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How far can one boost Lorentz… in Dirac matter

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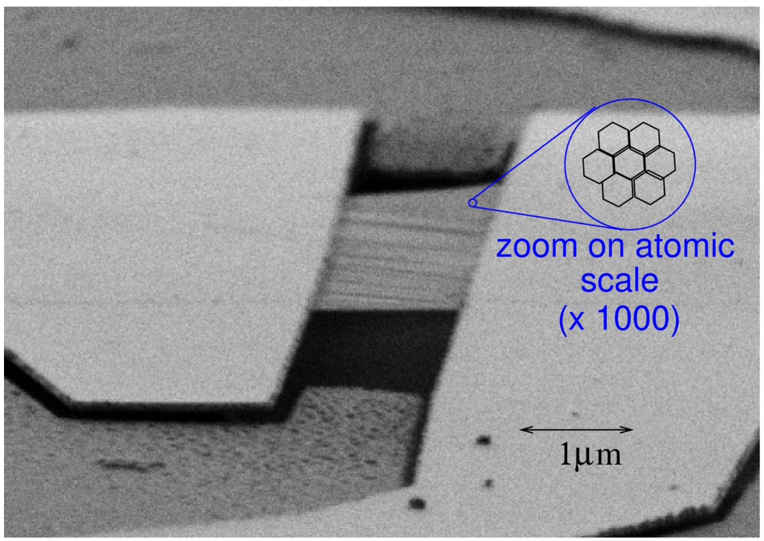
Prehistory: Frédéric Piéchon, Gilles Montambaux, Jean-Noël Fuchs

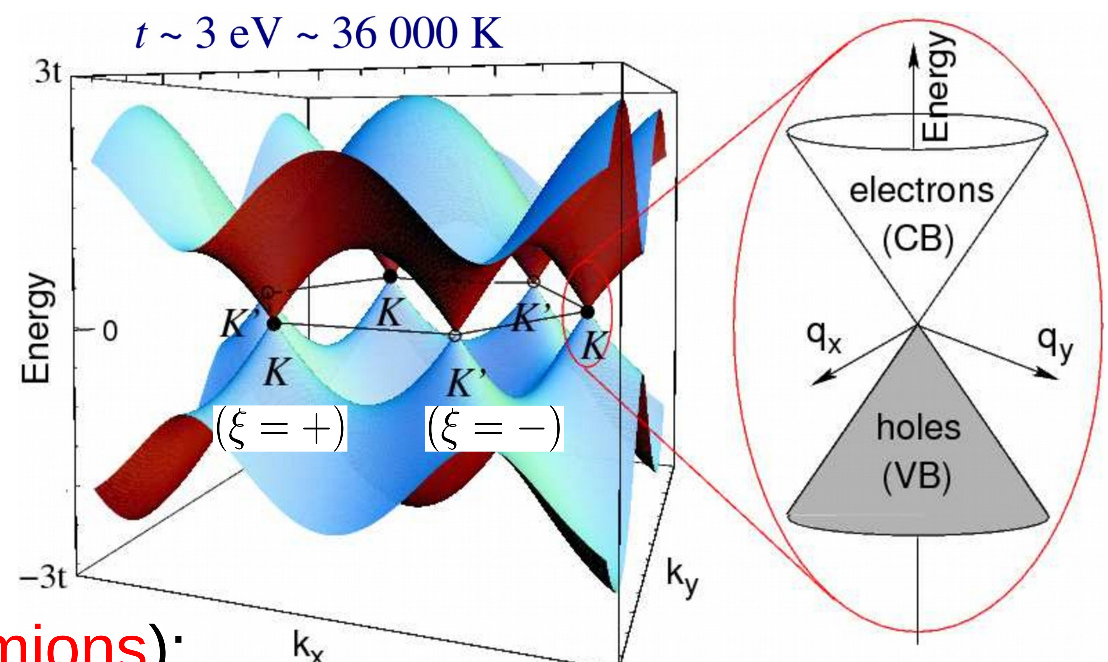
Collaborators (exp): *Jan Wyzula*, Milan Orlita, and… (LNCMI-Grenoble)
Andreas Inhofer, Bernard Plaçais, and… (LPENS)
Gautier Krizman, Joaquín Bermejo-Ortiz, Yves Guldner, ...

Le Studium Workshop, Tours, 05/07/2023

Emergence of relativistic (Dirac) electrons in graphene (2D graphite)



Chuan Li, physique mésoscopique, LPS, Orsay



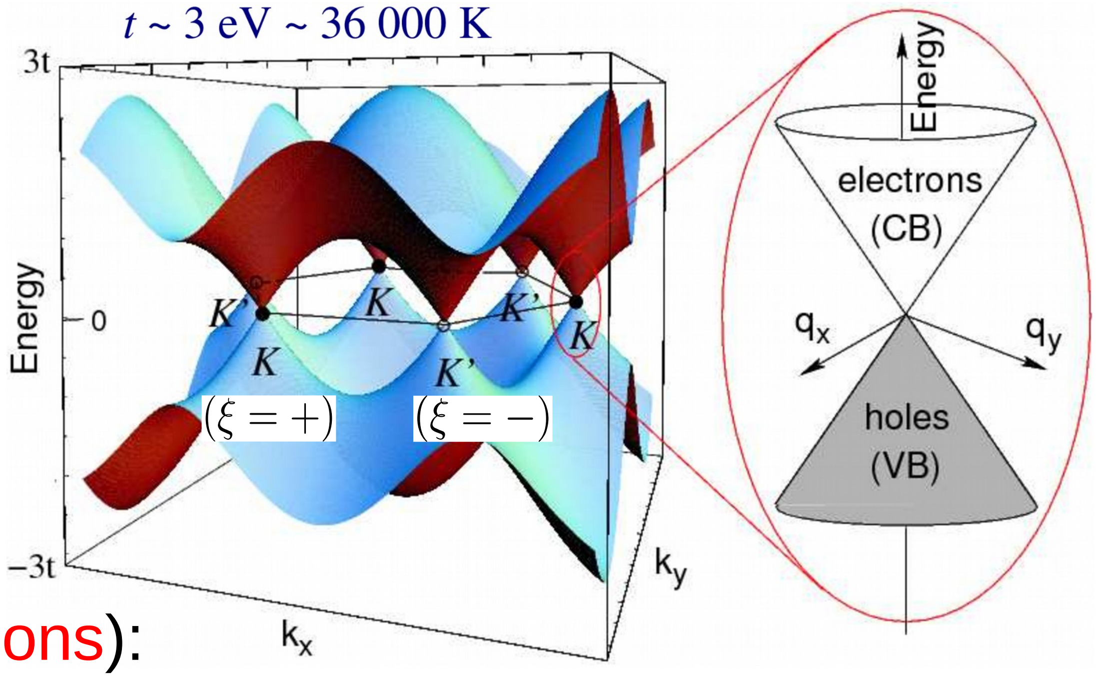
Dirac Hamiltonian (massless fermions):

$$H_\xi(\mathbf{q}) = \begin{pmatrix} 0 & \hbar v_F(\xi q_x - i q_y) \\ \hbar v_F(\xi q_x + i q_y) & 0 \end{pmatrix}$$

Emergence of relativistic (Dirac) electrons in graphene (2D graphite)

Dirac (relativistic) matter :

Electrons (in the vicinity of the Fermi level) are described in terms of a *Dirac equation* or ***variants*** of it instead of a *Schrödinger equation*.



speed of light → Fermi velocity

$$c \to v_F$$

Dirac Hamiltonian (massive fermions):

$$H_\xi(\mathbf{q}) = \begin{pmatrix} \Delta & \hbar v_F(\xi q_x - i q_y) \\ \hbar v_F(\xi q_x + i q_y) & -\Delta \end{pmatrix}$$

graphene :

$$\Delta = 0$$

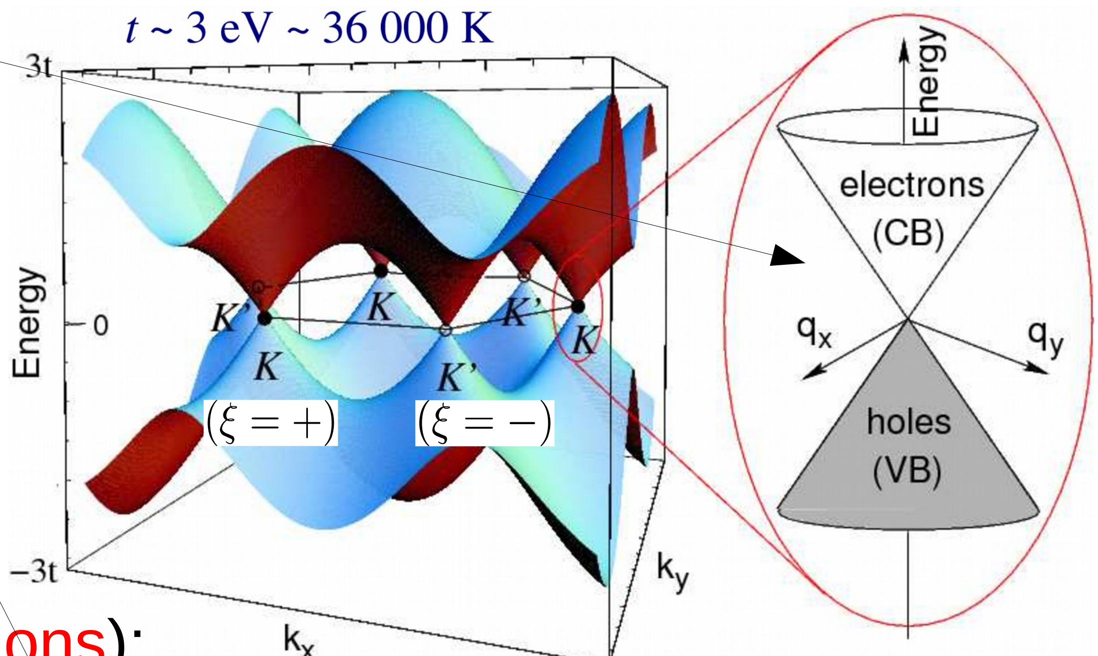
Emergence of relativistic (Dirac) electrons in graphene (2D graphite)

→ *relativistic quantum mechanics beyond the spectrum ?*

→ *what about Lorentz covariance ?*

speed of light → Fermi velocity

$$c \longrightarrow v_F$$



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$$\Delta = 0$$

Outline of the talk

- (Pseudo-)relativity in condensed matter: the example of electrons in crossed magnetic and electric fields
- Tilted Dirac cones and relation with pseudo-relativity and Lorentz boosts
- Unveiling Lorentz boosts in magneto-optical spectroscopy
- Pseudo-relativity in surface states of topological matter

Outline of the talk

- *(Pseudo-)relativity in condensed matter: the example of electrons in crossed magnetic and electric fields*
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2D electrons in crossed magnetic and electric fields

Lukose et al., PRL (2007)

Hamiltonian for 2D electrons in crossed fields $\mathbf{B} = B\mathbf{u}_z = \nabla \times \mathbf{A}(\mathbf{r})$

and $\mathbf{E} = E\mathbf{u}_y$

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

2D electrons in crossed magnetic and electric fields

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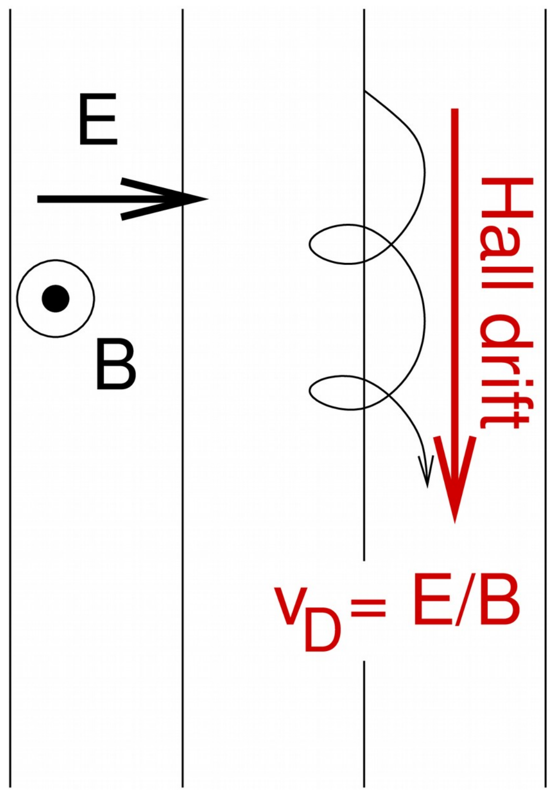
$$H_0(\hbar\mathbf{q}) \to H_0(\mathbf{p} + e\mathbf{A}(\mathbf{r})) - eEy$$

→ Non-relativistic (Schrödinger) fermions: *Galilei transformation* to comoving frame of reference with velocity $v_D = E/B$



→ Landau levels:

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

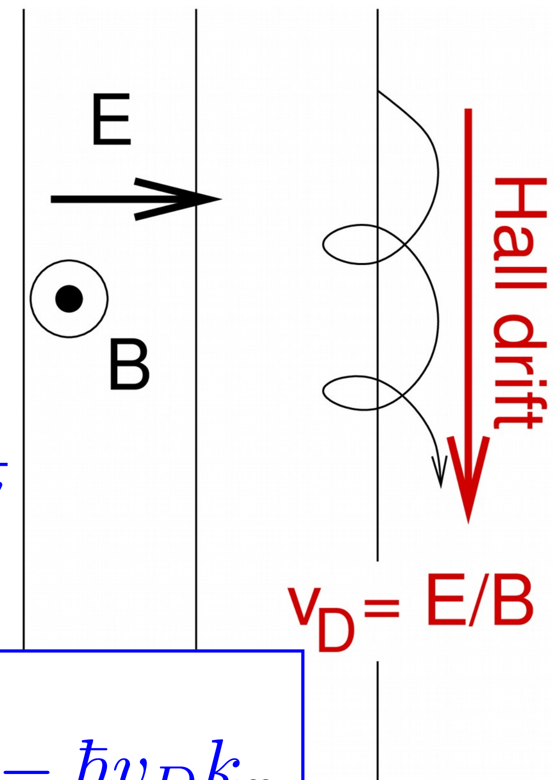
2D electrons in crossed magnetic and electric fields

Lukose et al., PRL (2007)

Hamiltonian for 2D electrons in crossed fields $\mathbf{B} = B\mathbf{u}_z = \nabla \times \mathbf{A}(\mathbf{r})$

and $\mathbf{E} = E\mathbf{u}_y$

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



→ Relativistic (Dirac) fermions:
Lorentz transformation to comoving frame of reference with velocity $v_D = E/B$

