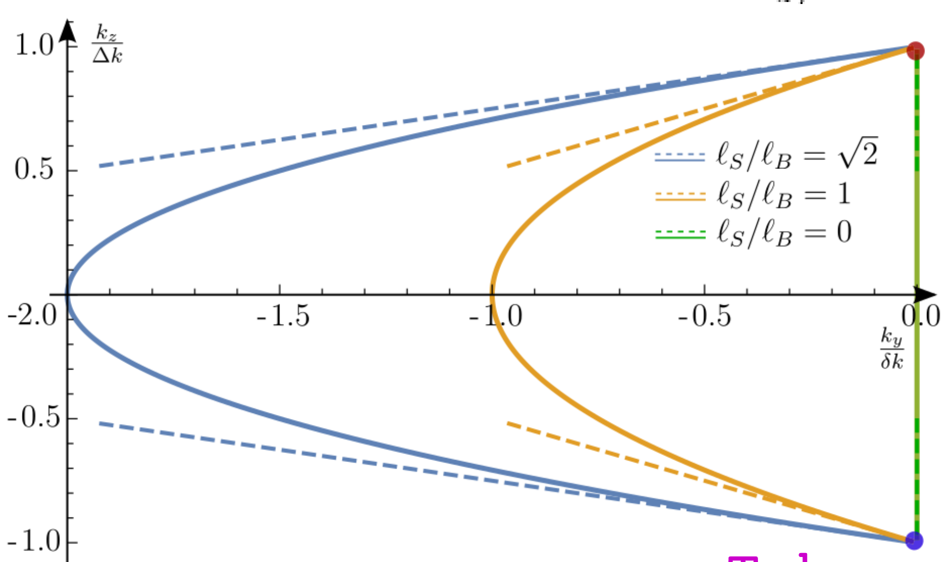
$$E_{\lambda, n\neq 0}(k_y) = \lambda \hbar v \sqrt{k_y^2 + 2n/\ell_S^2}$$ ← *massive VP states*



Tchoumakov, Civelli & MOG, PRB (2017)

Dispersing Fermi arcs



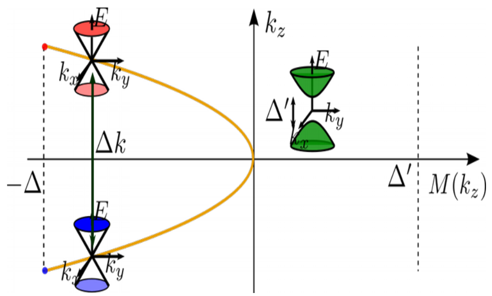


dispersion of Fermi arcs in k_z

→ magnetic field in interface (conspires with confinement)

Tchoumakov, Civelli & MOG, PRB (2017)

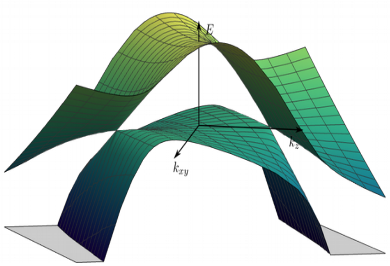
Surface states of tilted Weyl nodes



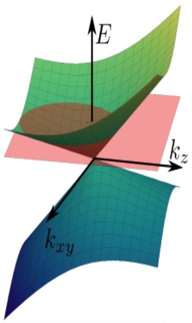
electric

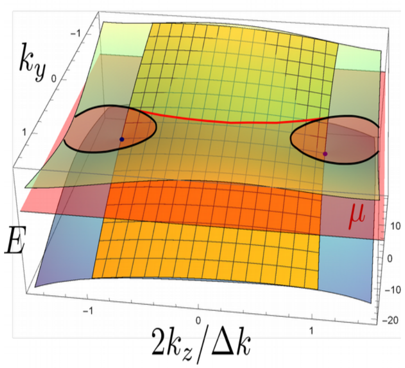
$$H = t_z(x)\left(\frac{k_z^2}{2m}-\Delta(x)\right)+\frac{v_F k_z}{\Delta k}\left(t_x k_x + t_y(x) k_y\right)$$
$$+ v_F(k_x\sigma_x + k_y\sigma_y) + \left[\frac{k_z^2}{2m}-\Delta(x)\right]\sigma_z$$

