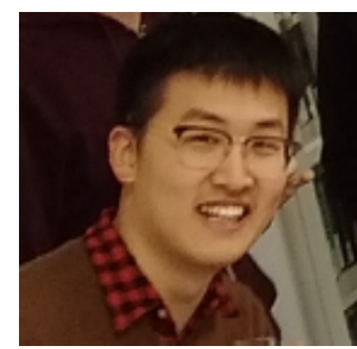
Bulk-edge correspondence in topological materials – Dirac fermions beyond chiral states (Part 1)

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)

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

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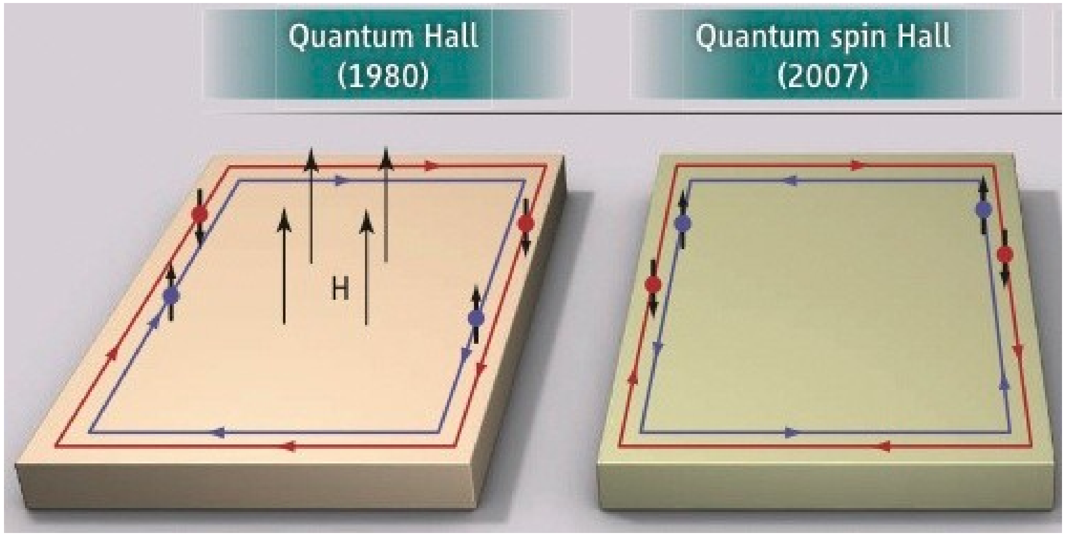
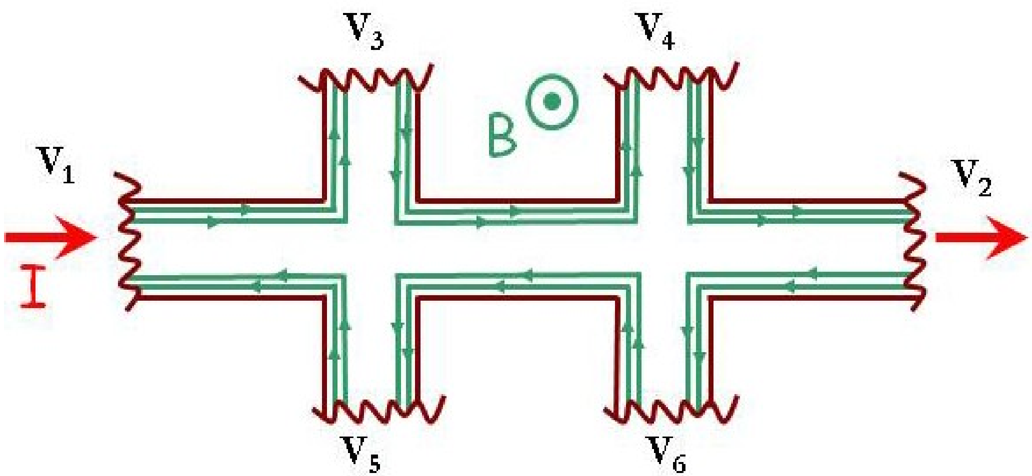
Topological insulators (1980→2007)



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

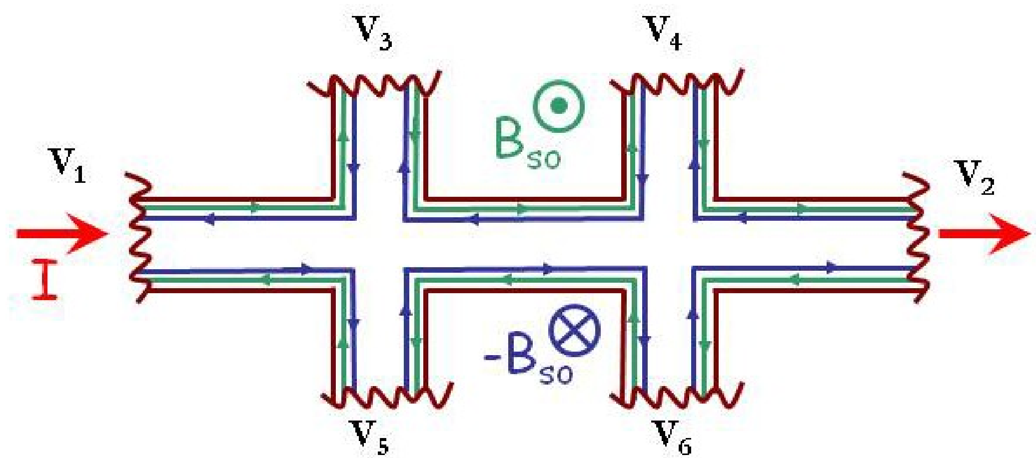
Topological insulator =
Bulk insulator +
Conducting edges (surfaces)

Quantum Hall effect



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

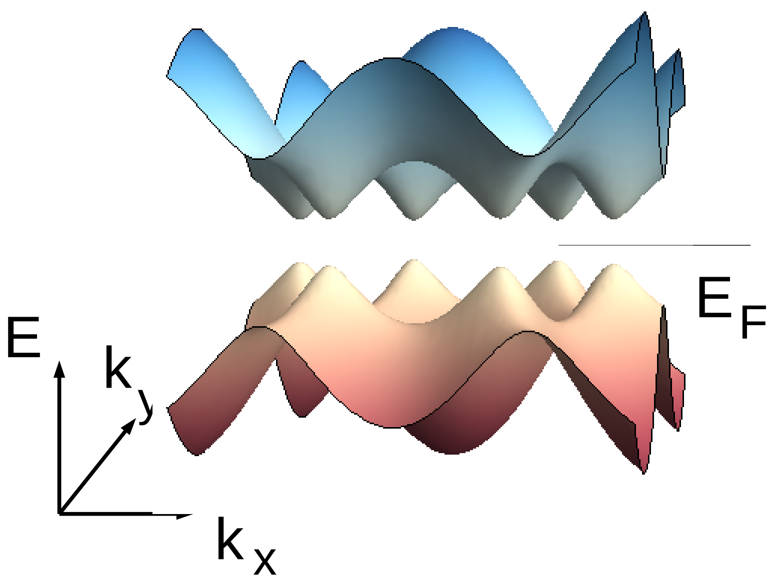
Quantum spin Hall effect



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

Gapped graphene as the prototype of a 2D insulator

band structure of insulating graphene

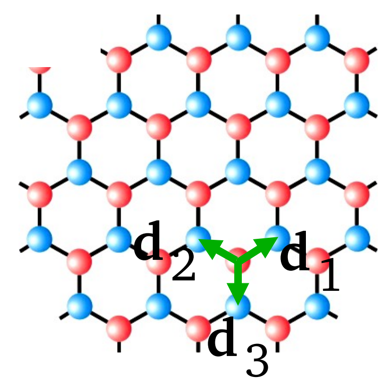


insulator gap = 2Δ

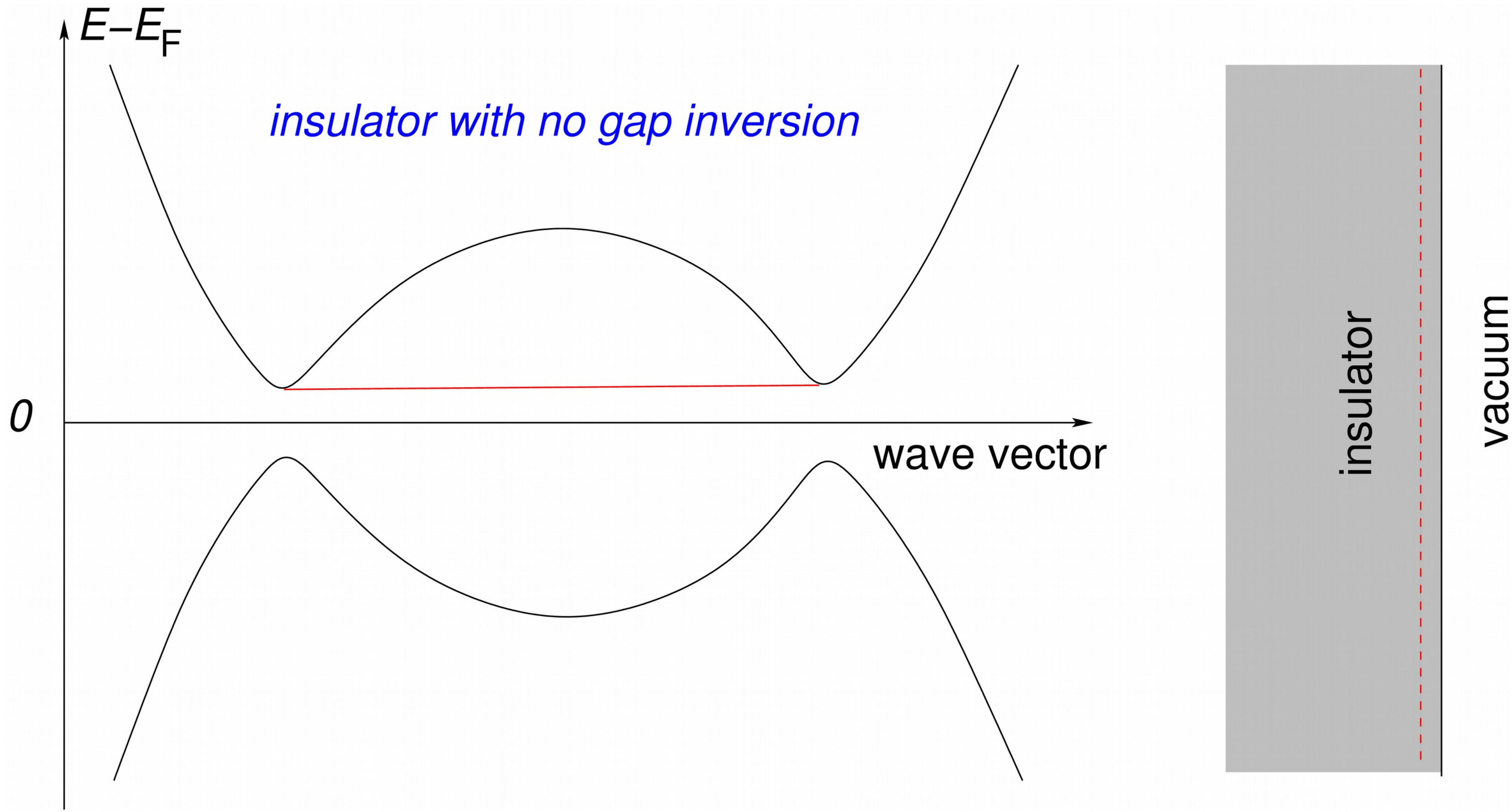
Hamiltonian (tight-binding model) :