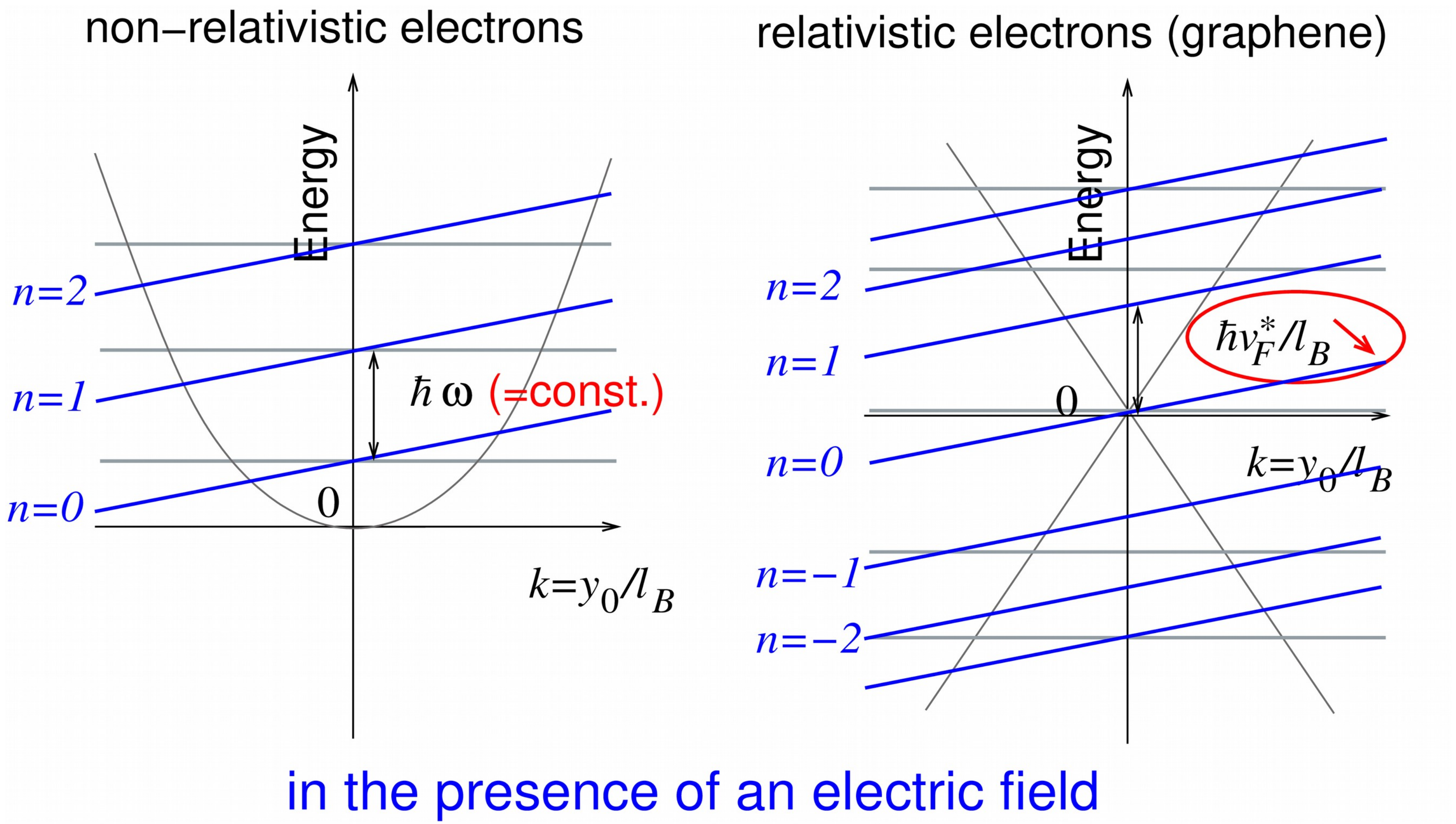
$$B \to B' = B\sqrt{1-(v_D/v)^2}$$

$$\epsilon \to \epsilon' = \epsilon/\sqrt{1-(v_D/v)^2} \propto 1/l_{B'} \propto \sqrt{B'}$$

→ Landau levels (in lab frame):

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

2D electrons in crossed magnetic and electric fields



Cyclotron resonance (theory and exp) in narrow-gap semiconductors (InSb)

Lukose et al., PRL (2007)
Zawadzki et al., PRL (1985)
+ even some papers before

Outline of the talk

- (Pseudo-)relativity in condensed matter: the example of electrons in crossed magnetic and electric fields *(just overture)*
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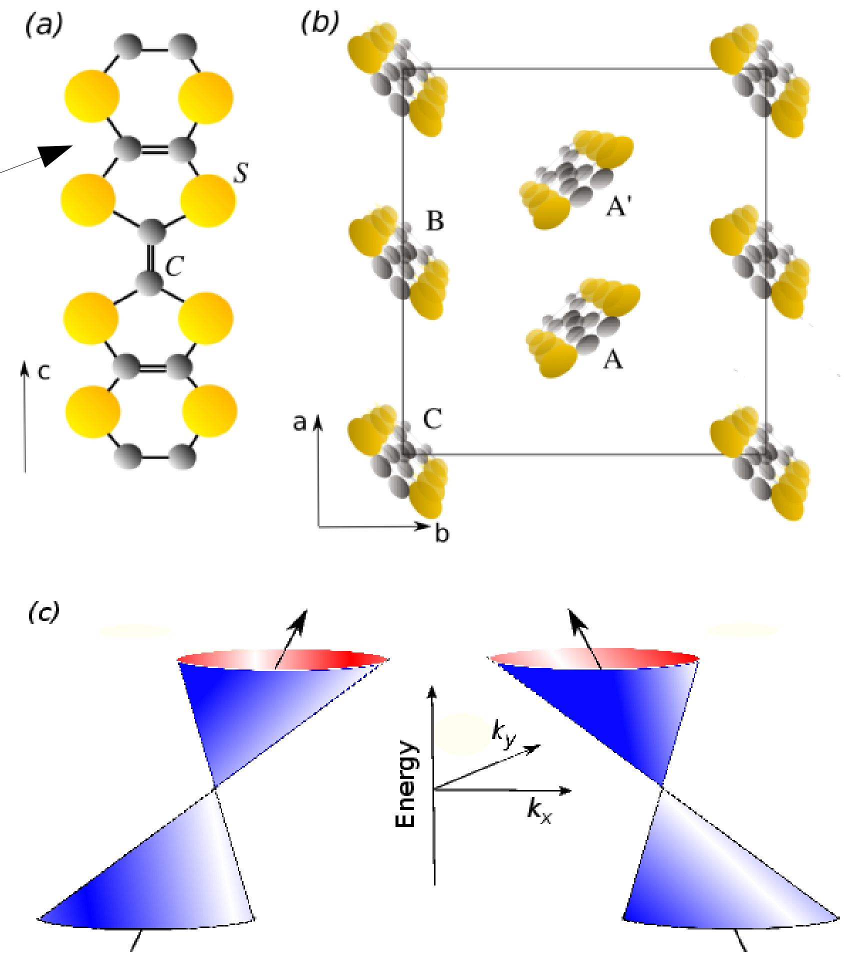
Beyond graphene: tilted Dirac cones in α-(BEDT-TTF)$_2$I$_3$

α-(BEDT-TTF)$_2$I$_3$

BEDT-TTF
=bis(ethylenedithio)tetrafulvalene
(organic molecule)



→ quasi-2D crystal (stacked layers)

→ 4 molecules/unit cell → 4 bands

→ electronic filling: ¾

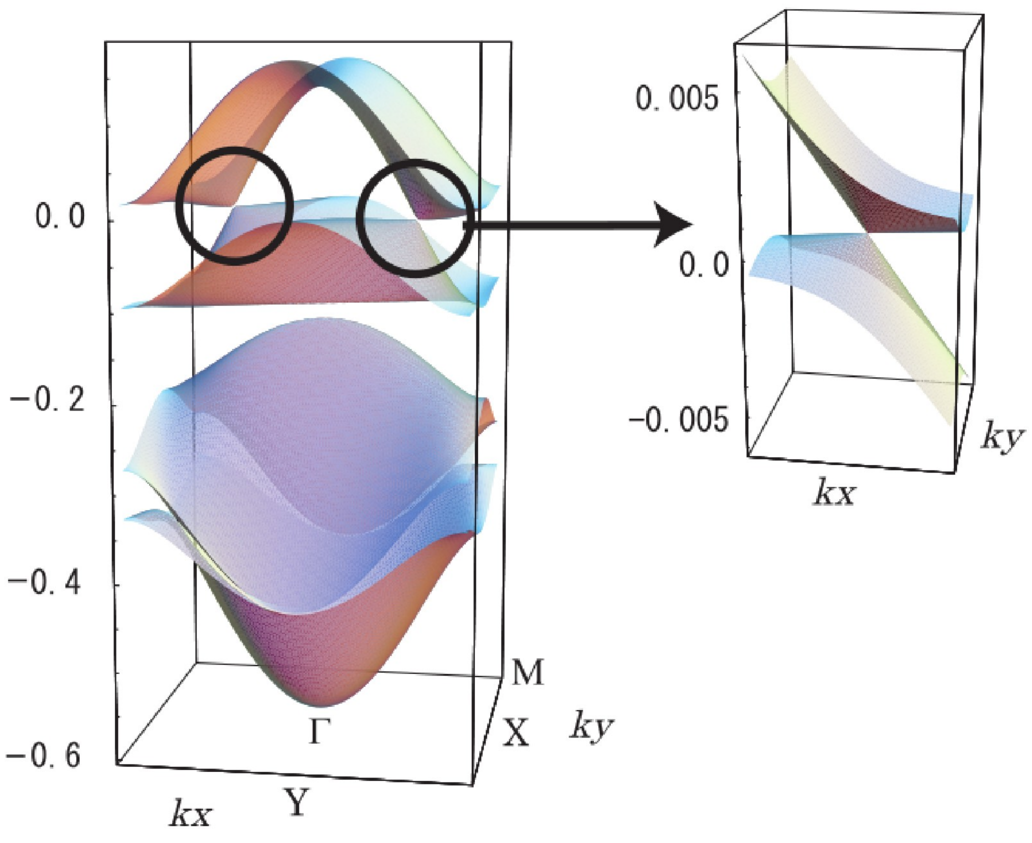
→ hopping parameters $t_i \sim 20 \ldots 140$ meV

→ *Tilted* Dirac semimetal under pressure

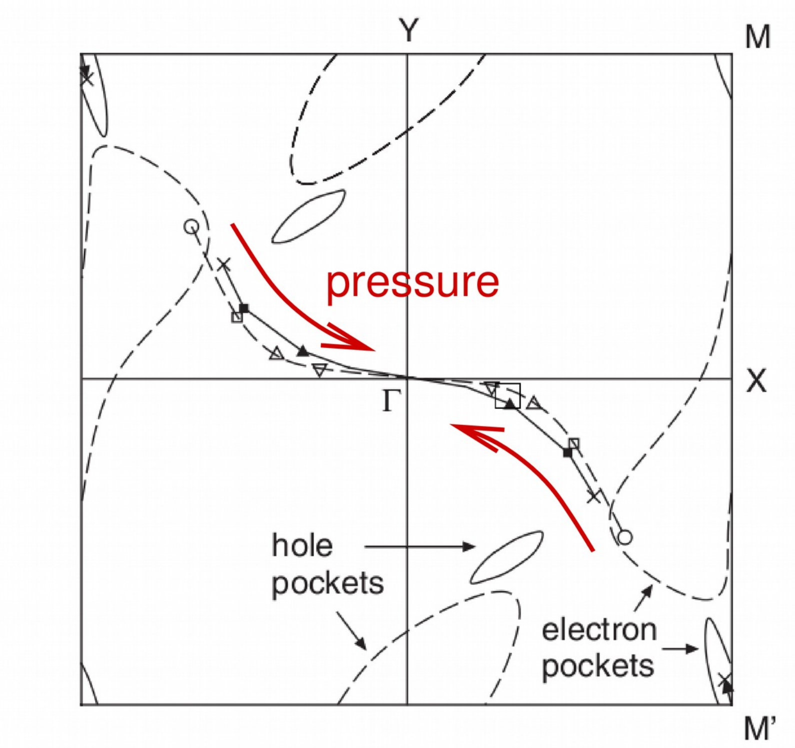
Katayama et al., JPSJ (2006)

α-(BEDT-TTF)$_2$I$_3$ bands under pressure

band structure (tight-binding model)



Brillouin zone



Katayama et al., JPSJ (2006)

Pseudo-covariance in tilted Dirac and Weyl cones

Generalised Dirac/Weyl Hamiltonian:

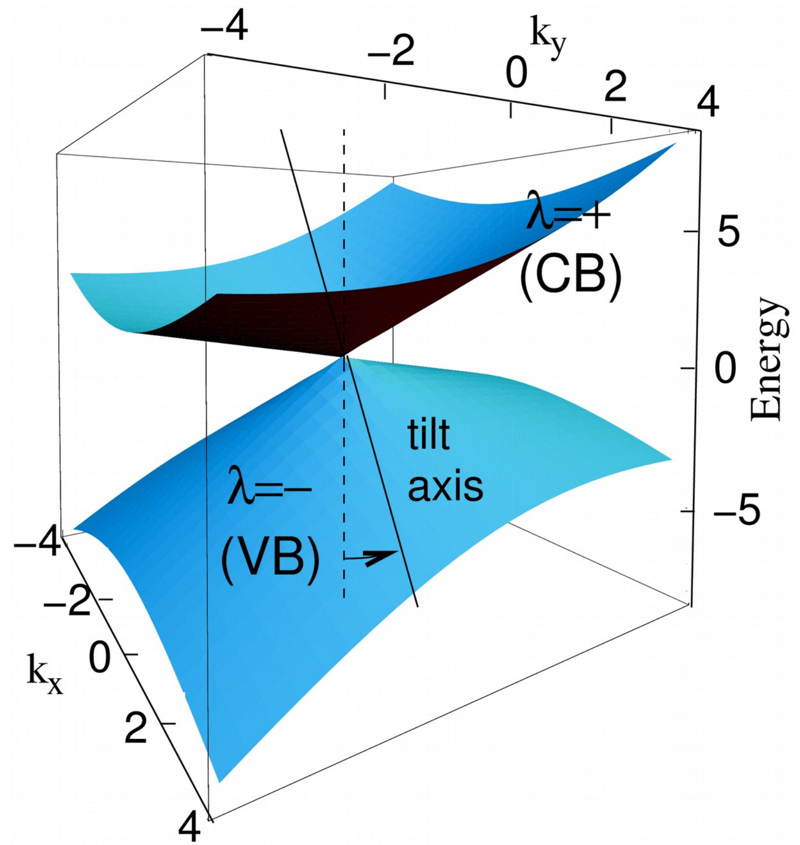
$$H_\xi = \xi\hbar v \left(q_x\sigma_x + \xi q_y\sigma_y + q_z\sigma_z\right) + \xi\hbar\mathbf{w}_0\cdot\mathbf{q}\sigma_0$$