magnetic

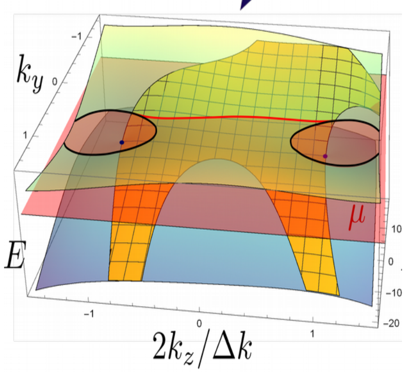


- Type-I Weyl semimetals



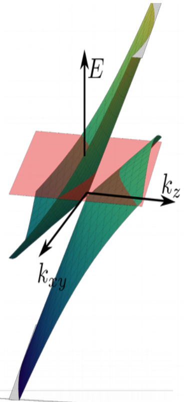


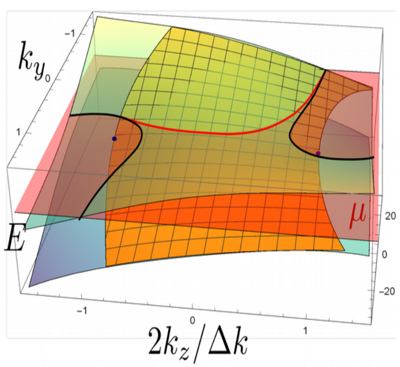
$\Delta' \gg \Delta$



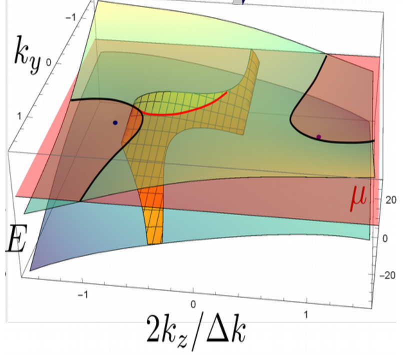
$\Delta' \sim \Delta$

- Type-II Weyl semimetals





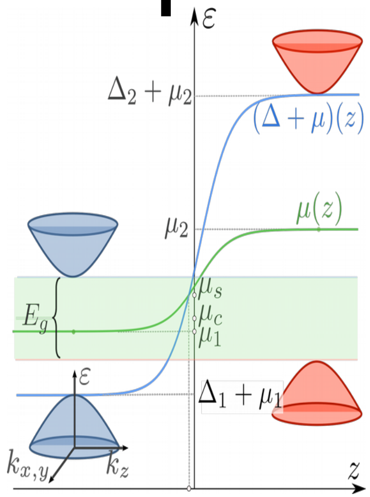
$\Delta' \gg \Delta$



$\Delta' \sim \Delta$

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

Special relativity in surface states

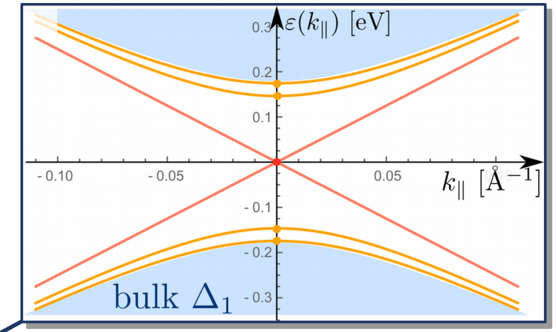


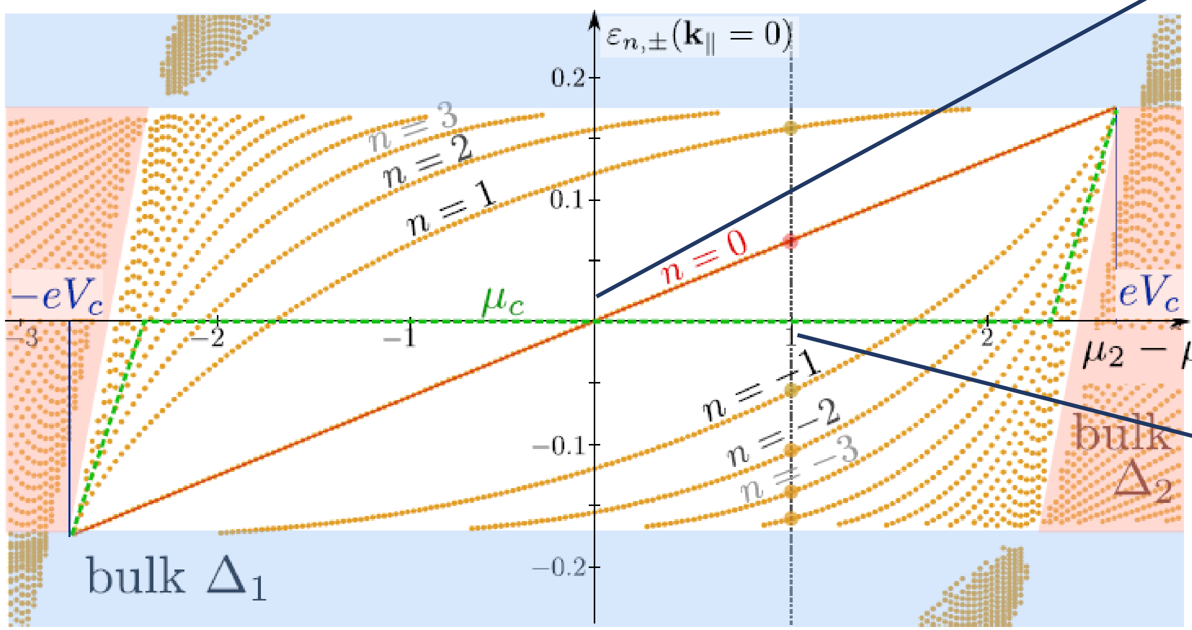
$$H = \boldsymbol{V(z)}\,\mathbb{1} + v_F(k_x\ \mathbb{1}\otimes\tau_y + (k_y\,\sigma_x - k_x\sigma_y)\otimes\tau_x) + \boldsymbol{\Delta(z)}\,\mathbb{1}\otimes\tau_z$$