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

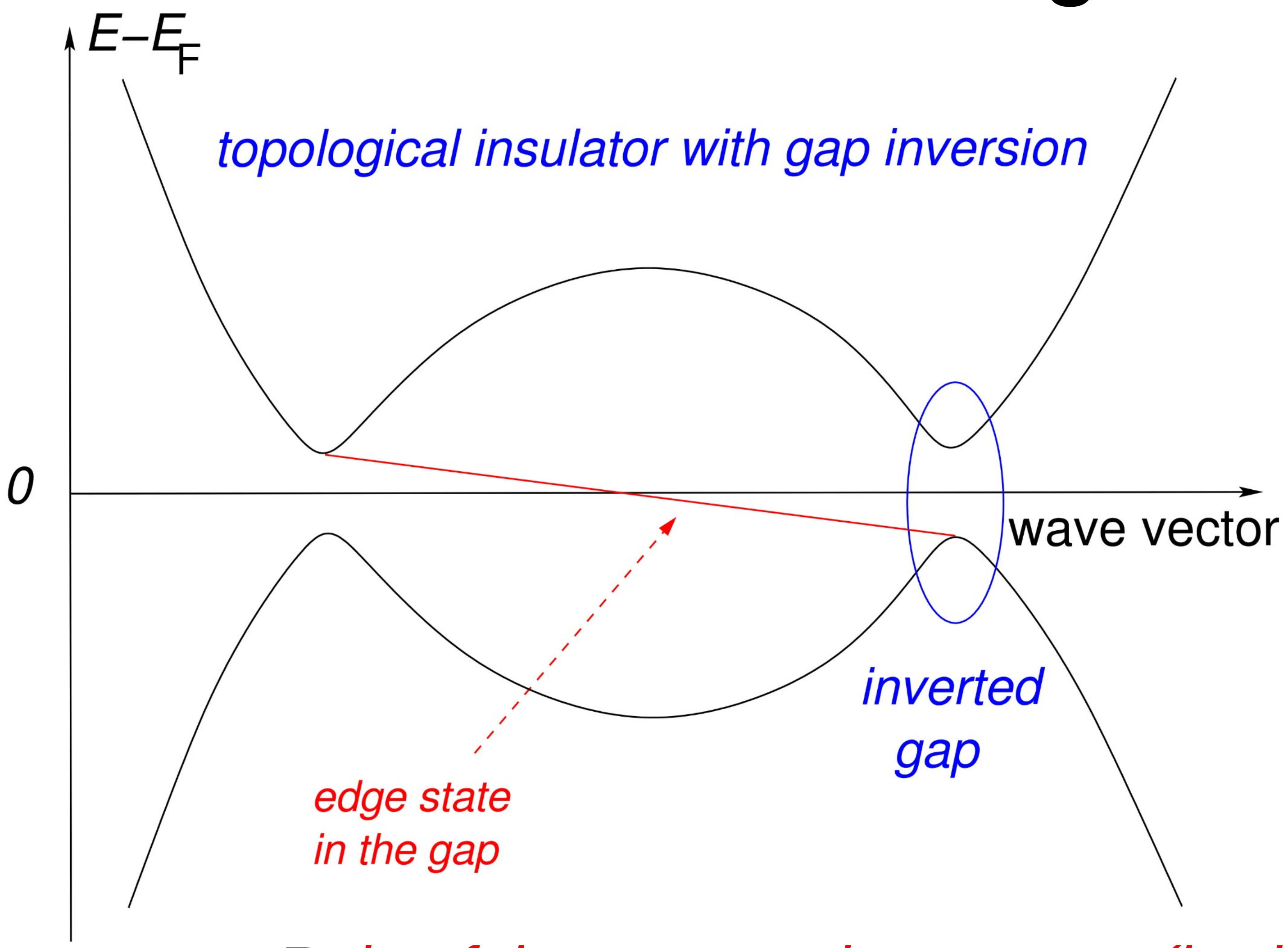
$$f(\mathbf{k}) = \sum_{j=1}^{3} e^{-i\mathbf{k}\cdot\mathbf{d}_j}$$

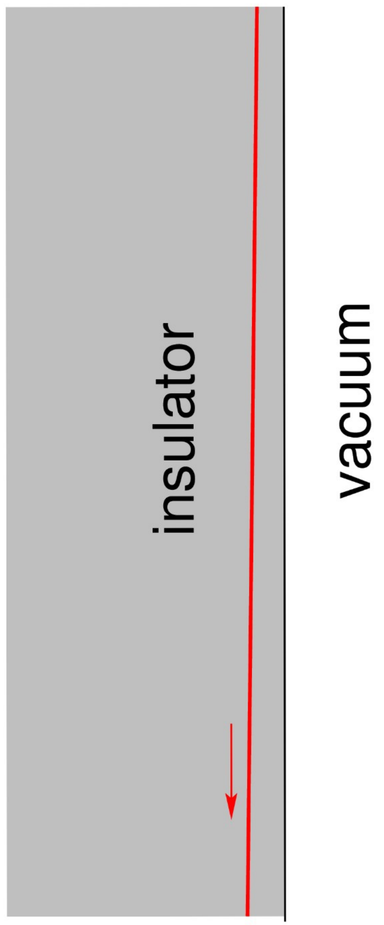


Gapped graphene as a normal insulator – adding an edge



Gapped graphene as a topological insulator – adding an edge





Role of time reversal symmetry (<u>broken here !</u>):

$$t \to -t \qquad k \to k \to -k \qquad E(k) = E(-k) \qquad v = \frac{\partial E}{\hbar \partial k} \to -v$$

Information beyond the spectrum

Wave functions (→ "spin"):

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

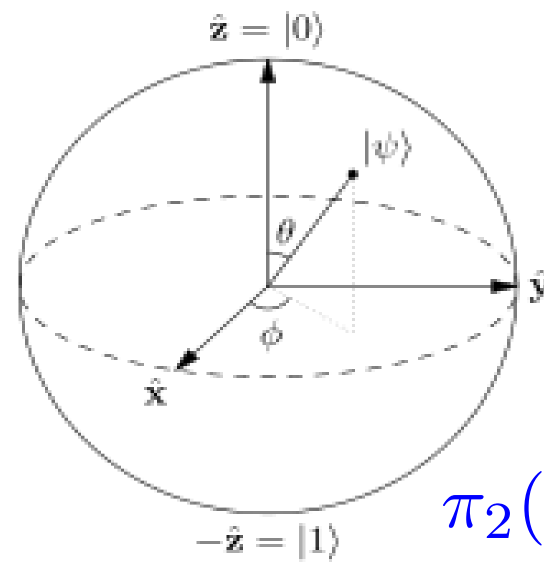
$$\psi_{+,\mathbf{k}} = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix} \qquad \psi_{-,\mathbf{k}} = \begin{pmatrix} -\sin\frac{\theta}{2} \\ e^{i\phi}\cos\frac{\theta}{2} \end{pmatrix}$$

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)

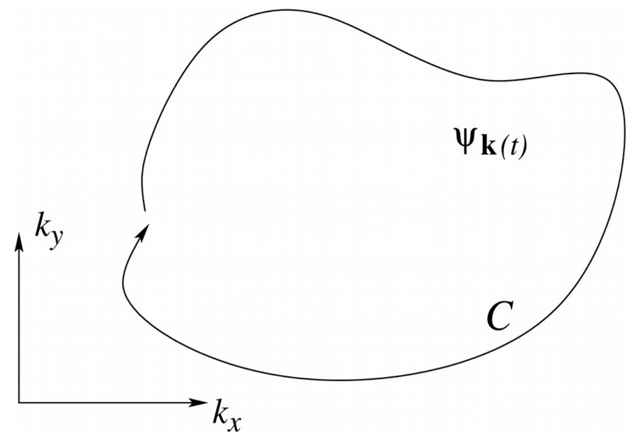
→ gap must change sign to have $n \neq 0$ *("gap inversion") !!*

Mathematical formulation (→ Berry)

Geometric (Berry) phase (~ magnetic flux):

$$\gamma_C = \int_C d\mathbf{k} \cdot \mathcal{A}_\lambda(\mathbf{k}) \qquad \psi_\lambda(t) = e^{-iEt/\hbar} e^{-i\gamma_C} \psi_{\lambda,\mathbf{k}(t)}$$

$\lambda = \pm$: 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):

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

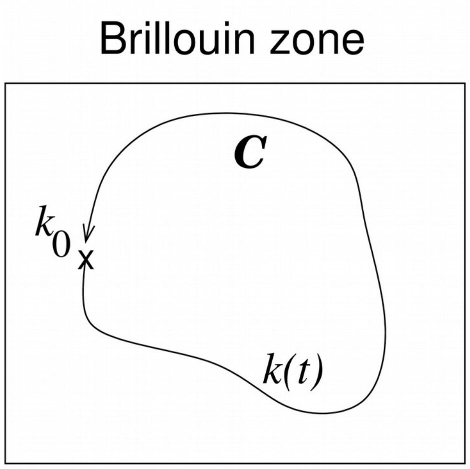
integer

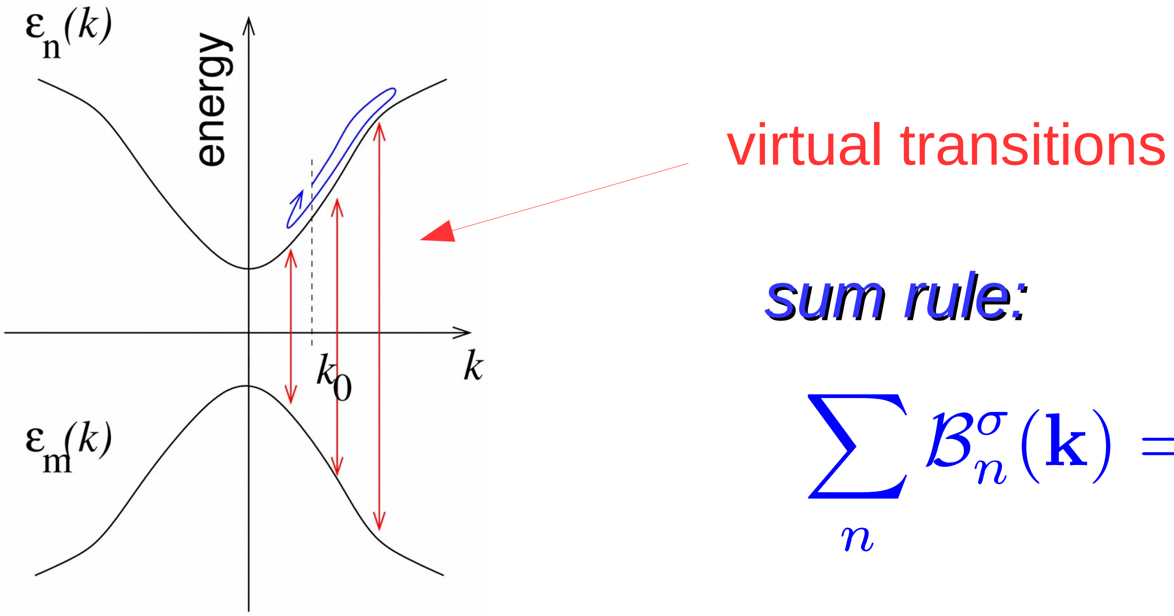
Berry curvature – some properties

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

→ link to perturbation theory :