$\mathbf{w}_0$ *: tilt velocity*

σ_0 *: 2x2 one matrix*

Energy dispersion:

$$\epsilon_\xi(\mathbf{q}) = \xi\hbar\mathbf{w}_0\cdot\mathbf{q} \pm \hbar v|\mathbf{q}|$$



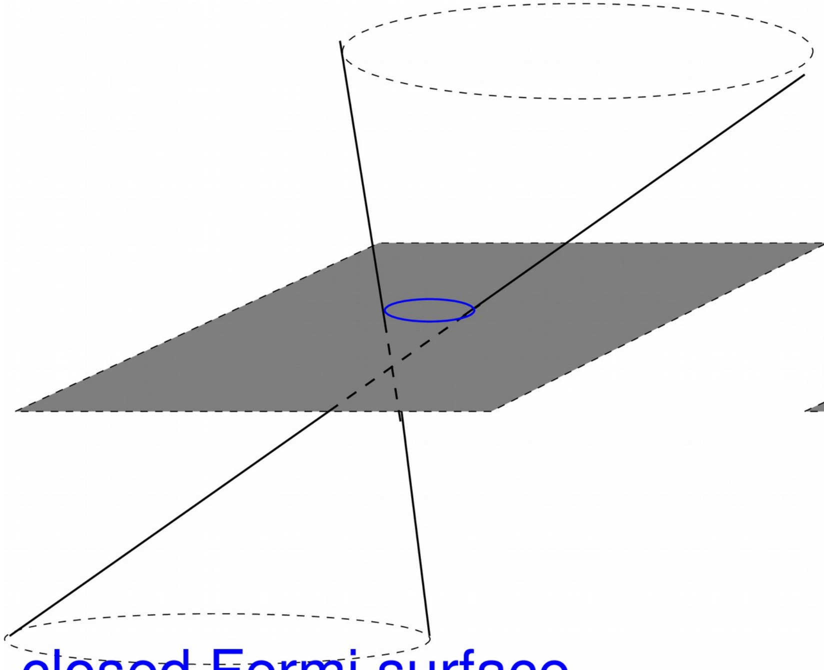
Criterion for maximal tilt or how not to spill your glass of Martini

$$w_{0x}^2 + w_{0y}^2 + w_{0z}^2 < v^2$$

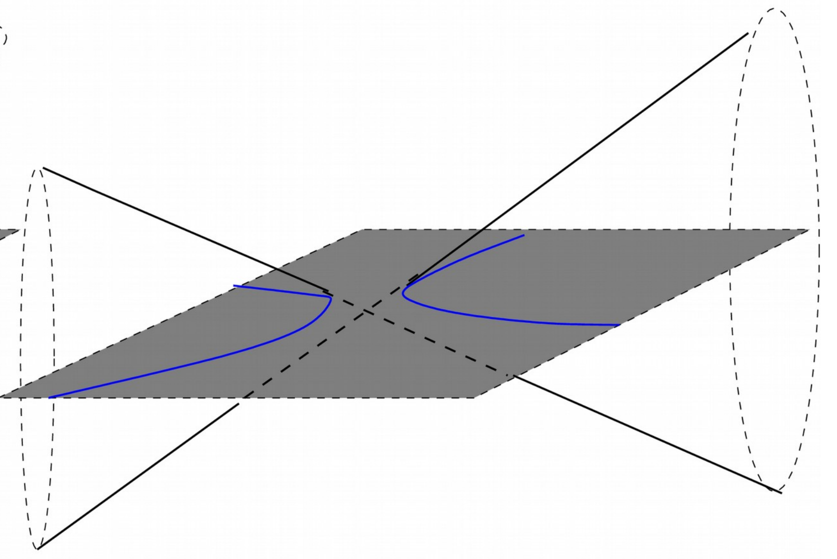
type-I Dirac/Weyl semimetal

$$w_{0x}^2 + w_{0y}^2 + w_{0z}^2 > v^2$$

type-II Dirac/Weyl semimetal



closed Fermi surface
(ellipse)



open Fermi surface
(hyperbolas)

M.O.G. et al., Phys. Rev. B (2008)
A.A. Soluyanov et al., Nature (2015)

Pseudo-covariance in tilted Dirac and Weyl cones

M.O.G. et al., EPL (2009)

Generalised Dirac/Weyl Hamiltonian (2D):

$$H_\xi = \xi\hbar v\left(q_x\sigma_x + \xi q_y\sigma_y + \tilde{w}_0 q_x\sigma_0\right)$$

Pseudo-covariance in tilted Dirac and Weyl cones in a magnetic field

M.O.G. et al., EPL (2009)

Generalised Dirac/Weyl Hamiltonian (2D):

$$H_\xi = \xi \hbar v \left(q_x \sigma_x + \xi q_y \sigma_y + \tilde{w}_0 q_x \sigma_0 \right)$$

in a magnetic field: $A_x = -By \qquad A_y = 0$

$$H_\xi = \xi \hbar v \left((q_x - eBy/\hbar)\sigma_x + \xi q_y \sigma_y + \tilde{w}_0 (q_x - eBy/\hbar)\sigma_0 \right)$$

$$= \underbrace{H_\xi^{cov}}_{\text{covariant part}} + \underbrace{\hbar w_0 q_x \sigma_0}_{\text{trivial part}}$$

Pseudo-covariance in tilted Dirac and Weyl cones in a magnetic field

M.O.G. et al., EPL (2009)

Generalised Dirac/Weyl Hamiltonian (2D):

$$H_\xi = \xi\hbar v\left(q_x\sigma_x + \xi q_y\sigma_y + \tilde{w}_0 q_x\sigma_0\right)$$

in a magnetic field:

$$A_x = -By \qquad A_y = 0$$

$$H_\xi = \xi\hbar v\left((q_x - eBy/\hbar)\sigma_x + \xi q_y\sigma_y + \tilde{w}_0(q_x - eBy/\hbar)\sigma_0\right)$$

$$= H_\xi^{cov} + \hbar w_0 q_x\sigma_0$$

trivial part

covariant part

$$\boxed{H_\xi^{cov} = \xi\hbar v\left((q_x - eBy/\hbar)\sigma_x + \xi q_y\sigma_y\right) - eE_{\text{eff}}\,y\sigma_0}$$

$$E_{\text{eff}} = w_0 B \quad \rightarrow \qquad w_0 = \tilde{w}_0 v = v_D$$ *: tilt = drift velocity !*

Pseudo-covariance in tilted Dirac and Weyl cones: Landau levels

$$H_\xi = \xi \hbar v \left((q_x - eBy/\hbar)\sigma_x + \xi q_y \sigma_y + \tilde{w}_0 (q_x - eBy/\hbar)\sigma_0 \right)$$

Diagonalisation yields Landau-level spectrum:

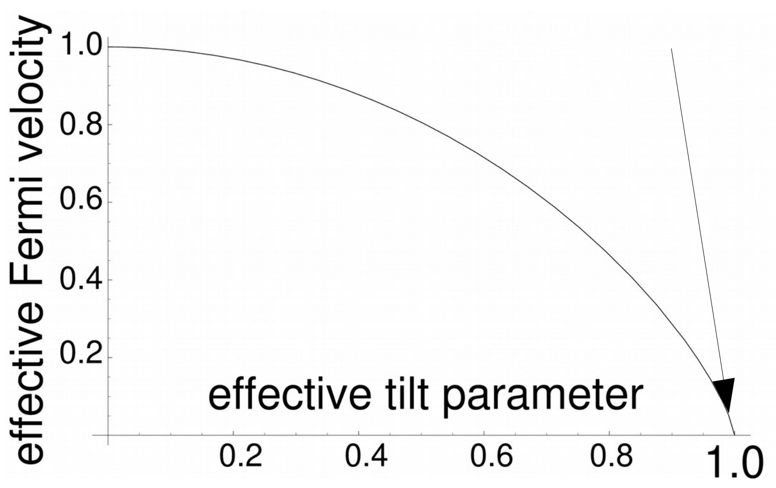
M.O.G. et al., Phys. Rev. B (2008)

$$\epsilon_{\pm n, q_x} = \pm \hbar \frac{v^*}{l_B} \sqrt{2n}$$

with renormalised velocity:

$$\boxed{v^* = v[1 - (w_0/v)^2]^{3/4}}$$

maximally allowed tilt



see also: *Morinari et al., JPSJ (2009)*

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Implications for LL spectroscopy

Motivation: *color shift* in relativity (*optical Doppler effect*)

Implications for LL spectroscopy

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→ Peierls substitution: $$\mathbf{q} \to \mathbf{q} + \frac{e}{\hbar}[\mathbf{A}(\mathbf{r}) + \mathbf{A}_{\mathrm{rad}}(t)]$$

magnetic field

radiation field

→ expansion of Hamiltonian to linear order in radiation field:

$$H(\mathbf{q}) \to H_B + e\mathbf{v} \cdot \mathbf{A}_{\mathrm{rad}}(t)$$

with velocity operator $\mathbf{v} = \nabla_{\mathbf{q}} H(\mathbf{q})/\hbar$

→ ***(magneto-)optical selection rules (matrix elements):***

$$\boxed{\psi^{\dagger}_{\lambda n} \mathbf{v} \psi_{\lambda' m}}$$

Light-matter coupling for straight cones (comoving frame)

(magneto-)optical selection rules (matrix elements):

$$\psi^\dagger_{\lambda n}\mathbf{v}\psi_{\lambda' m}$$

→ graphene (no tilt, no electric field): $m = (n \pm 1)$

dipolar selection rules (in comoving frame):

$$\lambda n \to \lambda'(n+1) \qquad \text{for} \quad \text{right-handed light} \qquad \circlearrowleft$$

$$\lambda n \to \lambda'(n-1) \qquad \text{for} \quad \text{left-handed light} \qquad \circlearrowright$$

Light-matter coupling for tilted Dirac cones

→ Lorentz boost in x direction, with $w_0 = E_{\rm eff}/B \qquad \tilde{w}_0 = w_0/v$

$$x'^{\mu} = \Lambda^{\mu}_{\nu} x^{\nu} \qquad x' = (w_0 t + \tilde{w}_0 x)/\sqrt{1-\tilde{w}_0^2}$$

(Lorentz transformation of a 4-vector)

→ transformation of wave function, with $\tanh\theta = \tilde{w}_0$:

$$\psi'(vt', x', y' = y) = S(\Lambda)\psi(vt, x, y) \qquad \text{with} \qquad S(\Lambda) = e^{\theta\sigma_x/2}$$

→ selection rules known in co-moving frame

$$\psi'^{\dagger}_{\lambda n}\mathbf{v}\psi'_{\lambda'(n\pm 1)}$$

WANTED: selection rules in lab frame !

Light-matter coupling for tilted Dirac cones

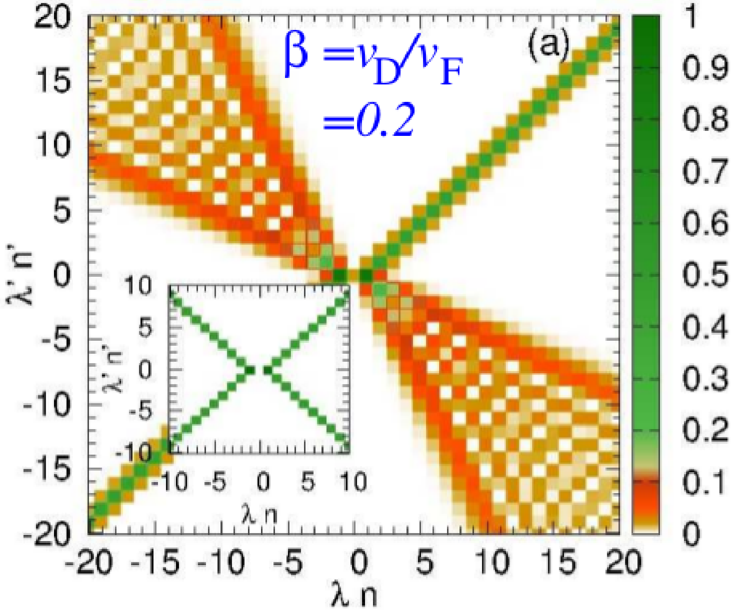
Sári, M.O.G. and Töke, PRB (2015)

- selection rules in comoving frame v_D (field $E = 0$)

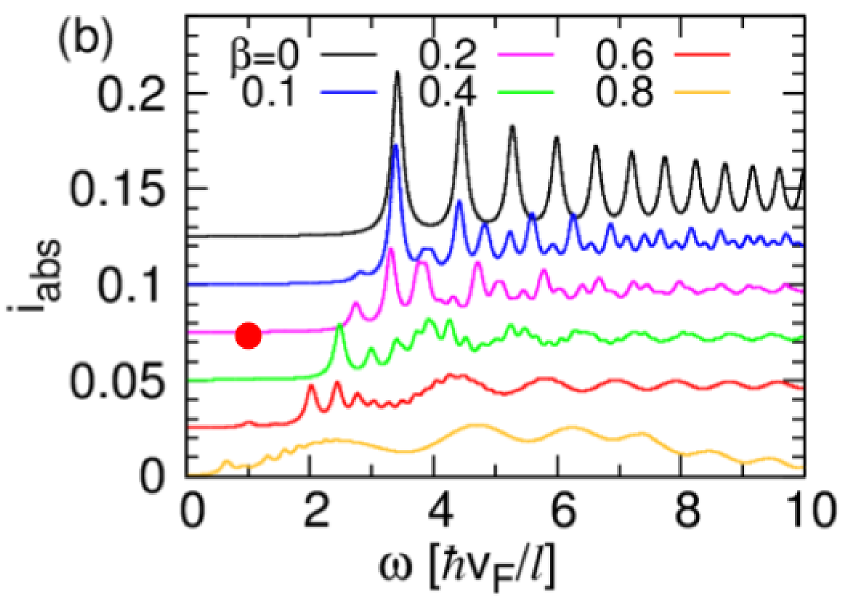
$$\lambda n \to \lambda'(n \pm 1)$$

$\Rightarrow$ new transitions in lab frame ($E \neq 0$)

matrix elements



absorption coefficient



$$\beta = \tilde{w}_0 = w_0/v$$

Light-matter coupling for tilted Dirac cones

Sári, M.O.G. and Töke, PRB (2015)