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

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

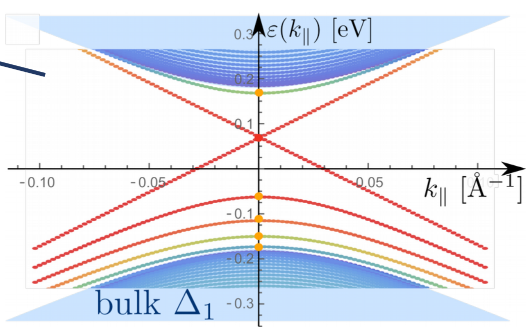
Magnetic field: $B \to B\sqrt{1-\beta^2}$





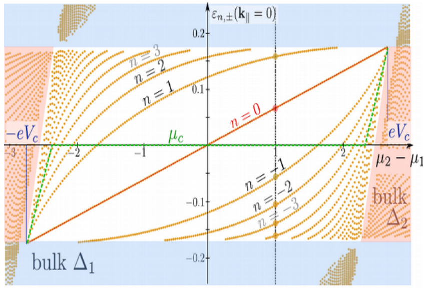
$$\Delta'_n \approx (1-\beta^2)^{3/4}\Delta_n$$

$$\mu'_s = -\beta\Delta_1$$



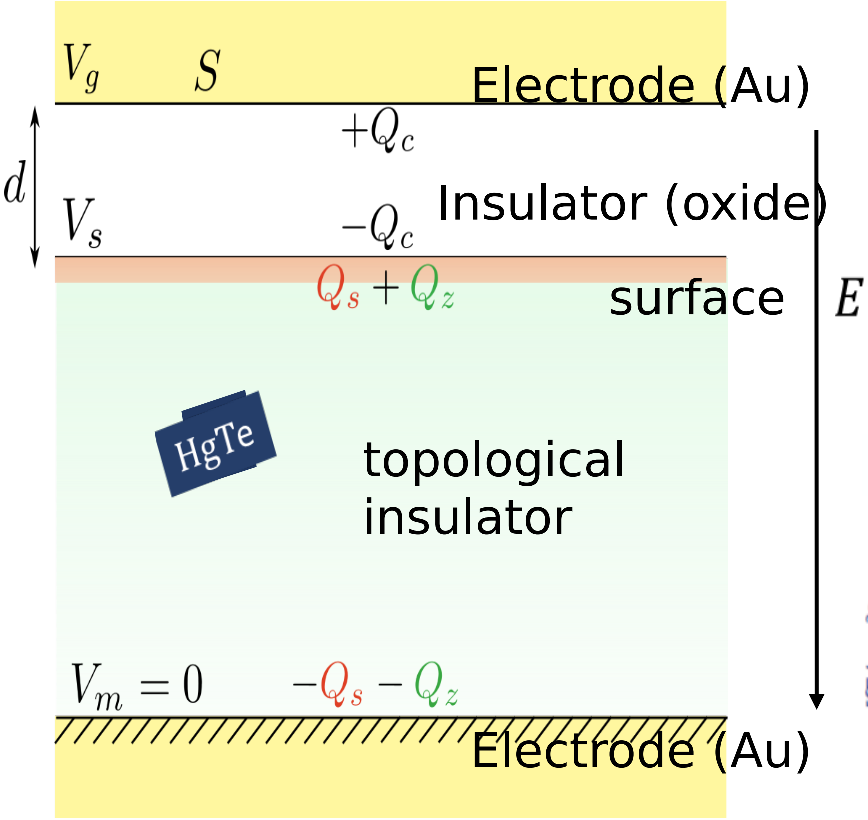
S. Tchoumakov, V. Jouffrey et al., PRB 96, 201302 (2017)