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



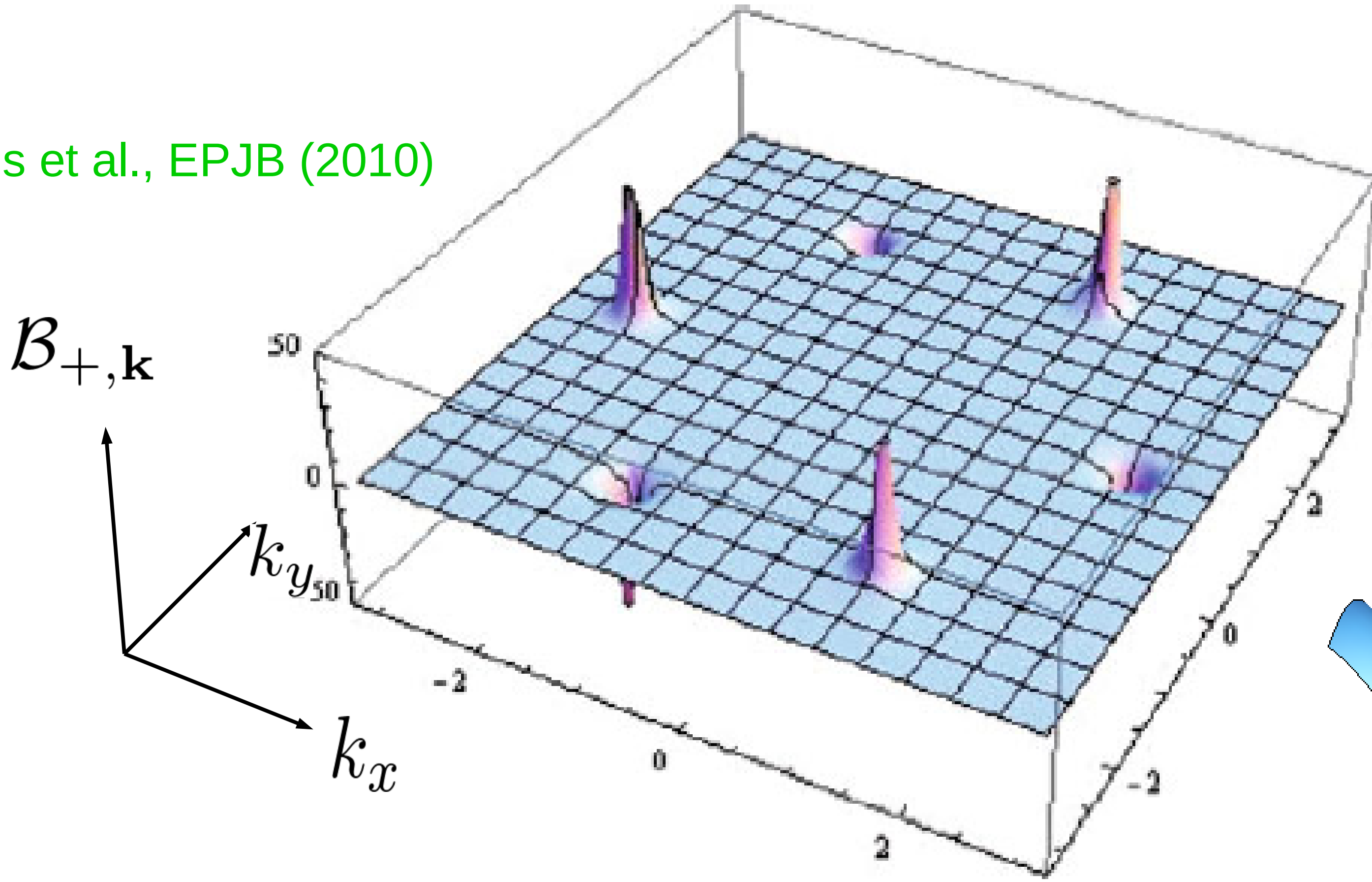


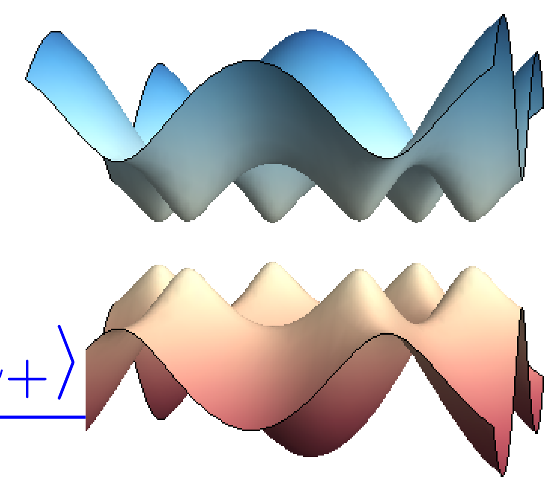
sum rule:

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

Berry curvature for insulating graphene

Fuchs et al., EPJB (2010)





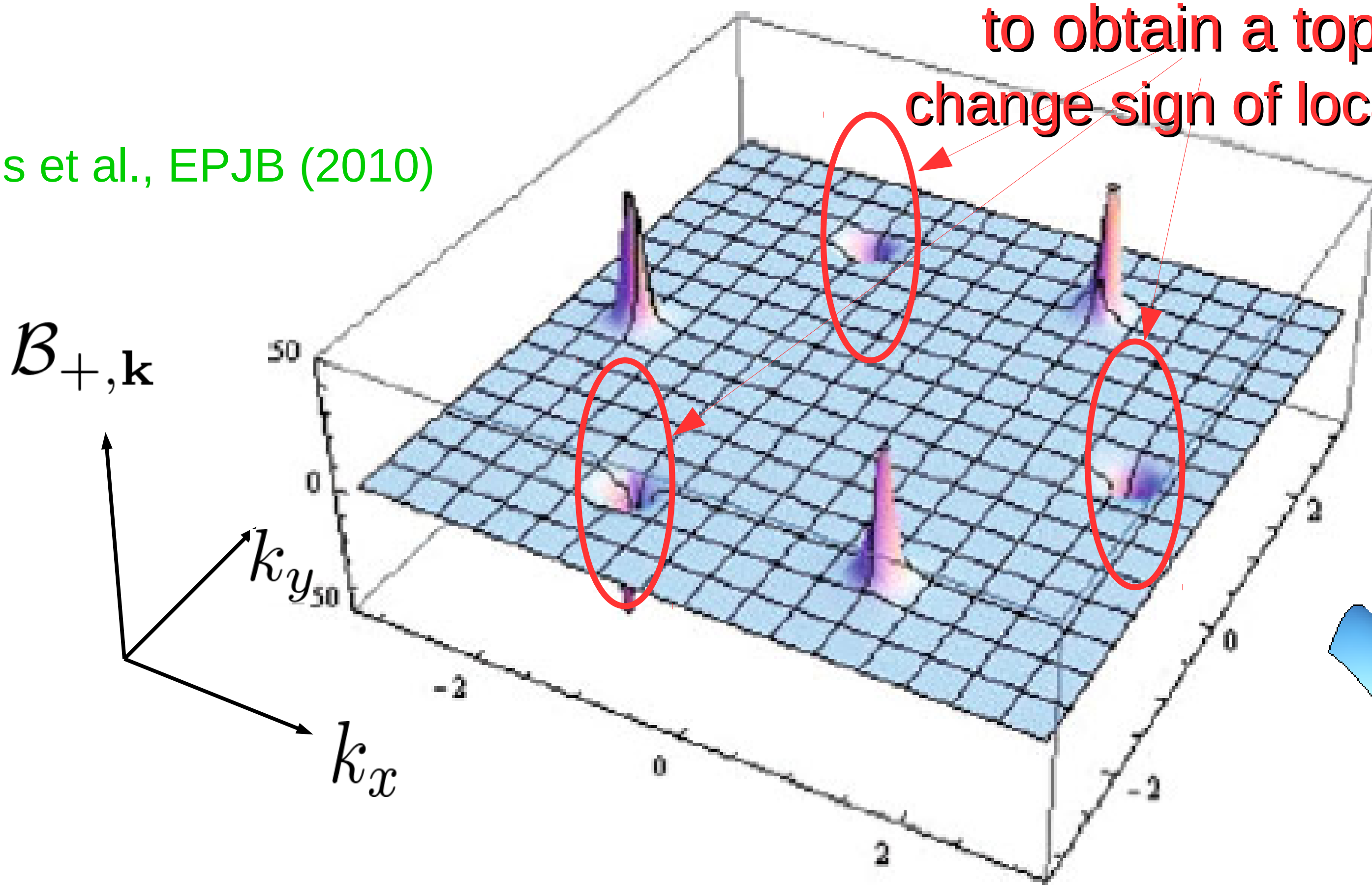
$$\mathcal{B}^{\sigma}_{+}(\mathbf{k}) = i\epsilon^{\sigma\mu\nu}\frac{\langle u_+|\partial_{k_\mu}H(\mathbf{k})|u_-\rangle\langle u_-|\partial_{k_\nu}H(\mathbf{k})|u_+\rangle}{[E_+(\mathbf{k})-E_-(\mathbf{k})]^2}$$

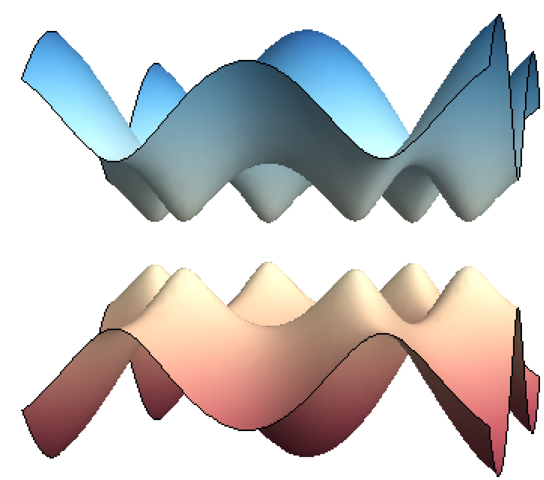
Berry curvature concentrated around Dirac points

Berry curvature for insulating graphene

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

Fuchs et al., EPJB (2010)





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

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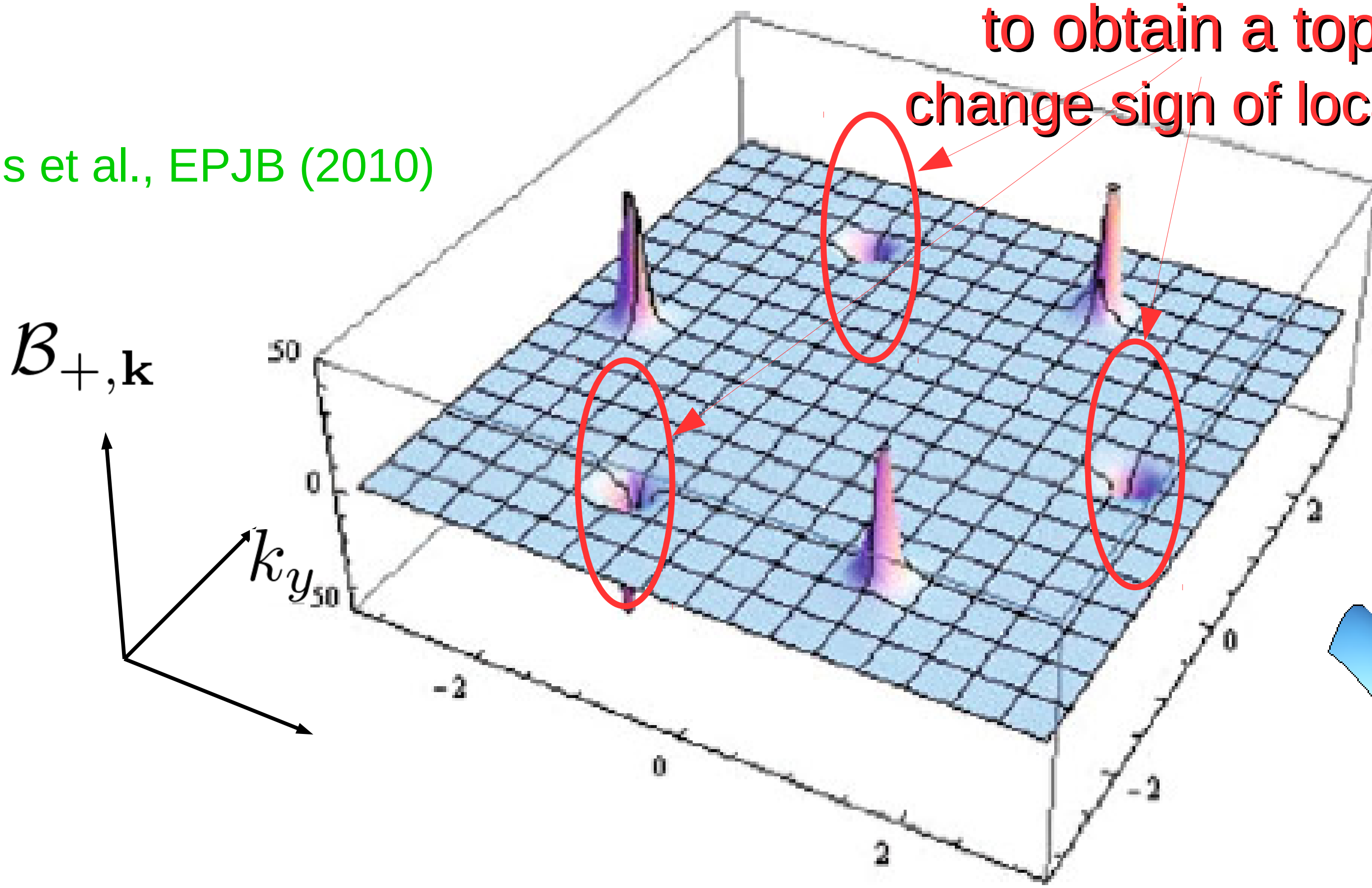
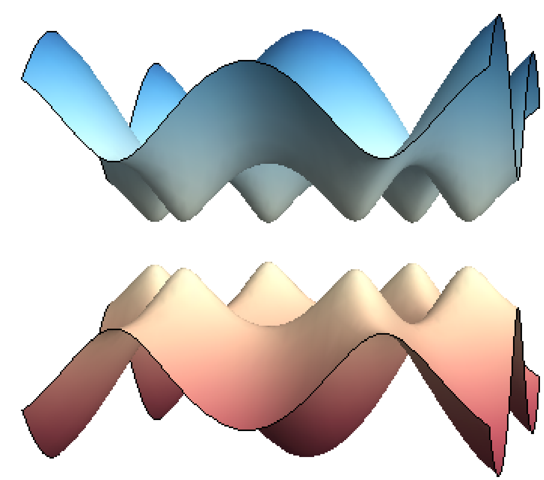