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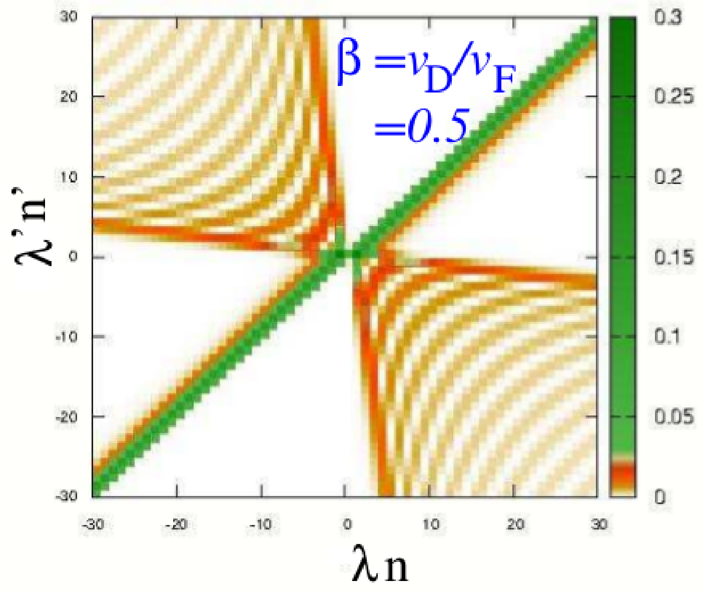

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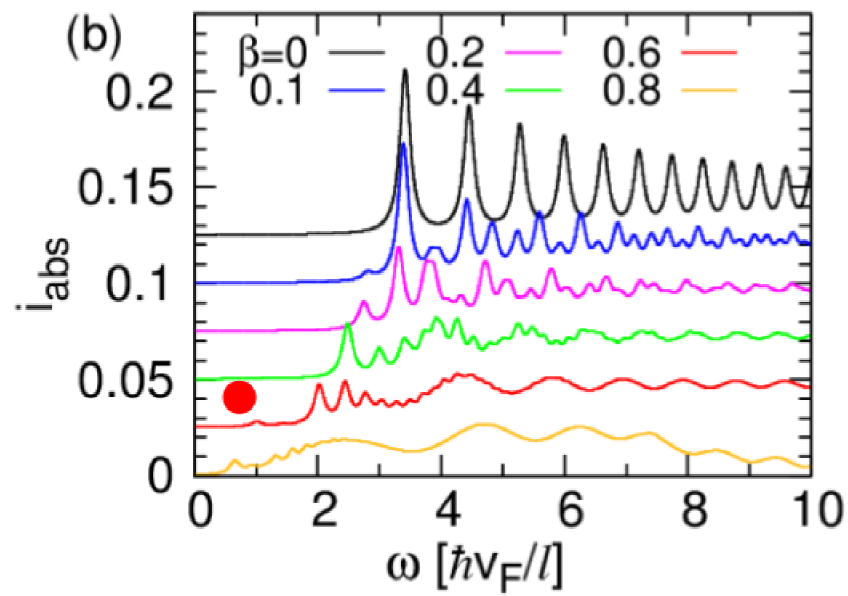


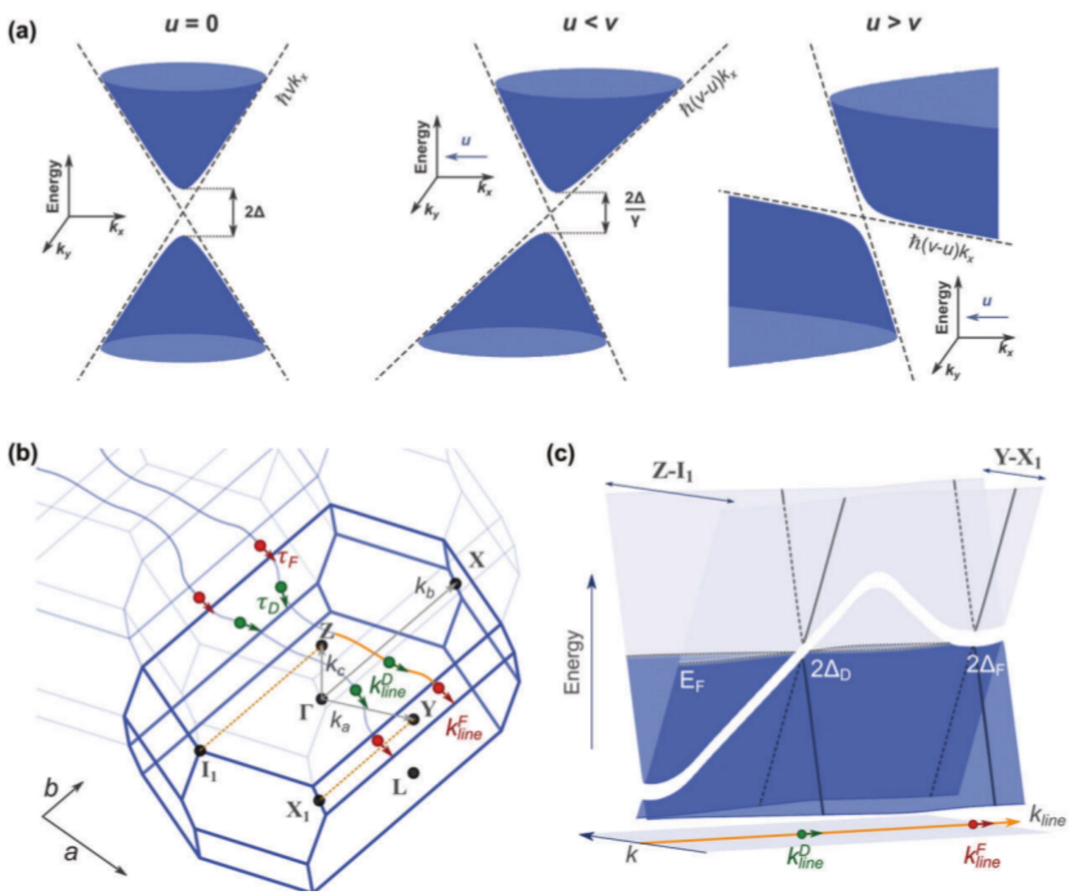
$$\beta = \tilde{w}_0 = w_0/v$$

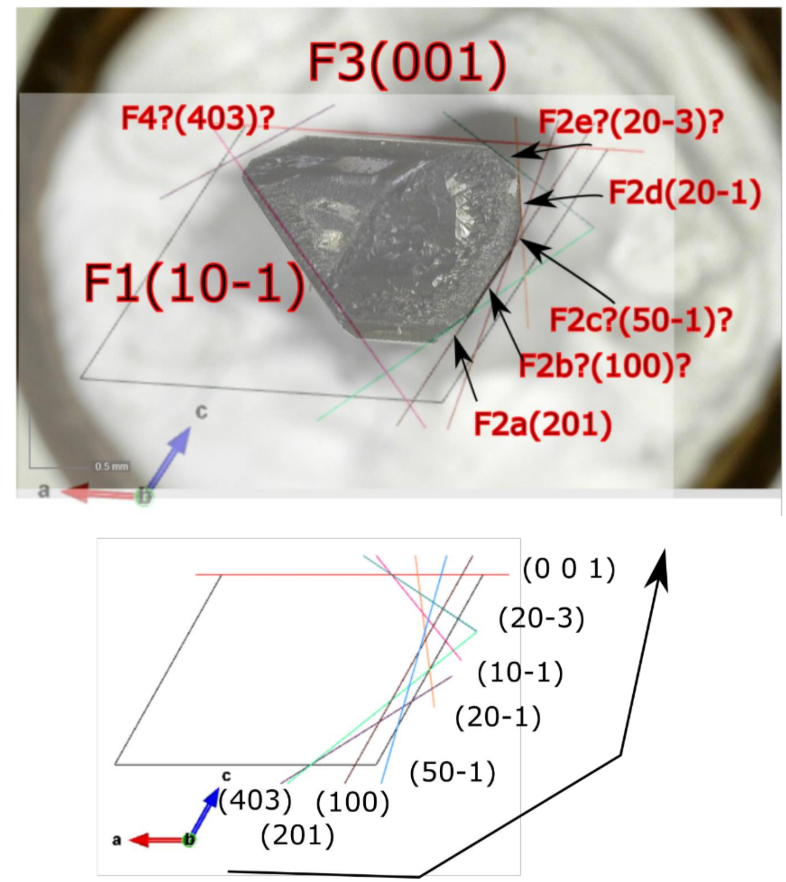
Generalization to 3D Weyl semimetals :
Tchoumakov, Civelli, MOG, PRL (2017)

Magneto-optical evidence for Lorentz boosts in $NbAs_2$

Wyzula, Lu, et al., Adv. Sci. (2022)

→ nodal-line semimetal with a (small) SO gap





<u>Faraday geometry</u> : B-field perpendicular to facets

~ *probing band structure in different planes in k-space*

Magneto-optical evidence for Lorentz boosts in $NbAs_2$

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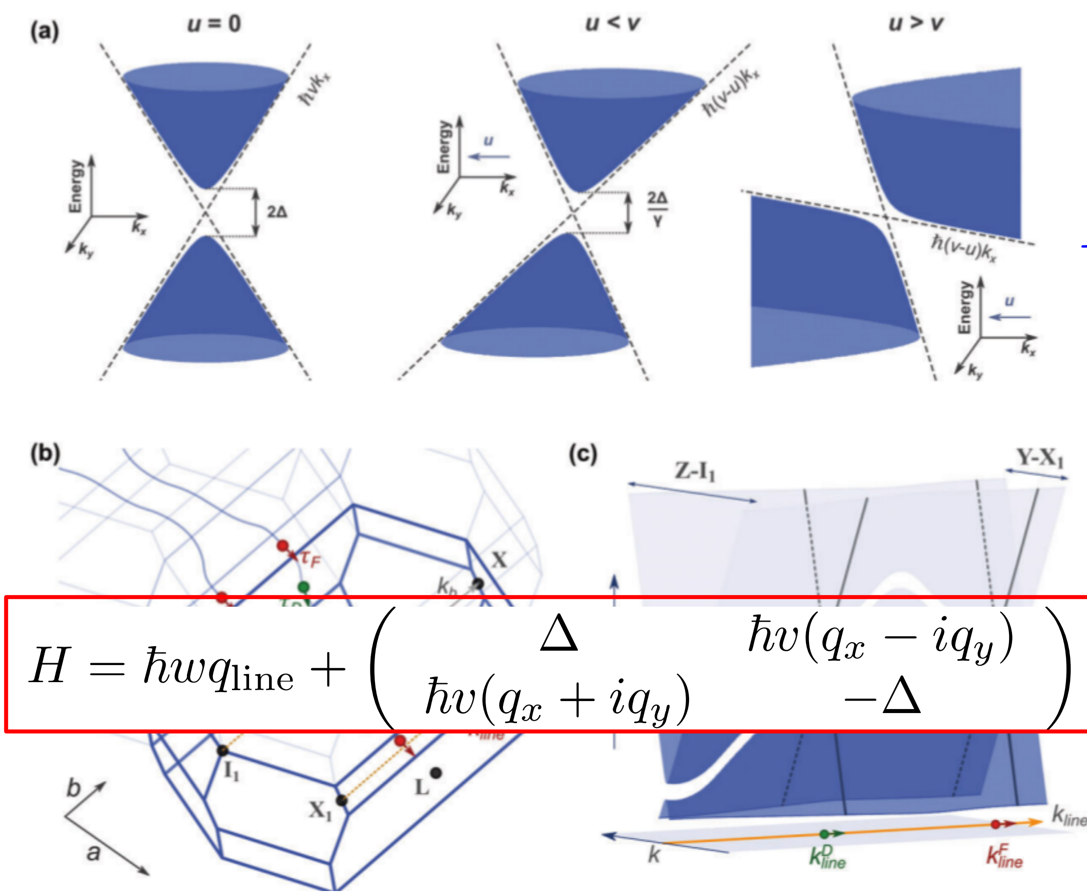

$$H = \hbar w q_{\mathrm{line}} + \begin{pmatrix} \Delta & \hbar v(q_x - i q_y) \\ \hbar v(q_x + i q_y) & -\Delta \end{pmatrix}$$

Landau levels (in the plane):

$$E_{\lambda,n} = \lambda\sqrt{\Delta^{*2} + 2e\hbar v^{*2} n}$$

with

$$\Delta^* = \Delta/\gamma \qquad v^* = \frac{v\sqrt{\cos\theta}}{\gamma^{3/2}}$$

$$\gamma = \frac{1}{\sqrt{1 - \frac{w^2}{v^2}\tan^2\theta}}$$

<u>Faraday geometry</u> : B-field perpendicular to facets

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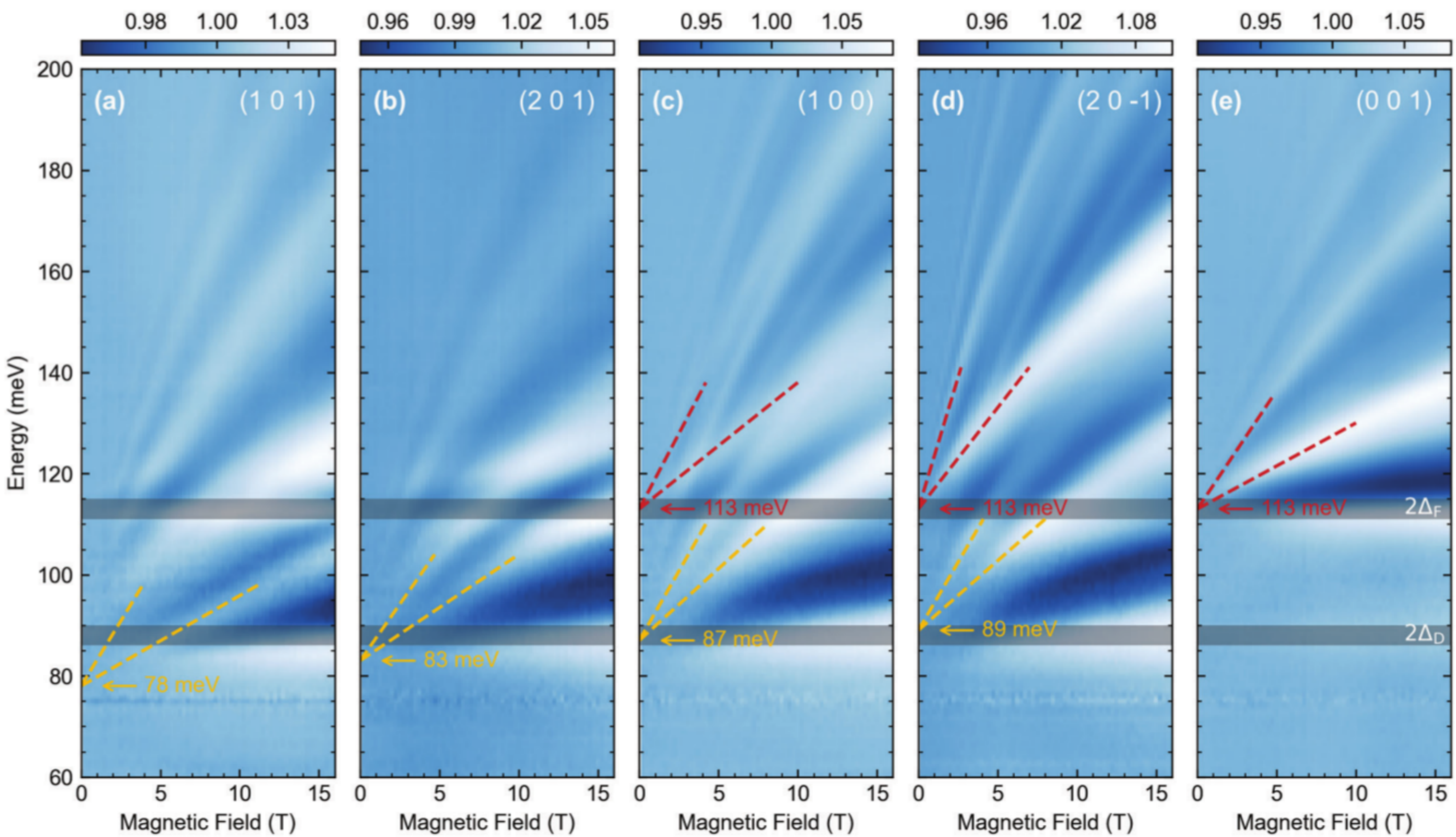