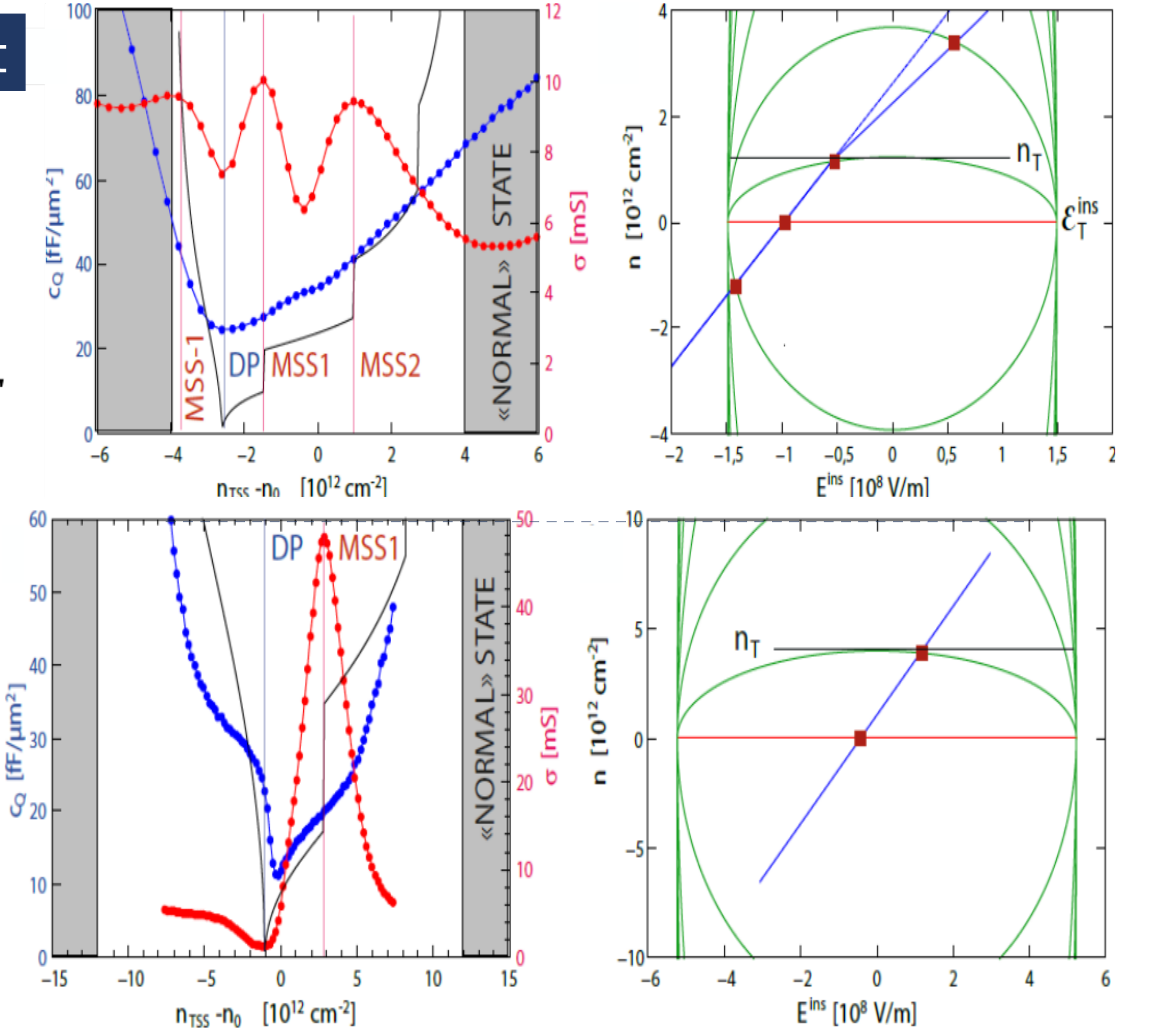
Experimental evidence



➢ Electrical resistance and capacitance of HgTe

Qualitative agreement





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