→ local gap inversion



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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:

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

→ *Chern number:*

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

“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

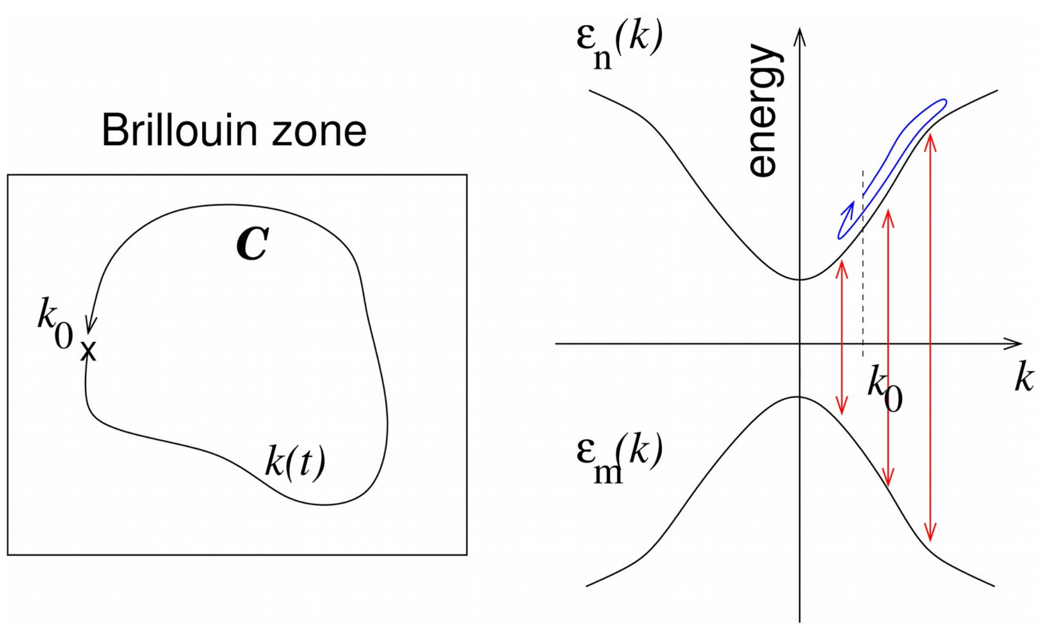
$$\mathcal{B}_{\sigma,\lambda,\xi}(\mathbf{q}) = -\frac{\lambda\sigma\xi}{2}\frac{\hbar^2 v^2 \Delta}{(\Delta^2 + \hbar^2 v^2 q^2)^{3/2}} \quad \xrightarrow{\mathbf{q}\to 0} \quad -\frac{\lambda\sigma\xi}{2}\ell_C^2$$

Berry curvature of a massive Dirac fermion → correlations

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

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

→ “minimal” length scale



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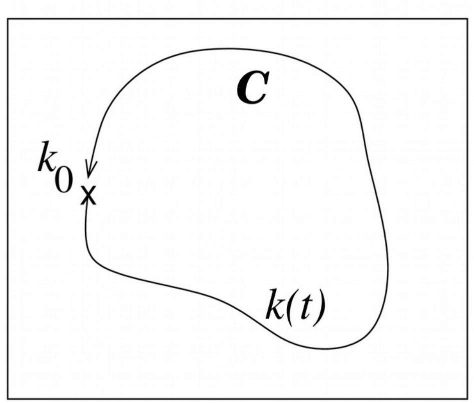
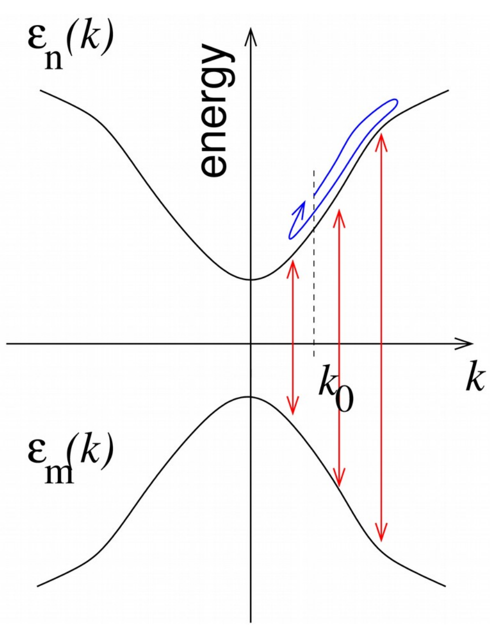
Brillouin zone





→ “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

Berry curvature of a massive Dirac fermion → correlations

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

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

→ 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***

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

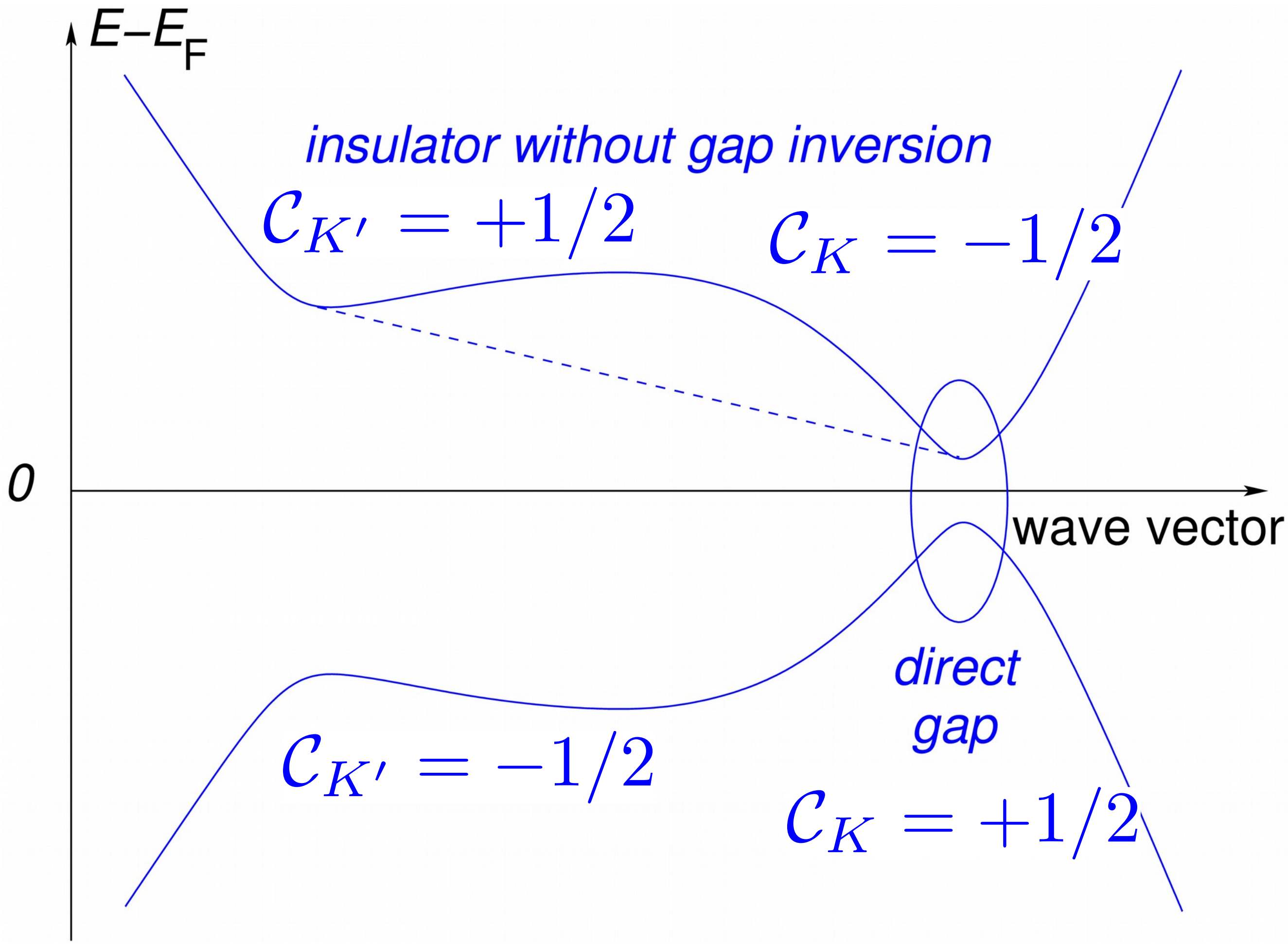
$$\alpha^* = \frac{e^2}{\hbar \epsilon v}$$

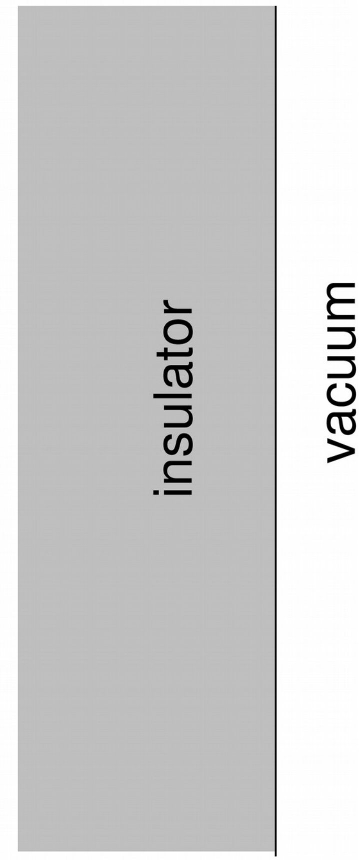
effective
fine-structure constant

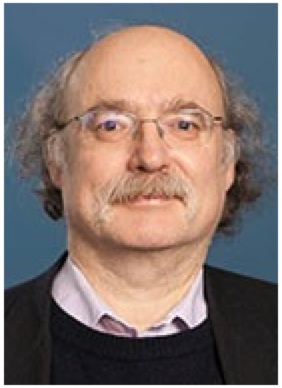
$$a_B^* = \frac{\hbar^2 \epsilon}{m_D e^2}$$

effective
Bohr radius

Haldane model (broken time-reversal symmetry, 1988)