Interband LL transitions : for $B \to 0$ extraction of $2\Delta^*$

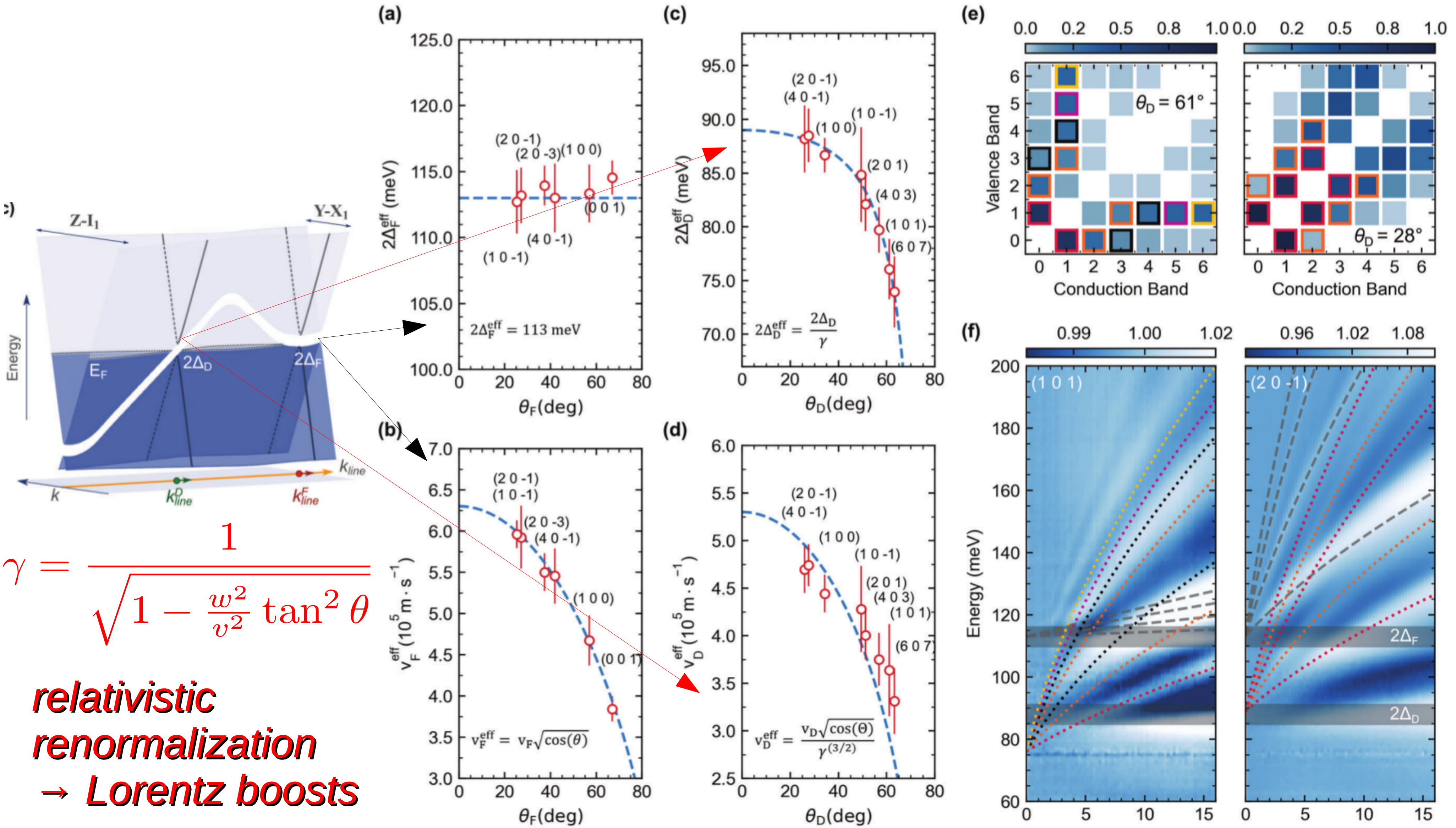
Theory-experiment relation

Theory

Experiment

Magneto-optical evidence for Lorentz boosts in $NbAs_2$

Wyzula, Lu, et al., Adv. Sci. (2022)



$$\gamma = \frac{1}{\sqrt{1 - \frac{w^2}{v^2}\tan^2\theta}}$$

relativistic renormalization → Lorentz boosts

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Bulk-edge correspondence in topological materials – in a nutshell

(topological chocolate bar)

+

= ?

Bulk-edge correspondence in topological materials – in a nutshell

(topological chocolate bar)

\+

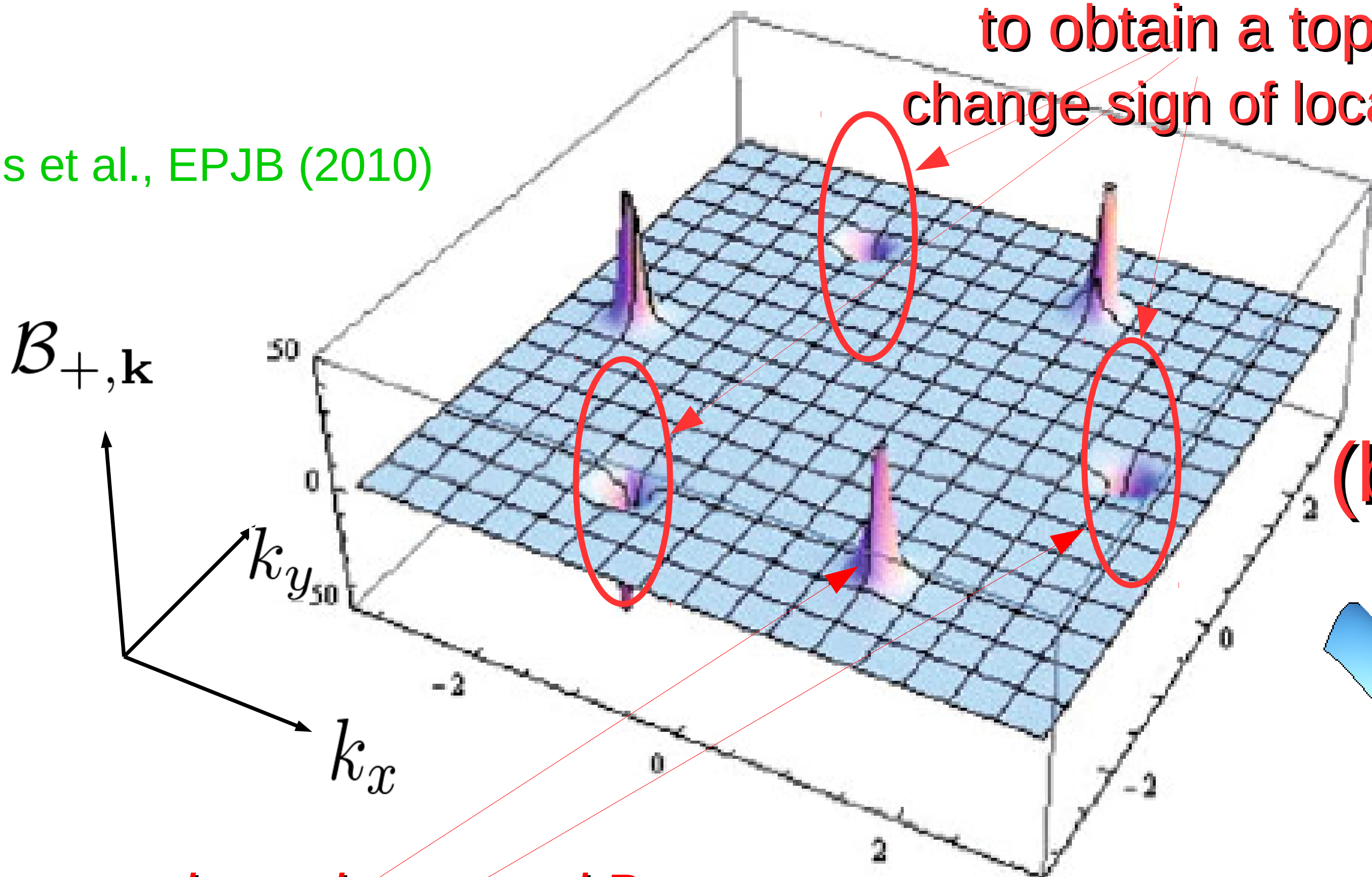
=

\+

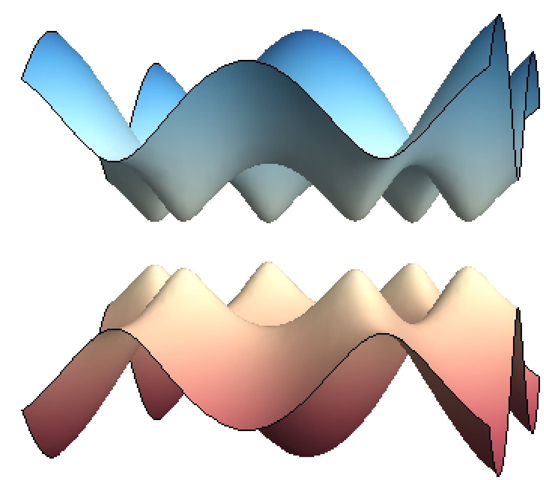
Berry curvature for insulating graphene

Fuchs et al., EPJB (2010)

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



→ local gap inversion (break TRS !)

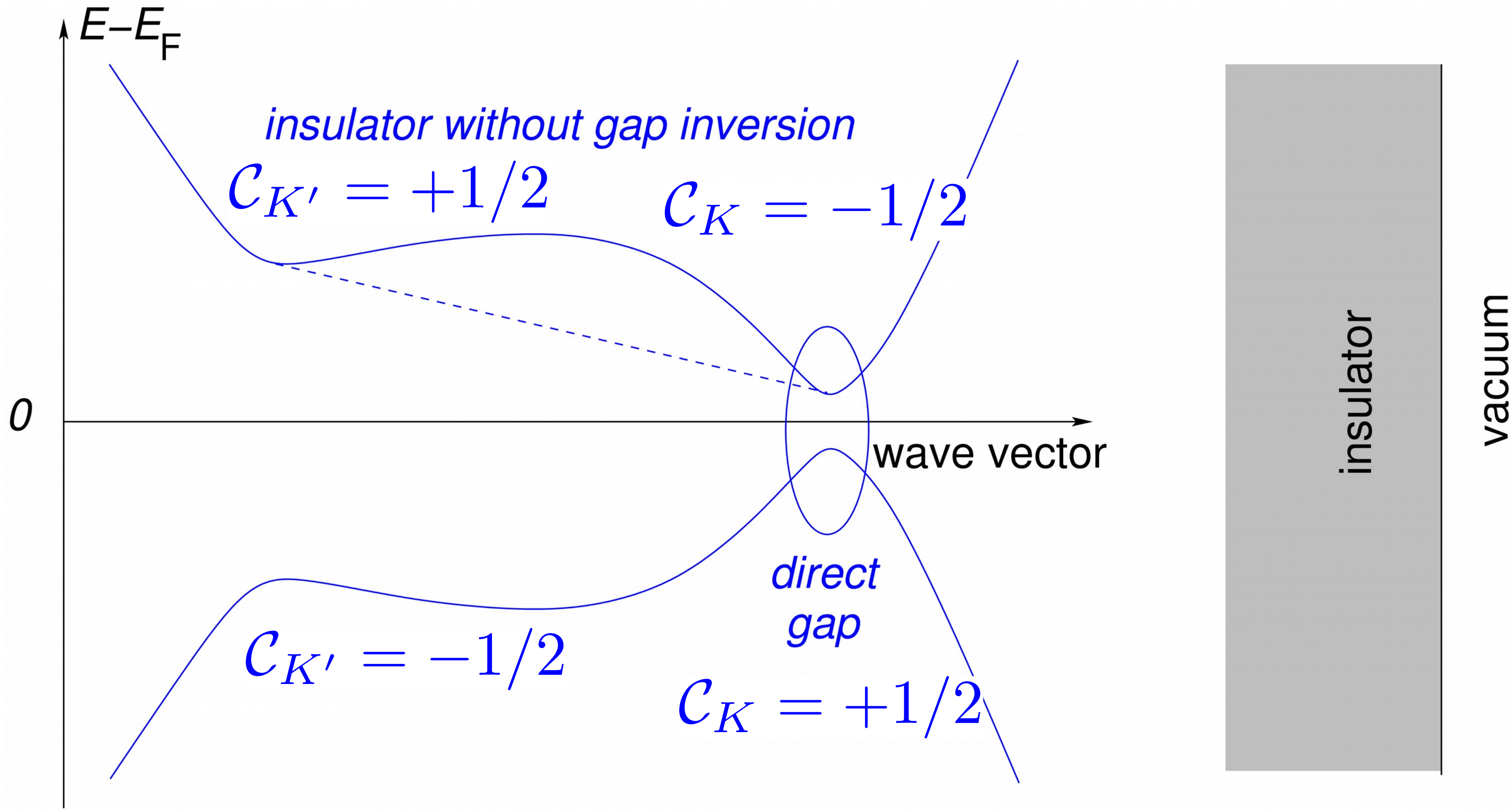


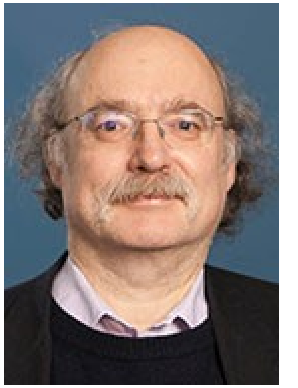
Chern number = integrated Berry curvature

$$C_\lambda = \tilde{C}_K + \tilde{C}_{K'} = \frac{1}{2} + \left(-\frac{1}{2}\right)$$

("topological invariant" = sum of contributions from both Dirac points)

Haldane model (broken time-reversal symmetry, 1988)

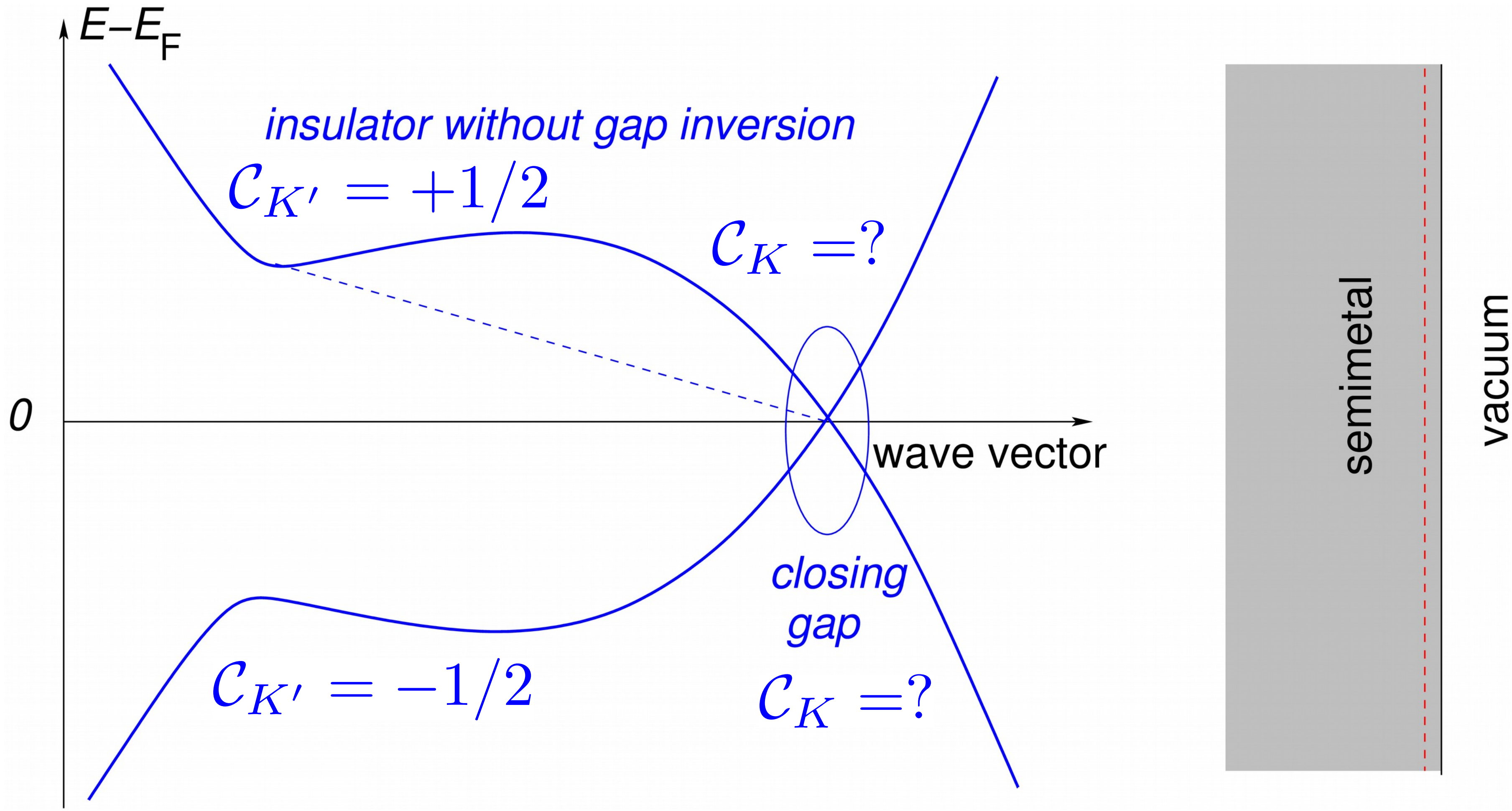




Broken TR symmetry : $E(\mathbf{k}) \neq E(-\mathbf{k})$

modify Dirac points independently from one another

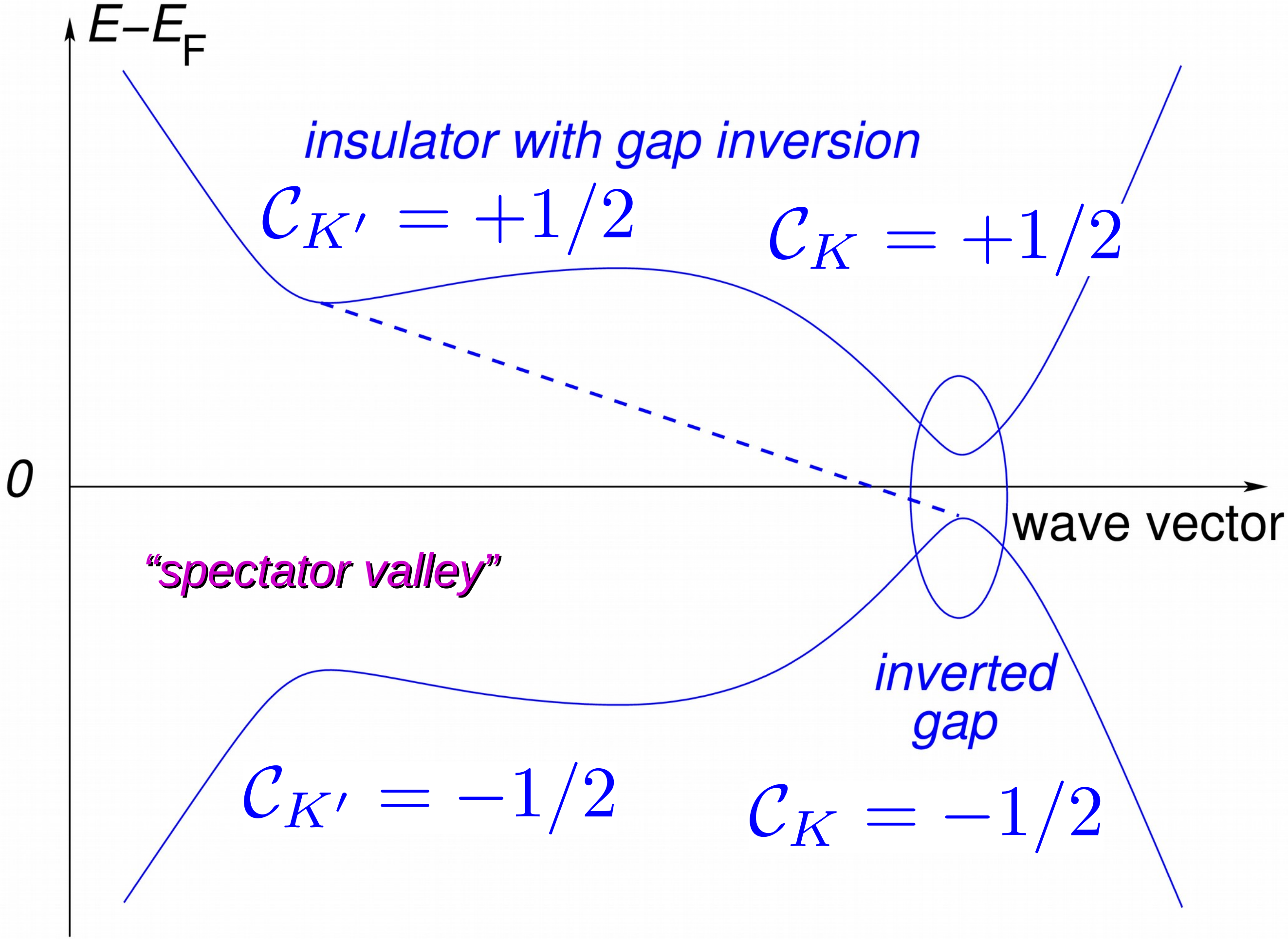
Haldane model (broken time-reversal symmetry, 1988)

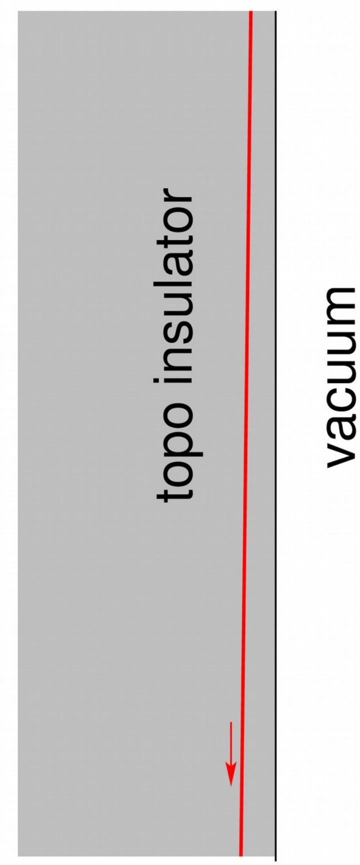


Broken TR symmetry : $E(\mathbf{k}) \neq E(-\mathbf{k})$

→ ***topological phase transition***

Haldane model (broken time-reversal symmetry, 1988)

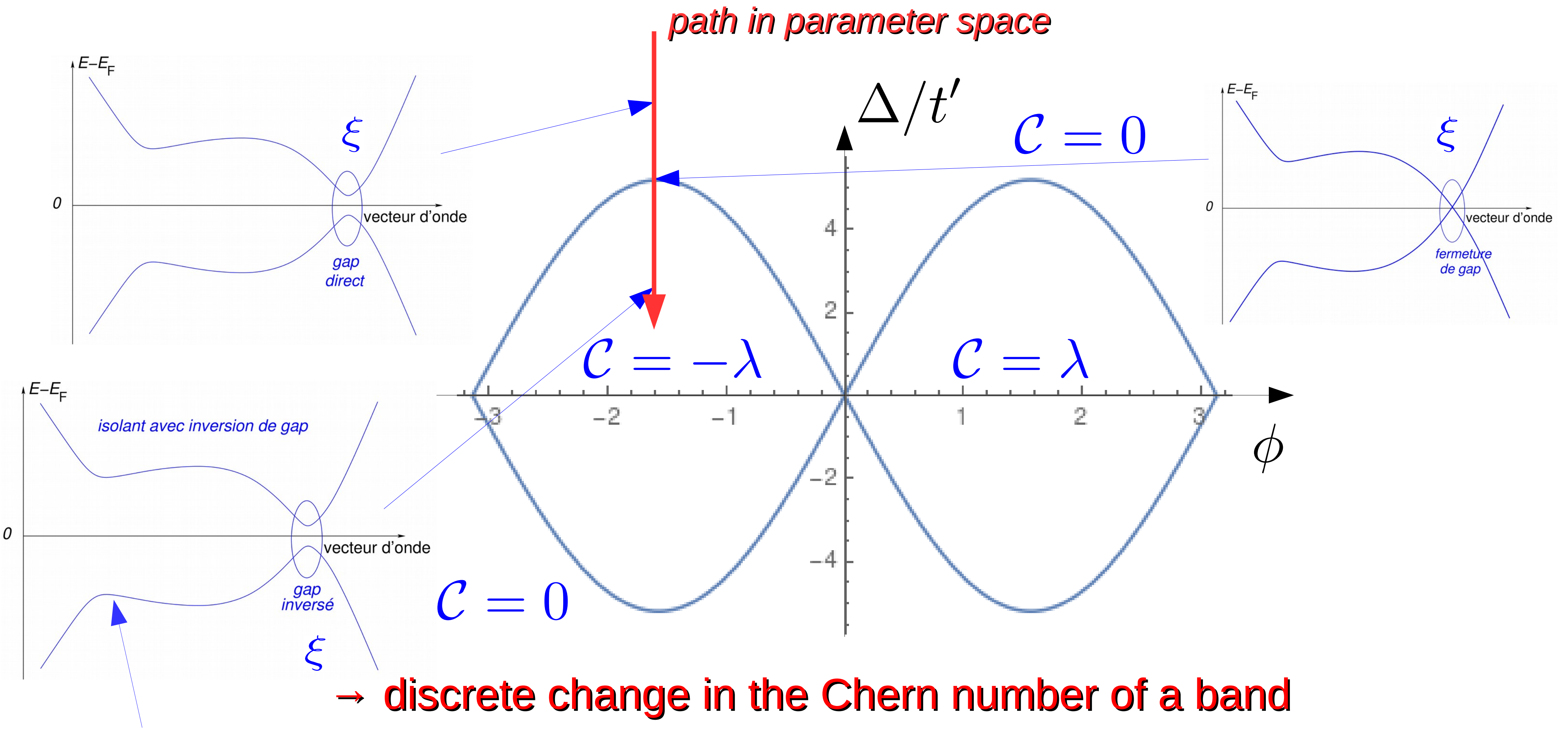




Change in total Chern number: $\Delta C = \Delta \mathcal{C}_K = \pm 1$

The gap is closed only in one (active) valley, while the other one is a pure spectator of the (topological) transition.