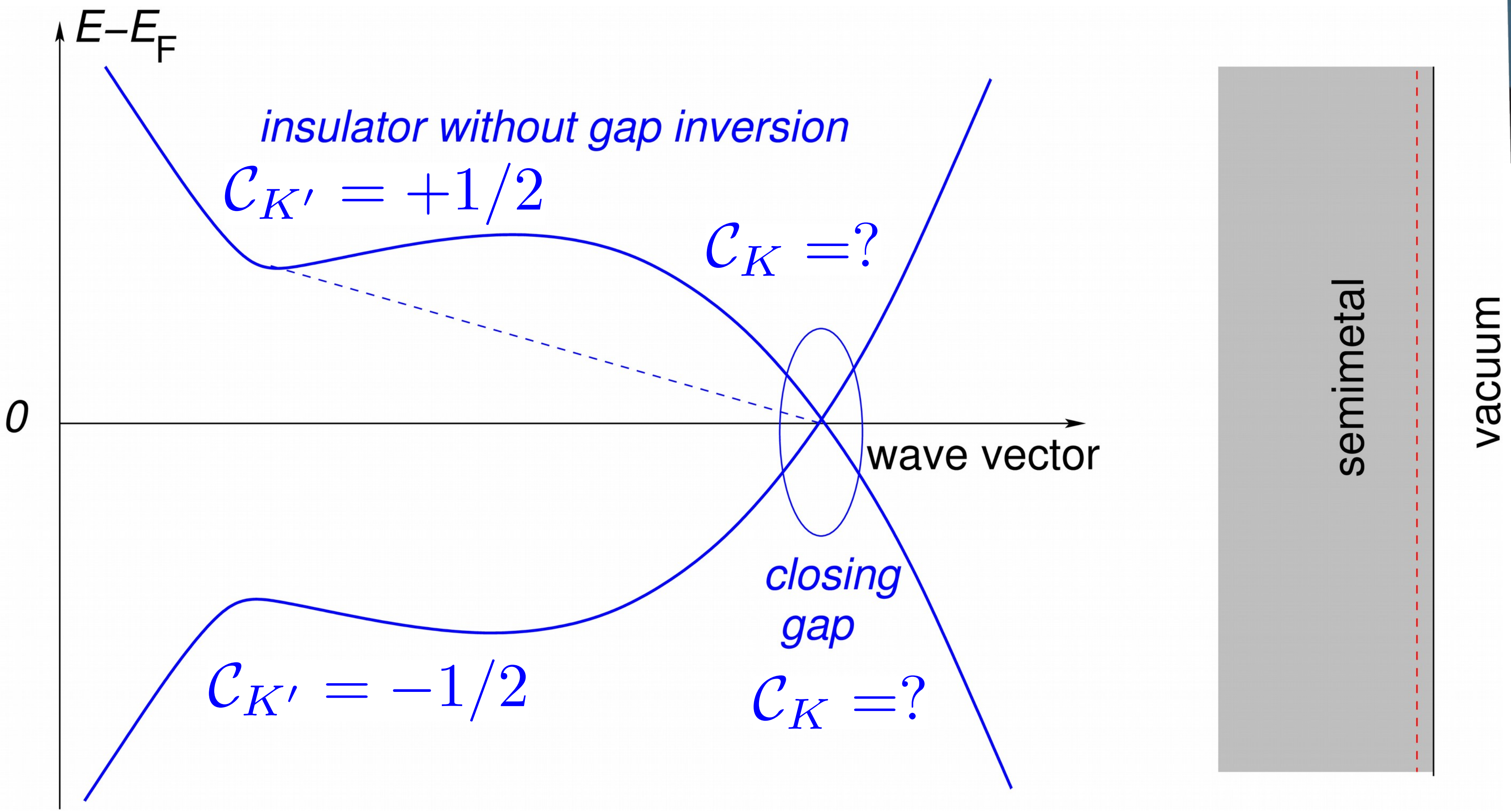




Broken TR symmetry : $E(\mathbf{k}) \neq E(-\mathbf{k})$

modify Dirac points independently from one another

Haldane model (broken time-reversal symmetry, 1988)



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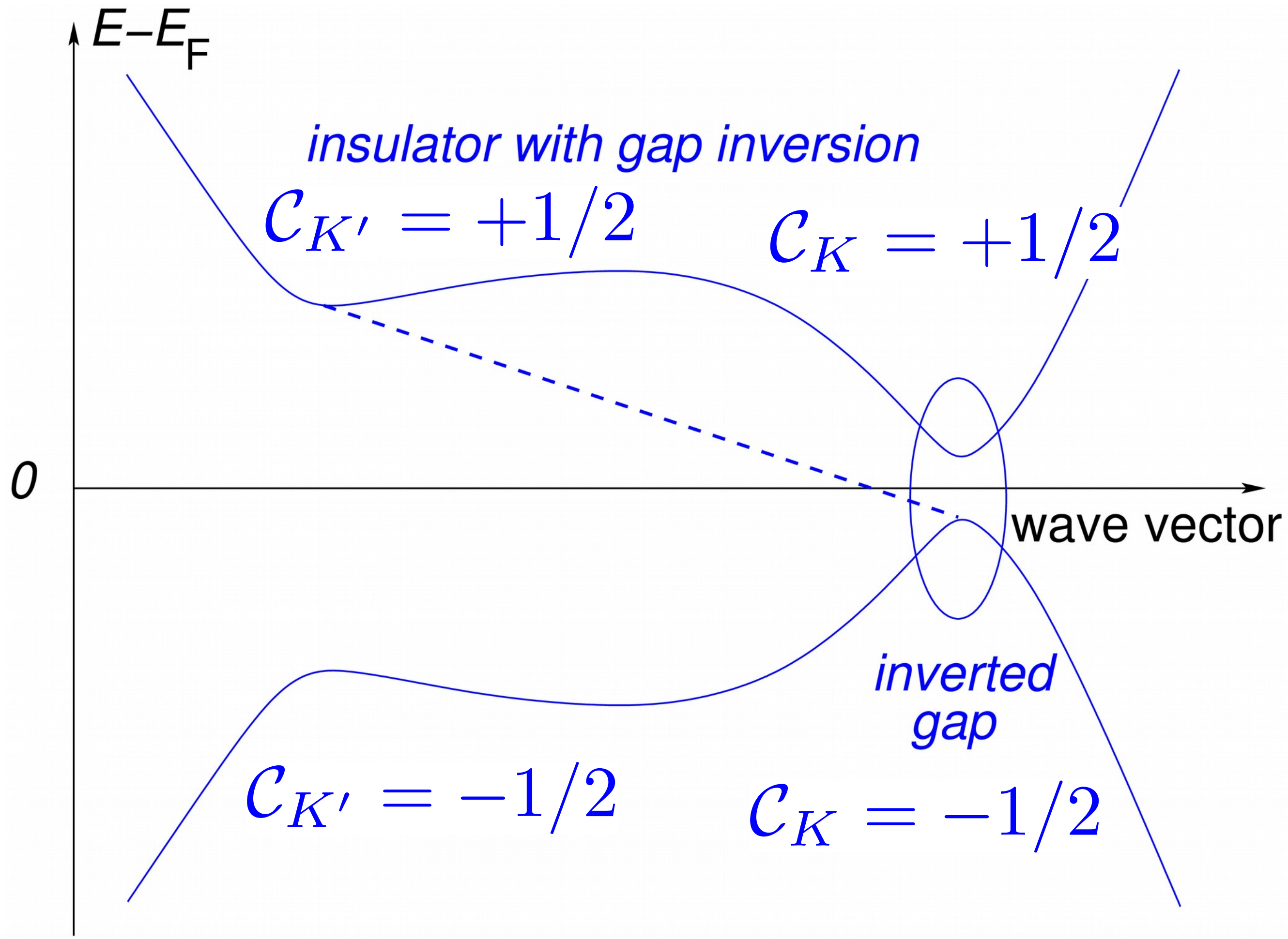
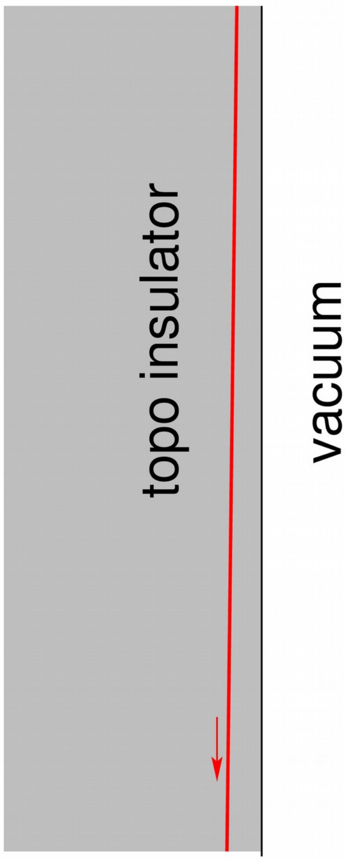




Broken TR symmetry : $E(\mathbf{k}) \neq E(-\mathbf{k})$

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

Intermediate summary

- Topological band transition → (unit) change in Chern number : $\Delta C_n = \pm 1$
- <u>(N.B.:</u> transitions with changes larger than one are possible)
- Continuum description of band closing via massive Dirac fermions with *half Chern number* and *gap inversion :*

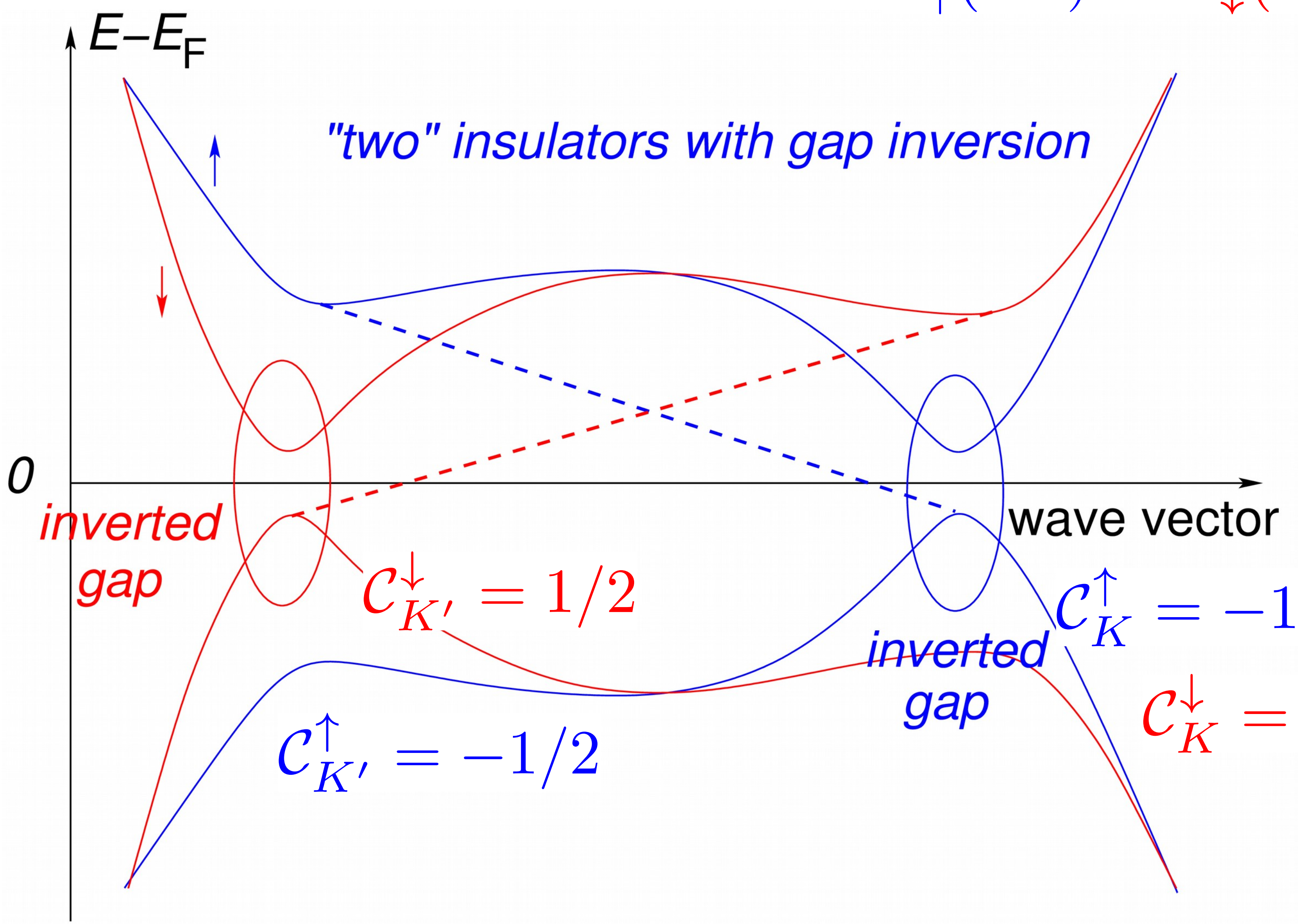
$$\mathcal{C} = +1/2 \to -1/2 \quad \text{or} \quad \mathcal{C} = -1/2 \to +1/2$$

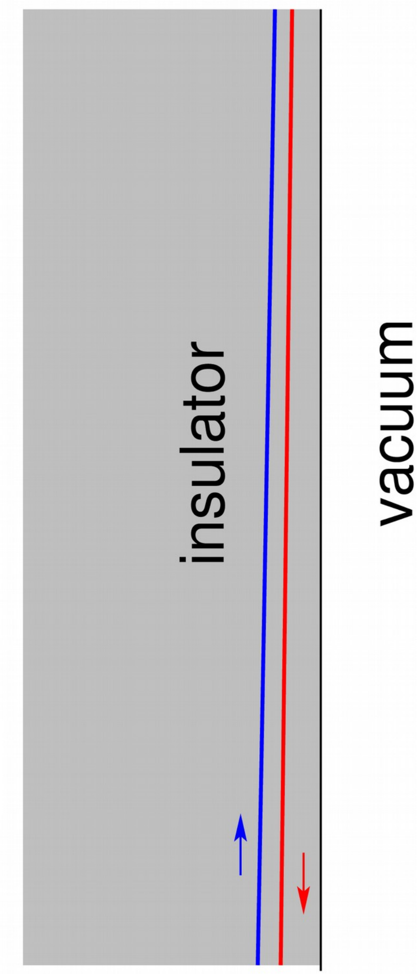
$$\Rightarrow \boxed{\Delta C_n = \Delta \mathcal{C} = \pm 1}$$

Kane-Mele model (2005)
→ TR symmetry respected

profit from spin !