Topological phase transition



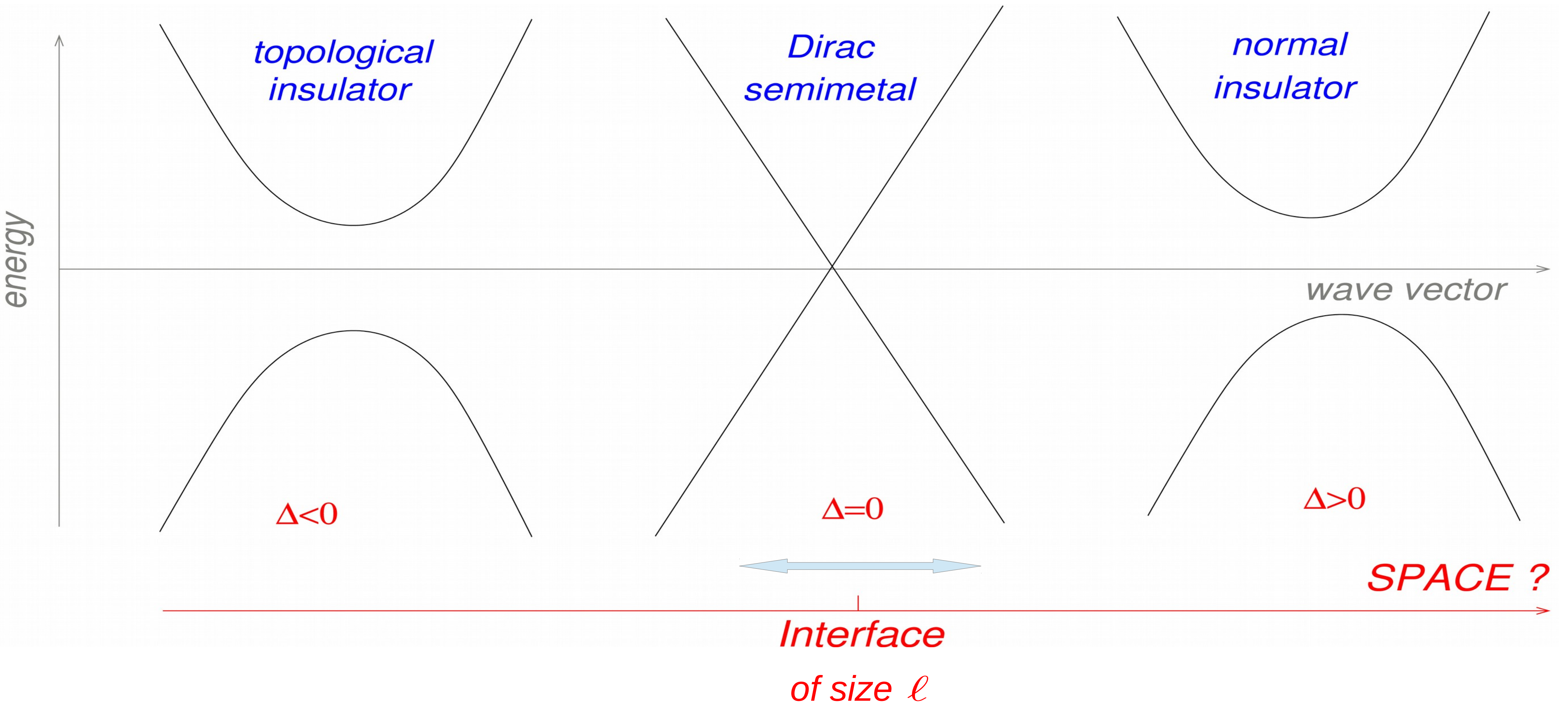
→ discrete change in the Chern number of a band

valley $-\xi$:
pure spectator

→ gap must close at the topological phase transition

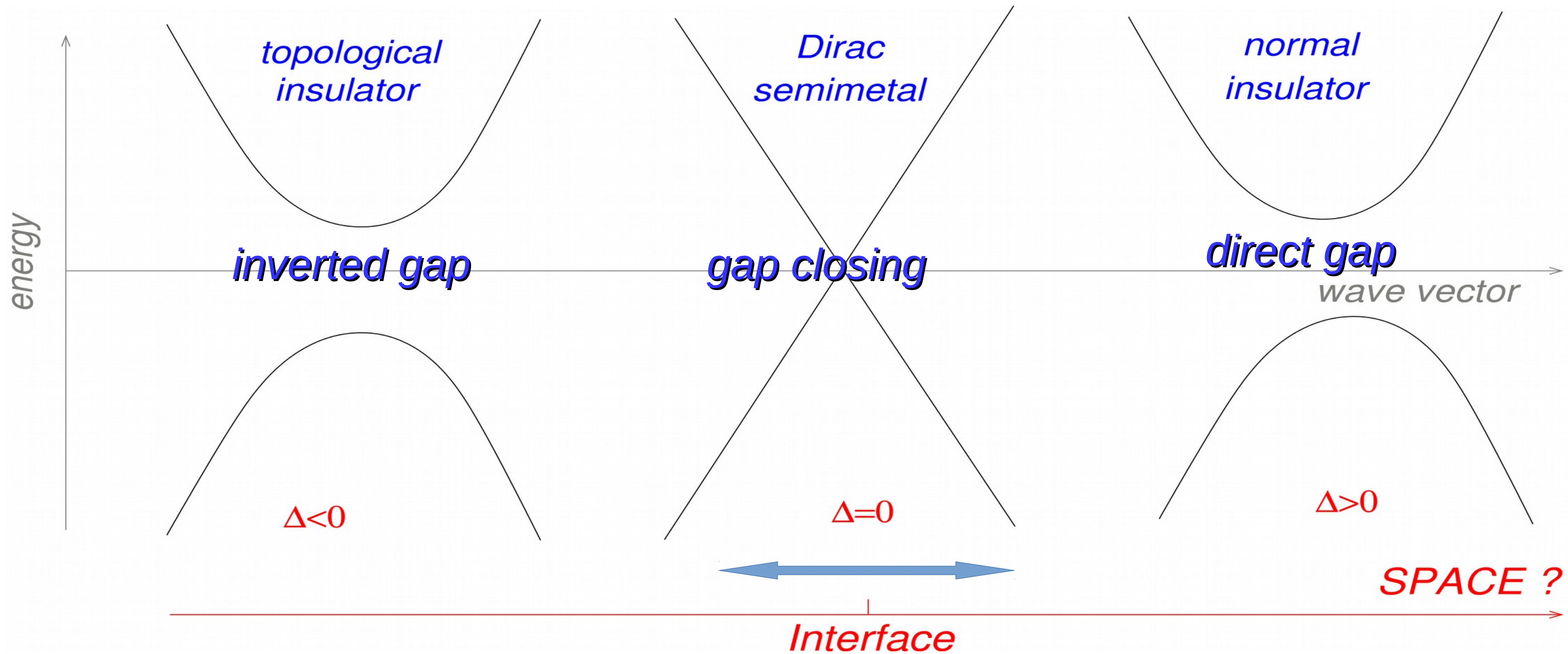
→ in the vicinity of a topological phase transition:
emergence of a (massless) Dirac fermion (sign change in mass)

How can we use this to describe an interface ?



$$\Delta \quad \rightarrow \quad \Delta\left(\frac{x}{\ell}\right) \simeq \Delta\frac{x}{\ell}$$

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:

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

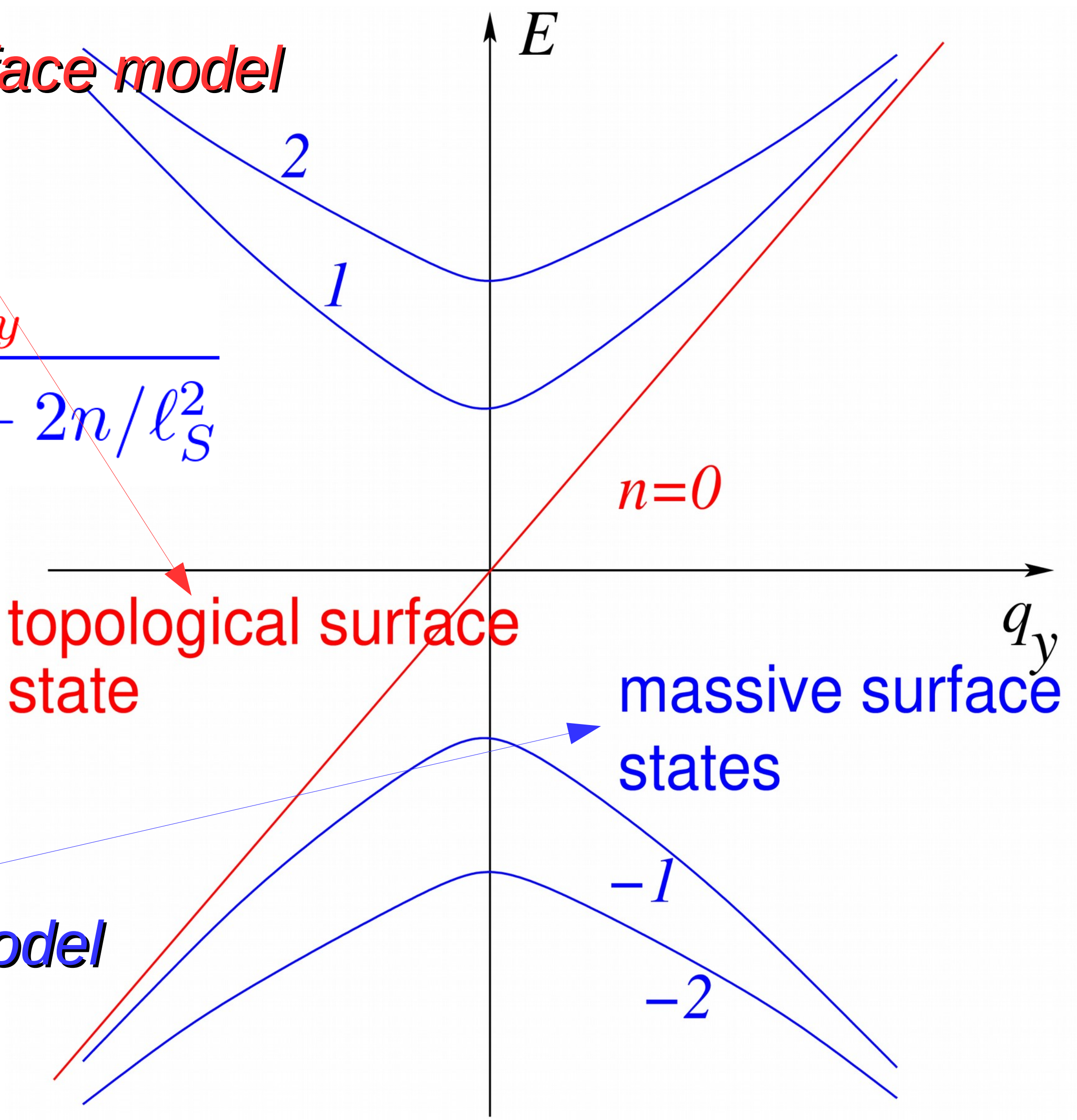
Tchoumakov et al., PRB (2017)

Surface (edge) states

independent of surface model

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

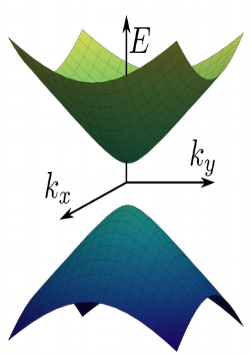
$$E_{\lambda,n\neq 0} = \lambda v\sqrt{q_y^2 + 2n/\ell_S^2}$$



depends on surface model

Surface states in 3D materials

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



Complication in 3D: 4x4 Hamiltonian

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

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

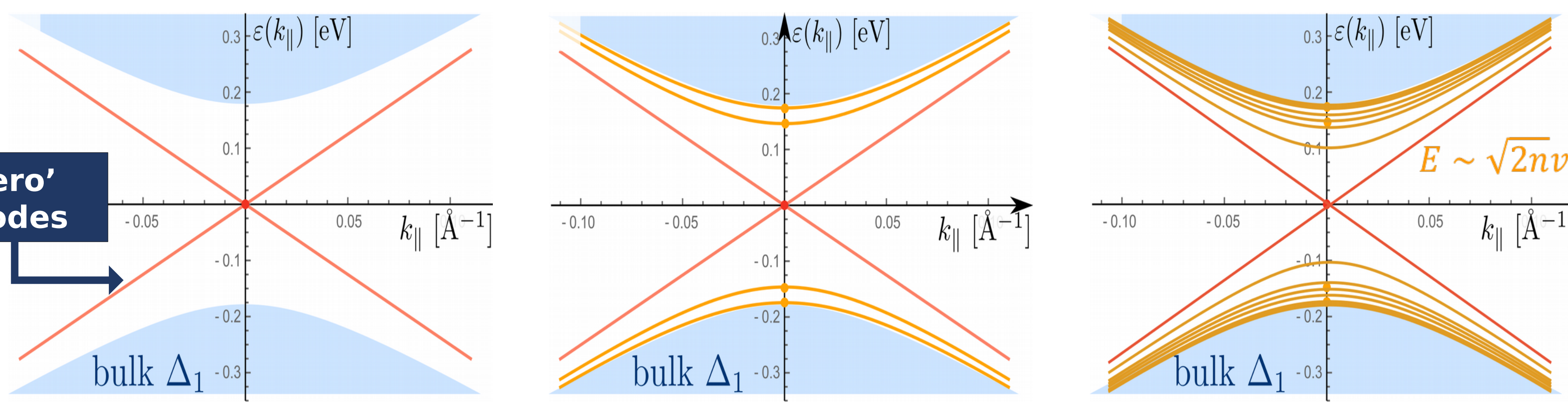
here: $$\Delta(z) = \Delta \tanh(z/\ell)$$