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





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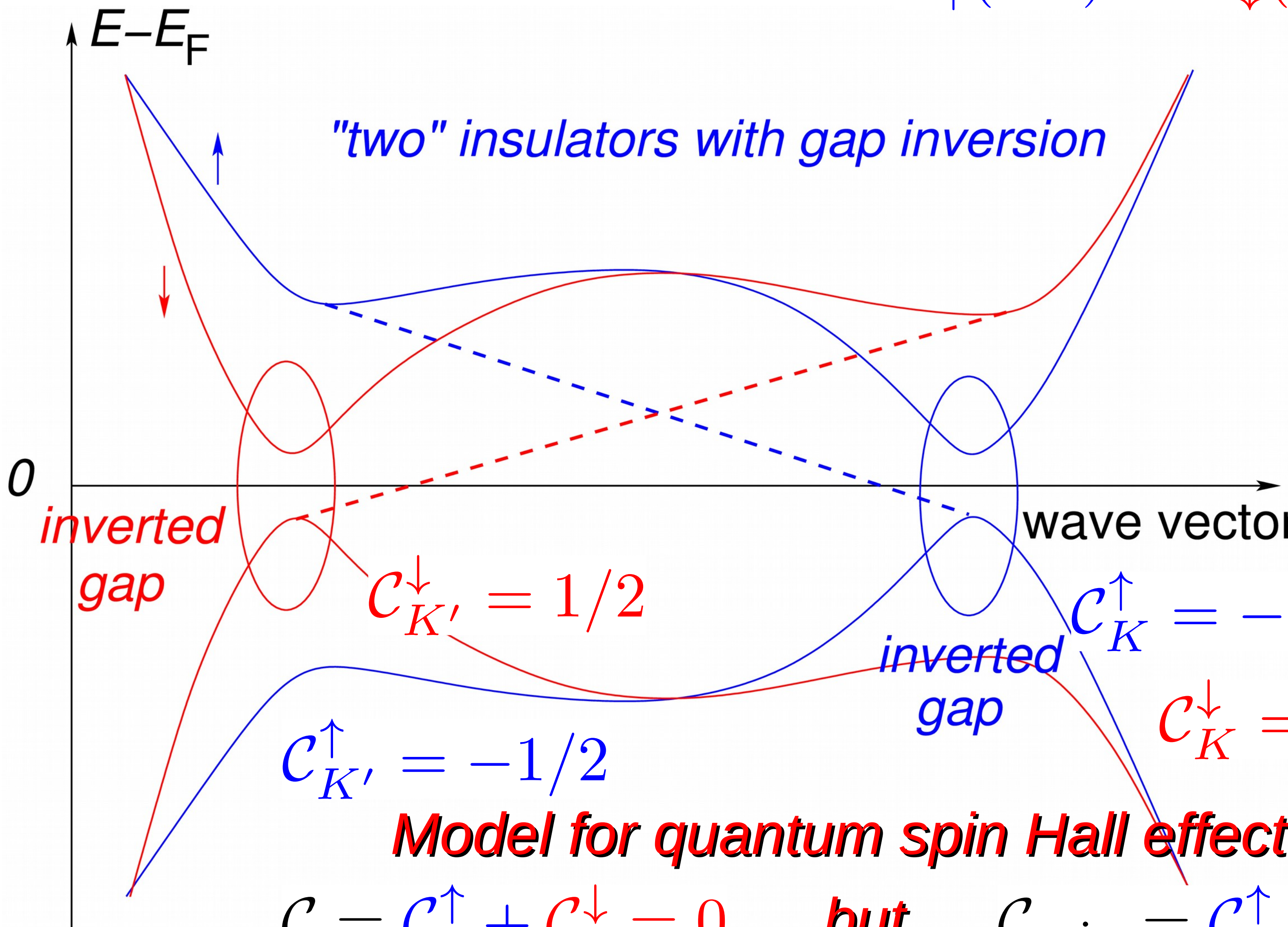

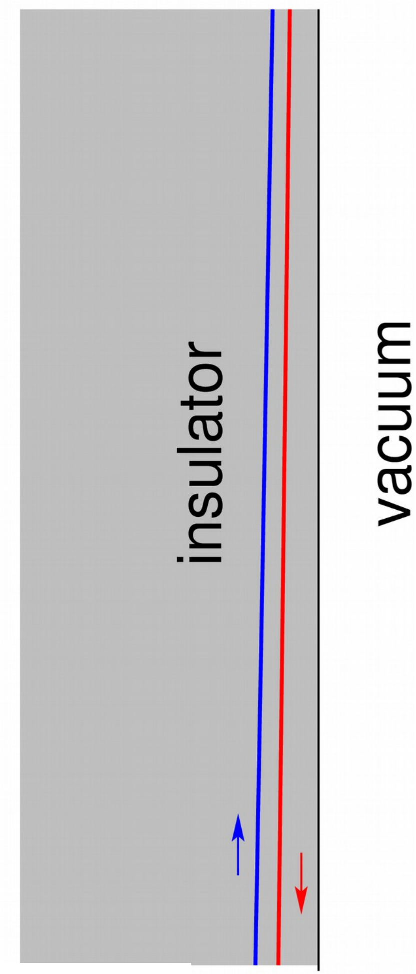

Model for quantum spin Hall effect

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

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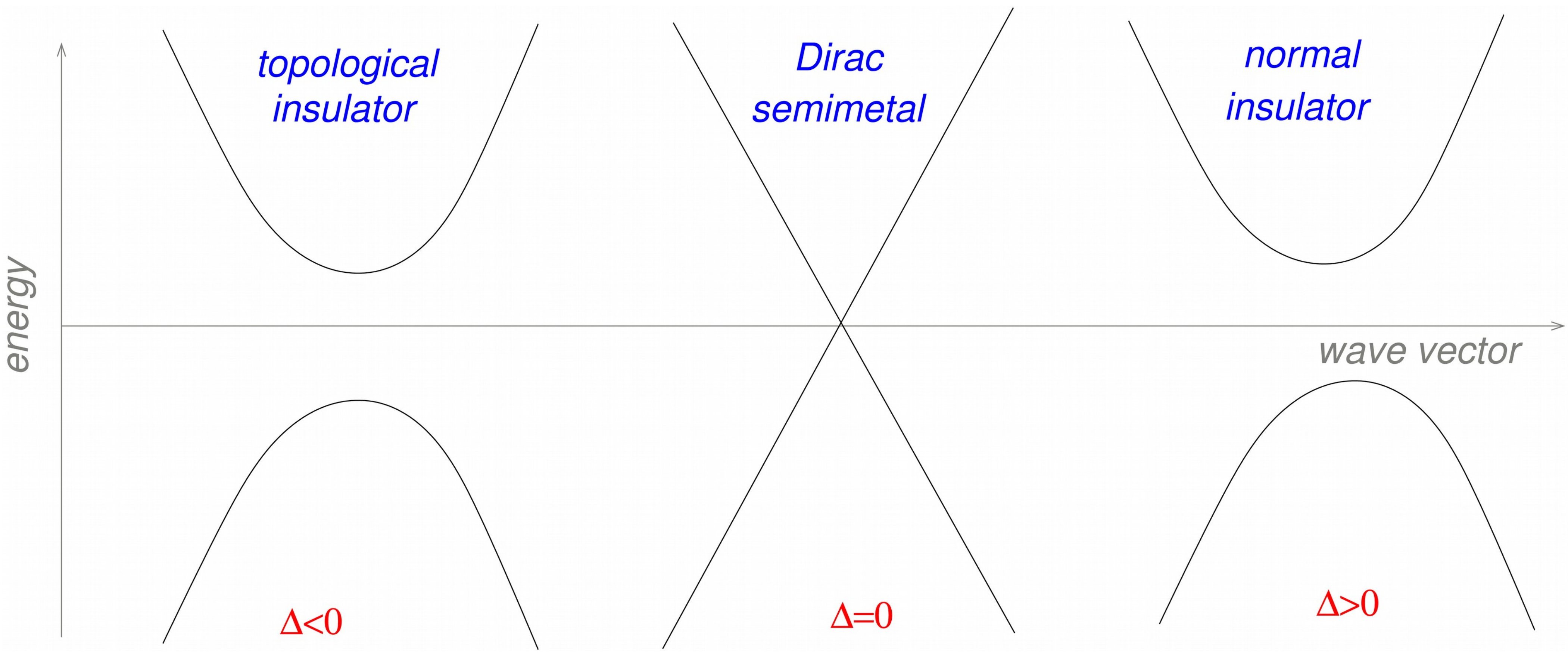
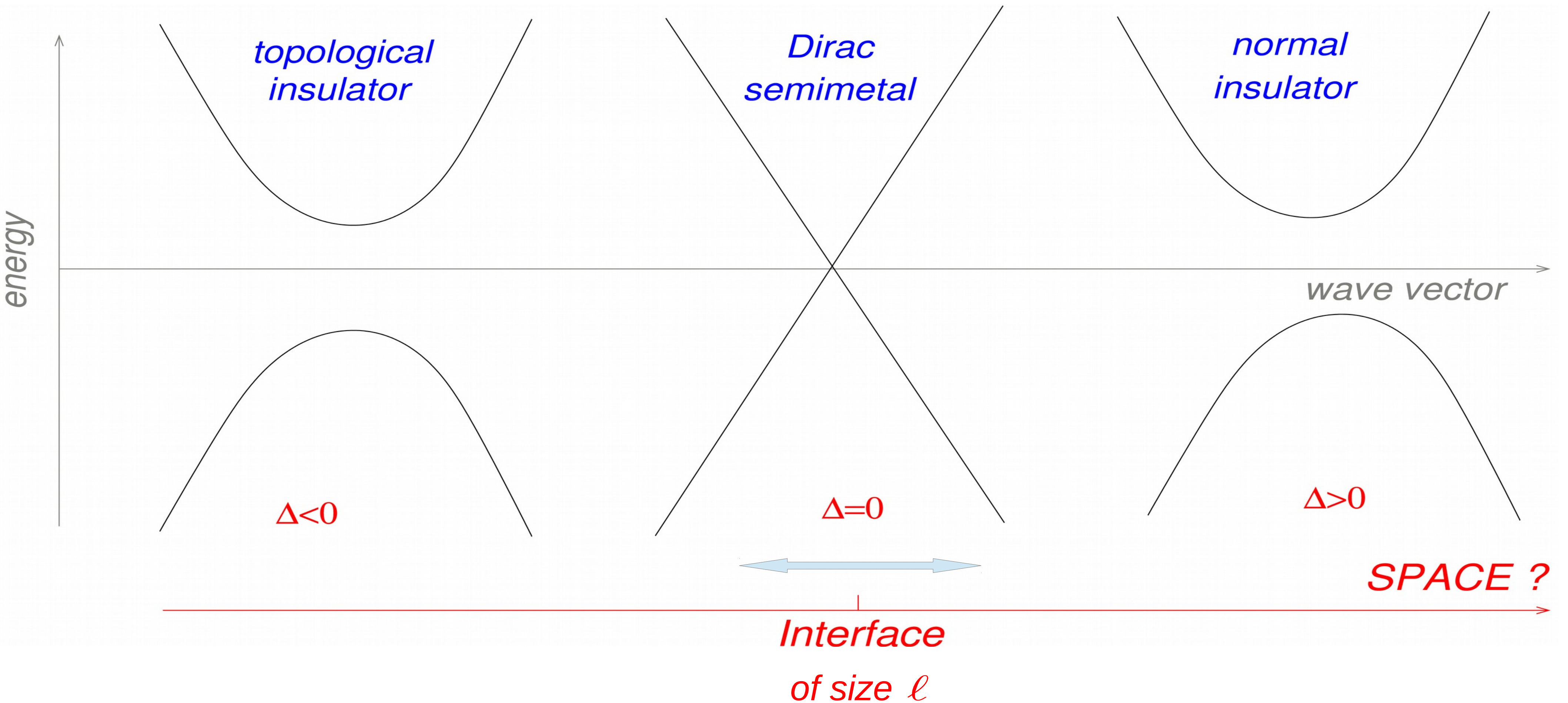
How can we use this to describe an interface ?



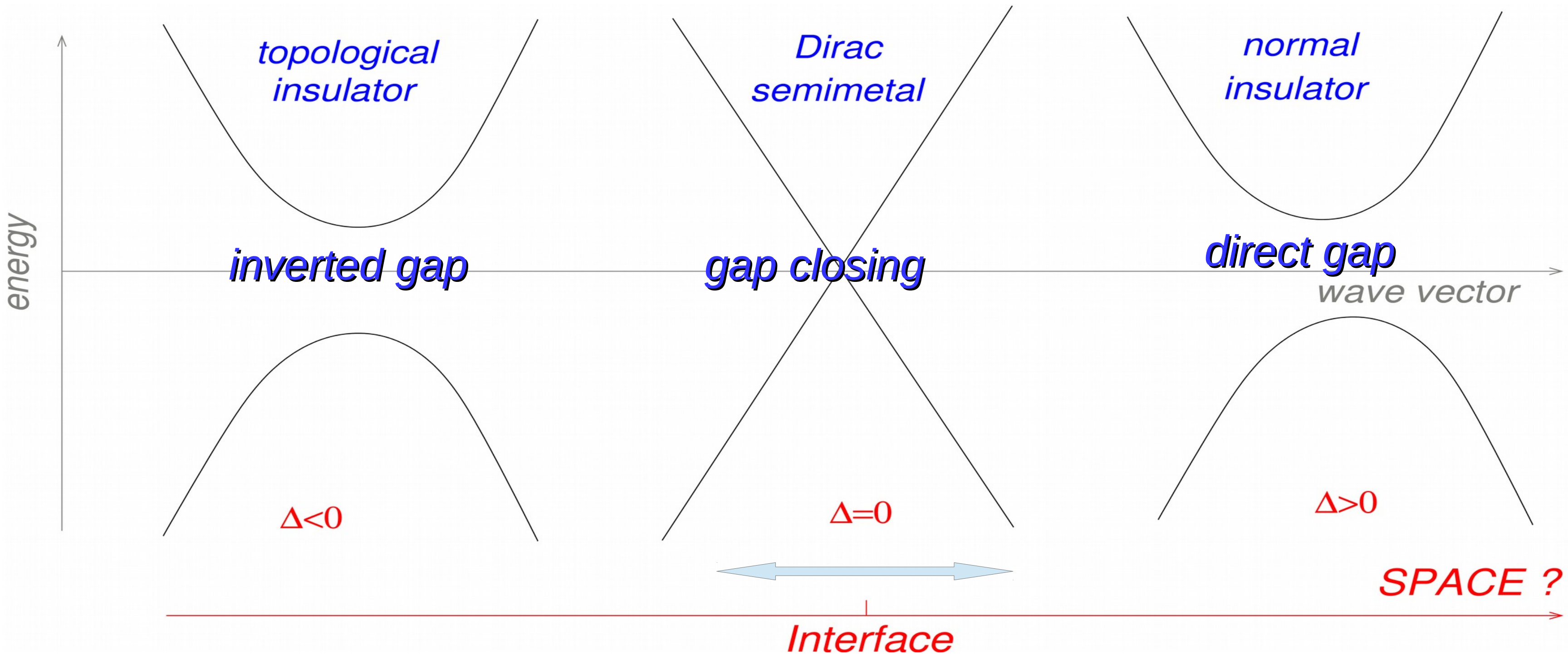
in parameter space

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)

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

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

… reminiscent of what ?

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

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

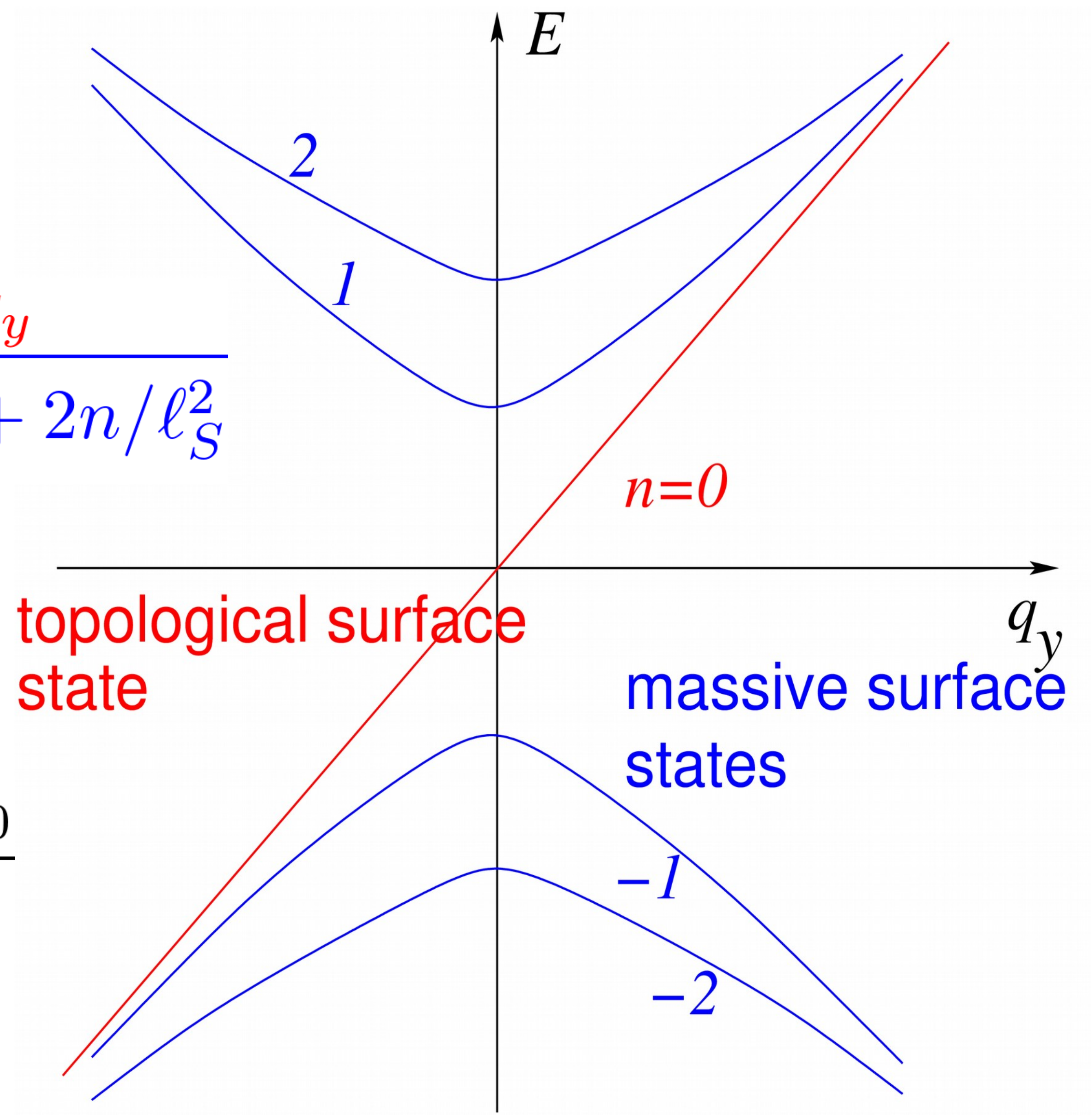
surface states ~ Landau levels

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

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 $\dfrac{\partial E_0}{\partial q_y}$

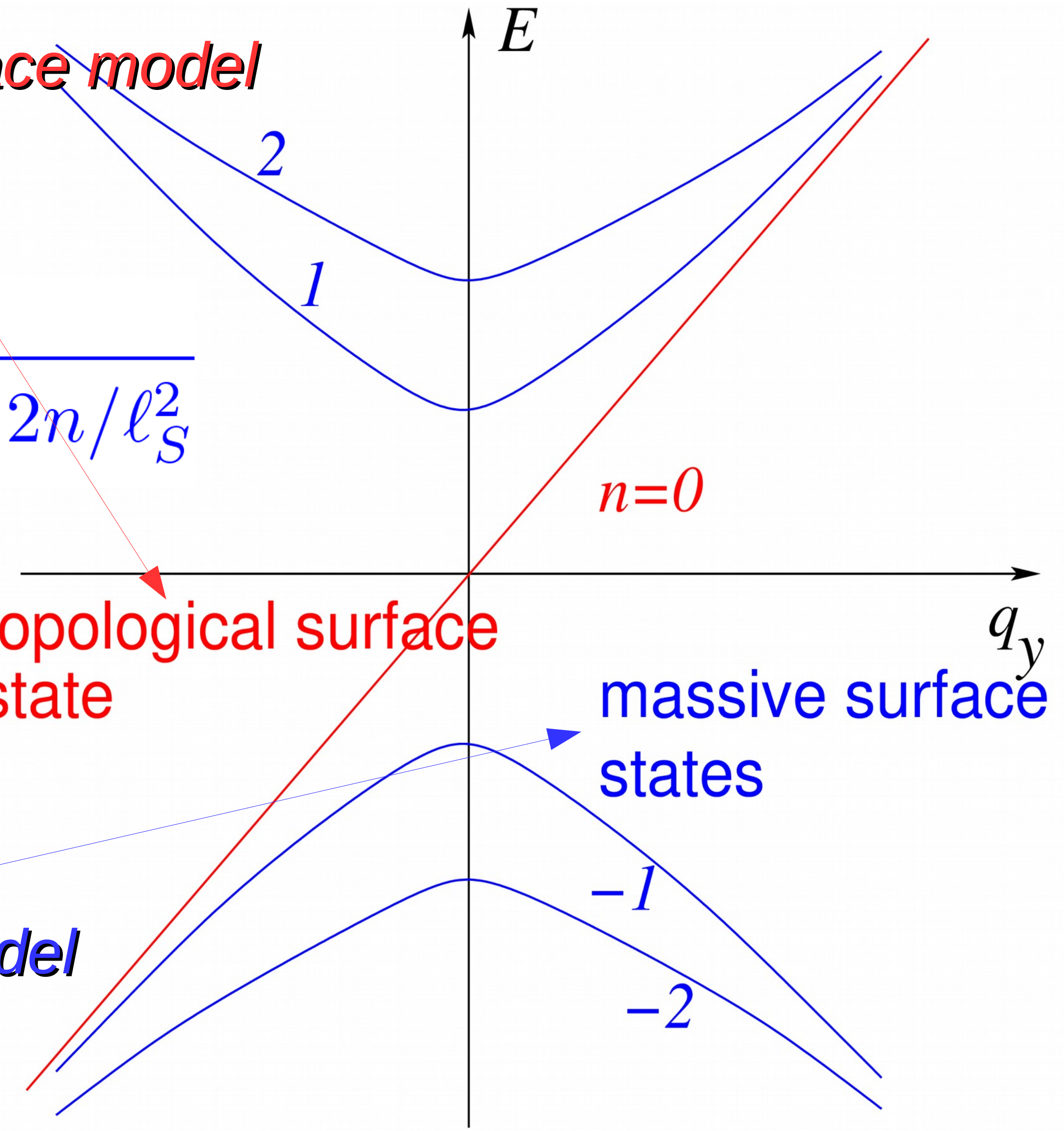


Surface (edge) states

independent of surface model

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

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



topological surface state

massive surface states

depends on surface model

Surface (edge) states

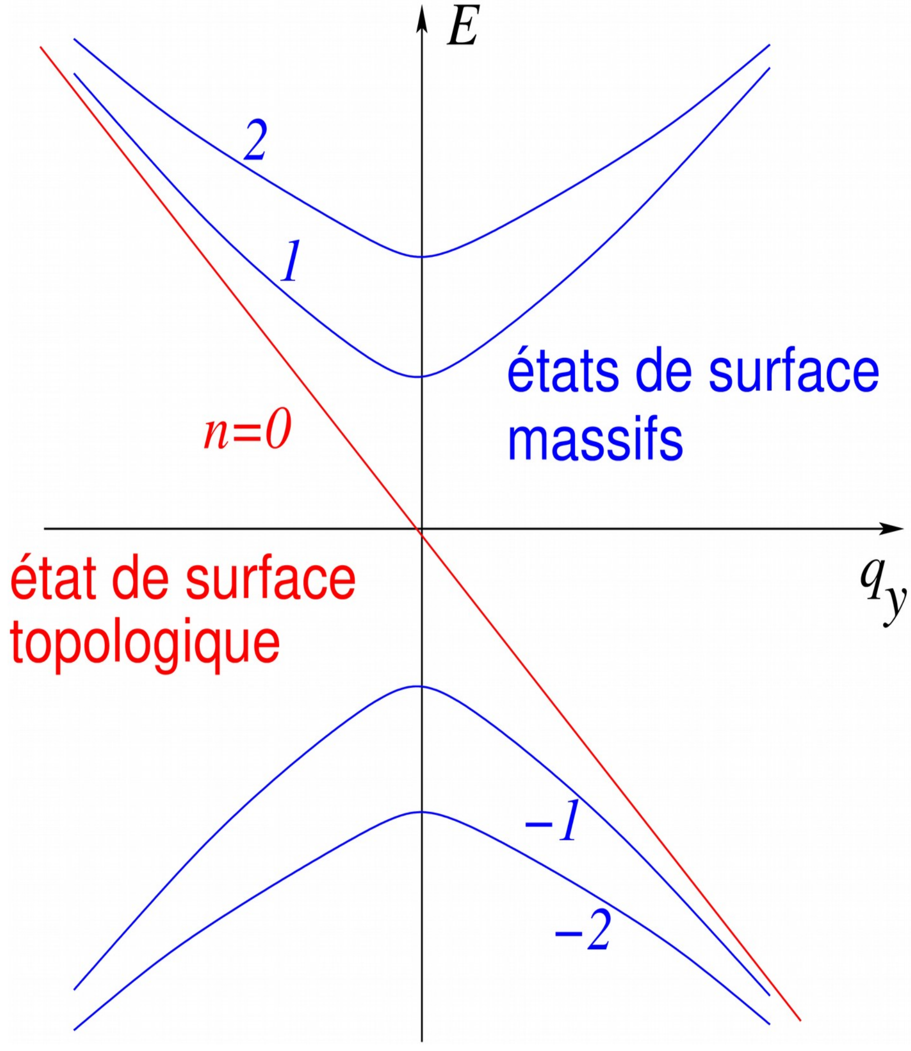
- How to change sign of chirality:

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

$$\xi \to -\xi$$

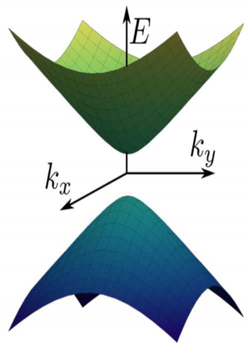
→ changing the edge (~ flipping orientation of “magnetic field”)

$$\ell \to -\ell$$



Surface states in 3D materials

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



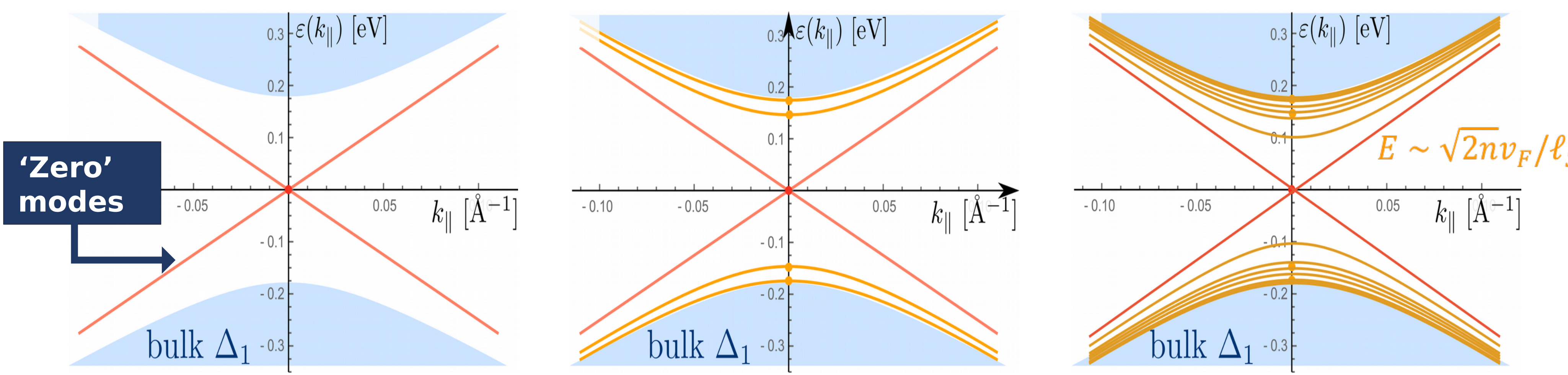
Complication in 3D: 4x4 Hamiltonian

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

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

ℓ/ξ

abrupt | intermediate | very smooth



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

Intermezzo: electrons in crossed B and E fields (I)

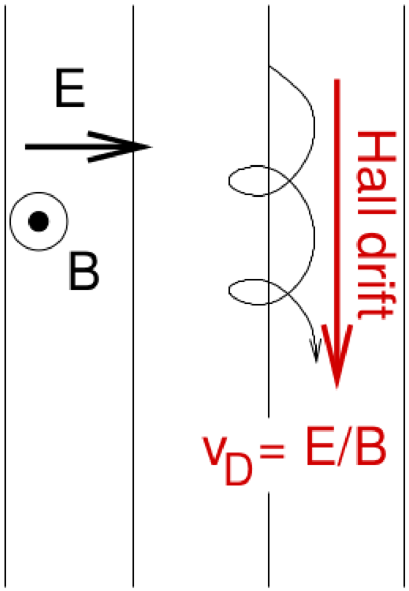
2D electrons in a perpendicular magnetic $\mathbf{B} = \nabla \times \mathbf{A}$ and inplane electric E fields

$$H_0(\hbar\mathbf{q}) \qquad \rightarrow \qquad H_0(\mathbf{p} + e\mathbf{A}(\mathbf{r})) - eEy$$

- (non-relativistic) Schrödinger fermions

$\rightarrow$ Galilei transformation to comoving frame of reference v_D

- Landau levels



$$\epsilon_{n,k} = \hbar\frac{eB}{m}\left(n + \frac{1}{2}\right) - \hbar v_D k$$

Intermezzo: electrons in crossed B and E fields (I)

2D electrons in a perpendicular magnetic $\mathbf{B} = \nabla \times \mathbf{A}$ and inplane electric E fields

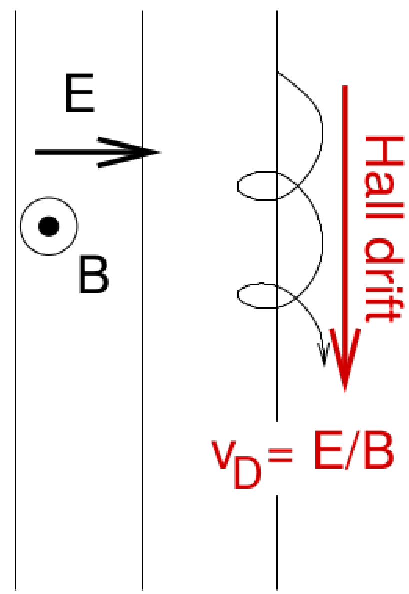
$$H_0(\hbar\mathbf{q}) \qquad \rightarrow \qquad H_0(\mathbf{p} + e\mathbf{A}(\mathbf{r})) - eEy$$

- relativistic electrons (graphene)

$\rightarrow$ Lorentz transformation to frame of reference v_D [Lukose et al., PRL 2007]

$$B \quad \rightarrow \quad B' = B\sqrt{1 - (v_D/v_F)^2}$$

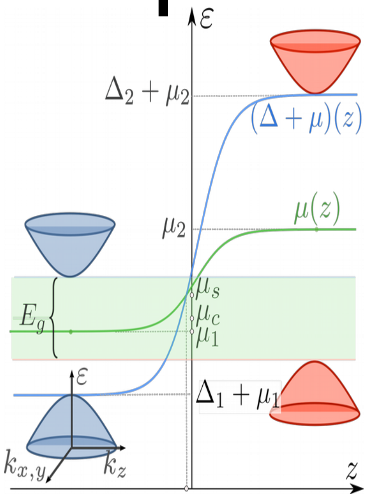
$$\epsilon \quad \rightarrow \quad \epsilon' \propto 1/l'_B \propto \sqrt{B'}$$



$\rightarrow$ energy in lab frame

$$\epsilon_{\pm n,k} = \pm\frac{\hbar v_F[1 - (v_D/v_F)^2]^{3/4}}{l_B}\sqrt{2n} - \hbar v_D k$$

Special relativity in surface states

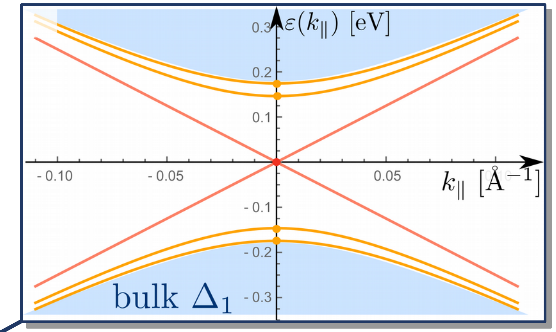


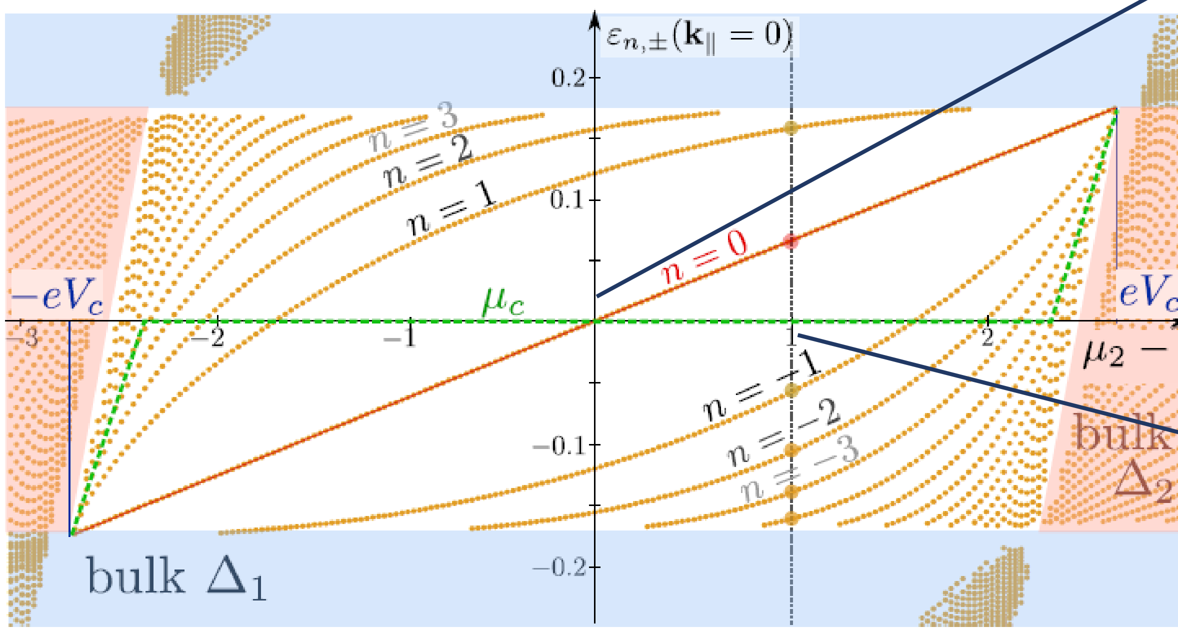
$$H = \color{blue}{\boldsymbol{V(z)}}\,\mathbb{1} + v_F(k_x\ \mathbb{1}\otimes\tau_y + (k_y\,\sigma_x - k_x\sigma_y)\otimes\tau_x) + \color{red}{\boldsymbol{\Delta(z)}}\,\mathbb{1}\otimes\tau_z$$

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

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

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





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

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