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

ℓ/ξ

abrupt | intermediate | very smooth

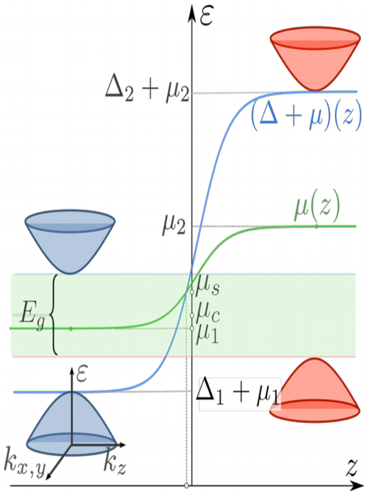
'Zero' modes



$E \sim \sqrt{2n}v_F/\ell_S$

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

Special relativity in surface states

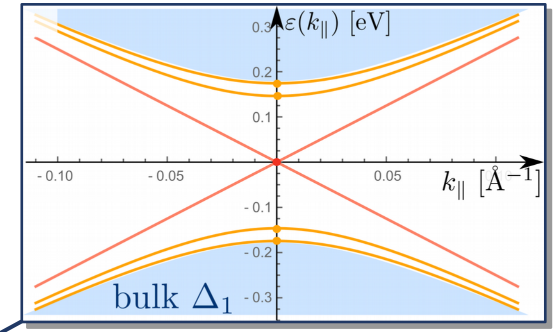


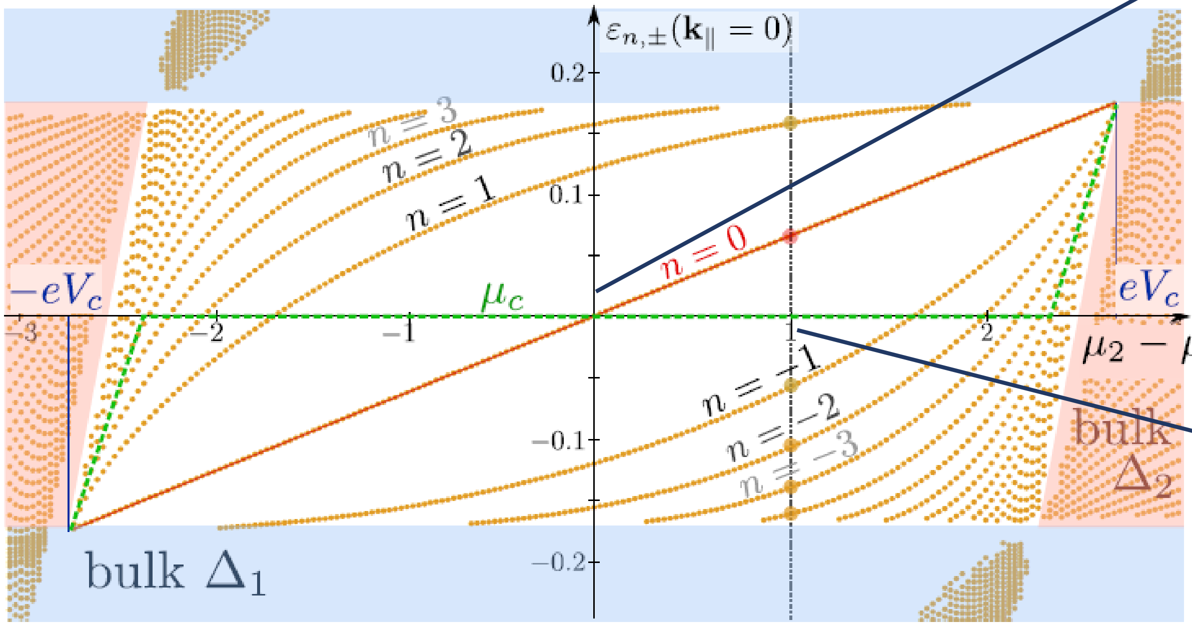
$$H = V(z)\,\mathbb{1} + v_F(k_x\,\mathbb{1}\otimes\tau_y + (k_y\,\sigma_x - k_x\sigma_y)\otimes\tau_x) + \Delta(z)\,\mathbb{1}\otimes\tau_z$$

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

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

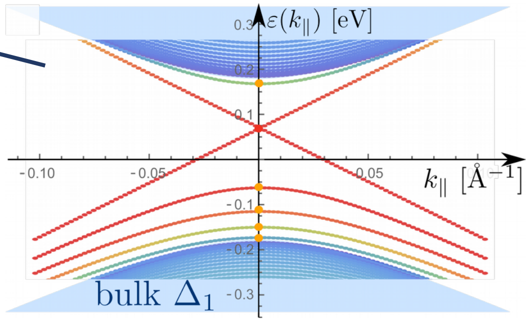
Magnetic field: $B \to B\sqrt{1-\beta^2}$





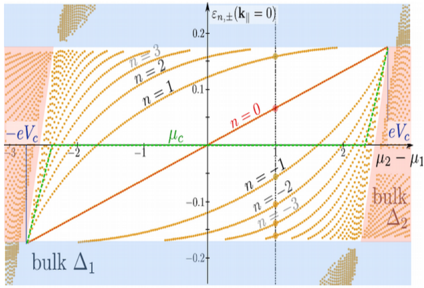
$$\Delta'_n \approx (1-\beta^2)^{3/4}\Delta_n$$

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



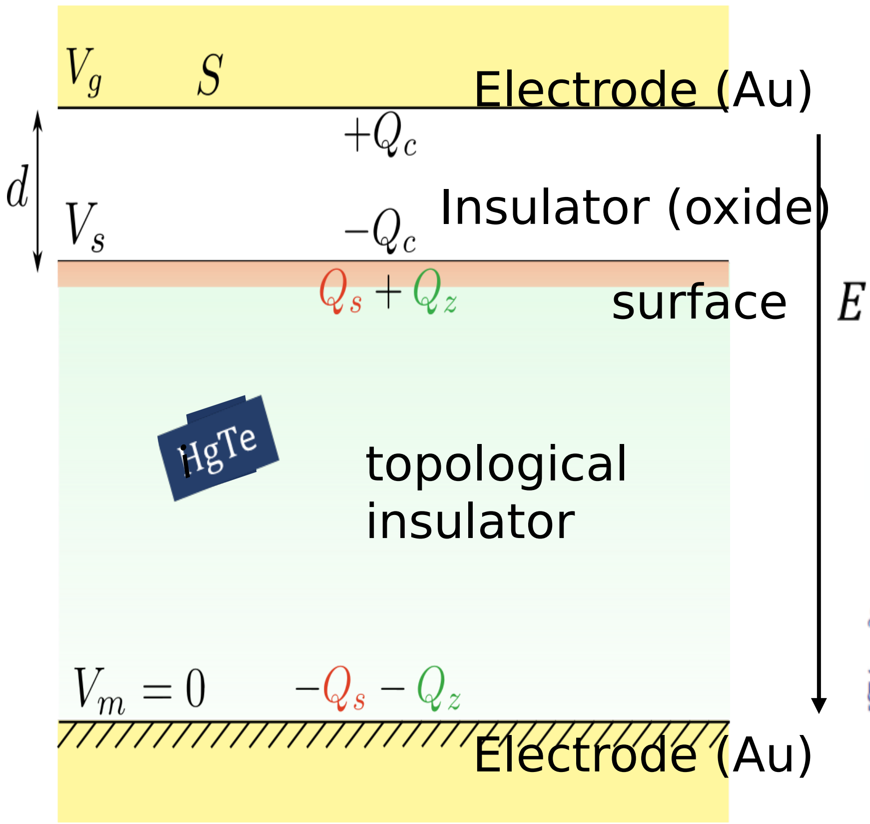
S. Tchoumakov, V. Jouffrey et al., PRB 96, 201302 (2017)

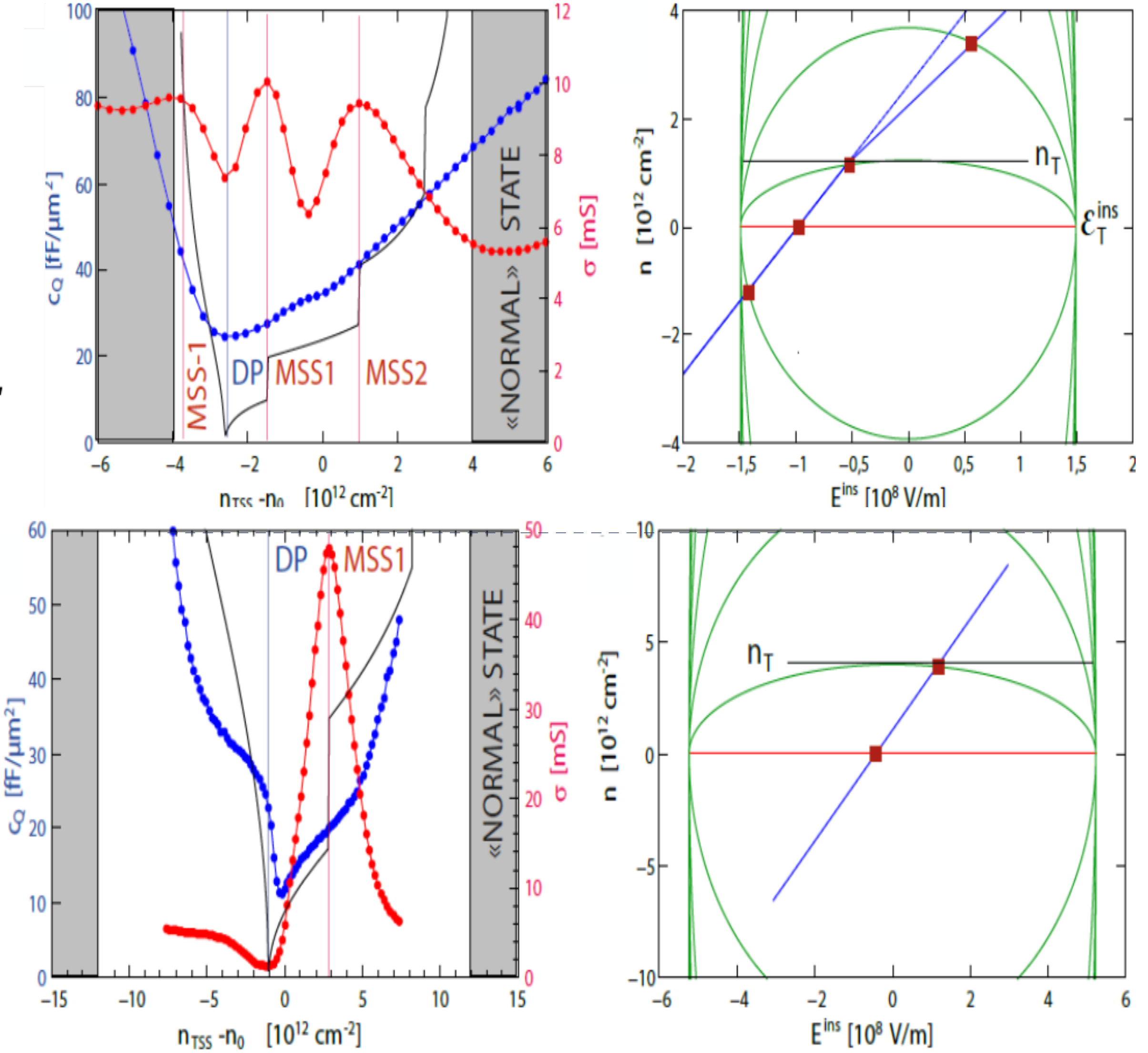
Experimental evidence (transport)



- Electrical resistance and capacitance of HgTe

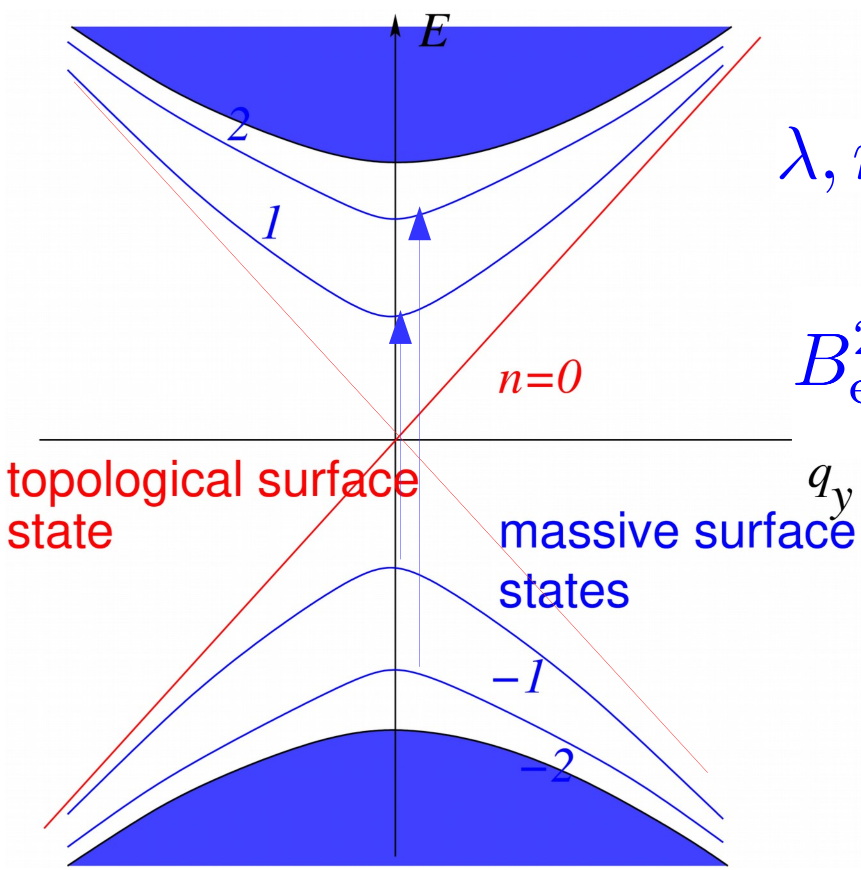
Qualitative agreement





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

Magneto-optical signatures of surface states in 3D (B field in surface) *X. Lu, MOG, EPL 126, 67004 (2019)*



selection rules:

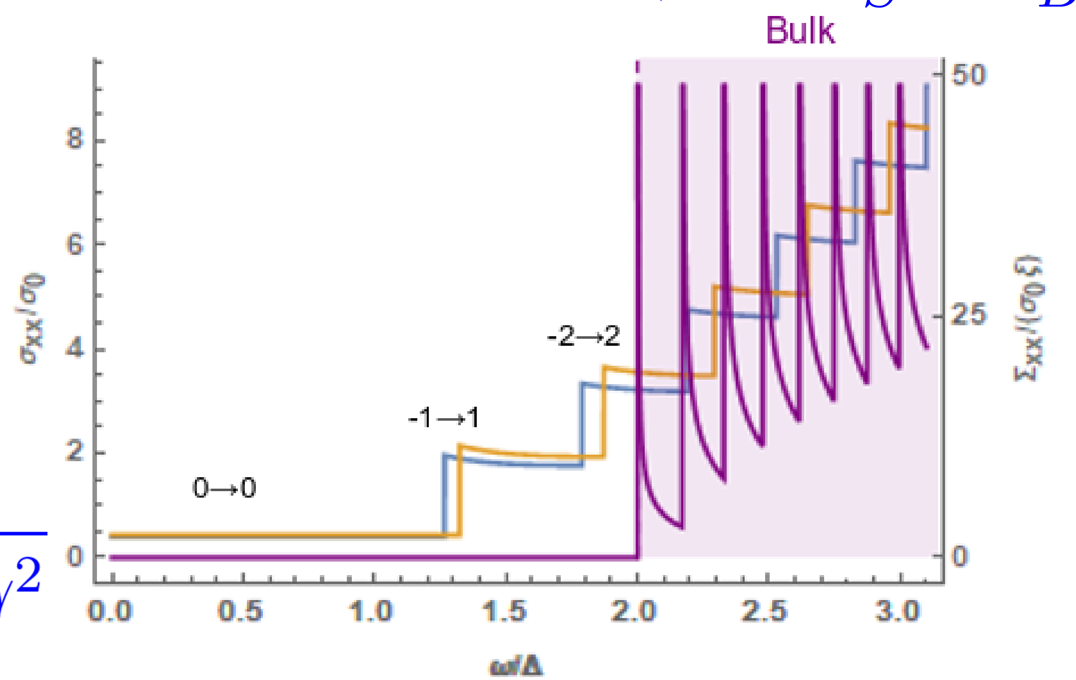
$$\lambda, n \to \lambda', n \qquad \text{for} \qquad \sigma_{xx}$$

(polarisation in surface)

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

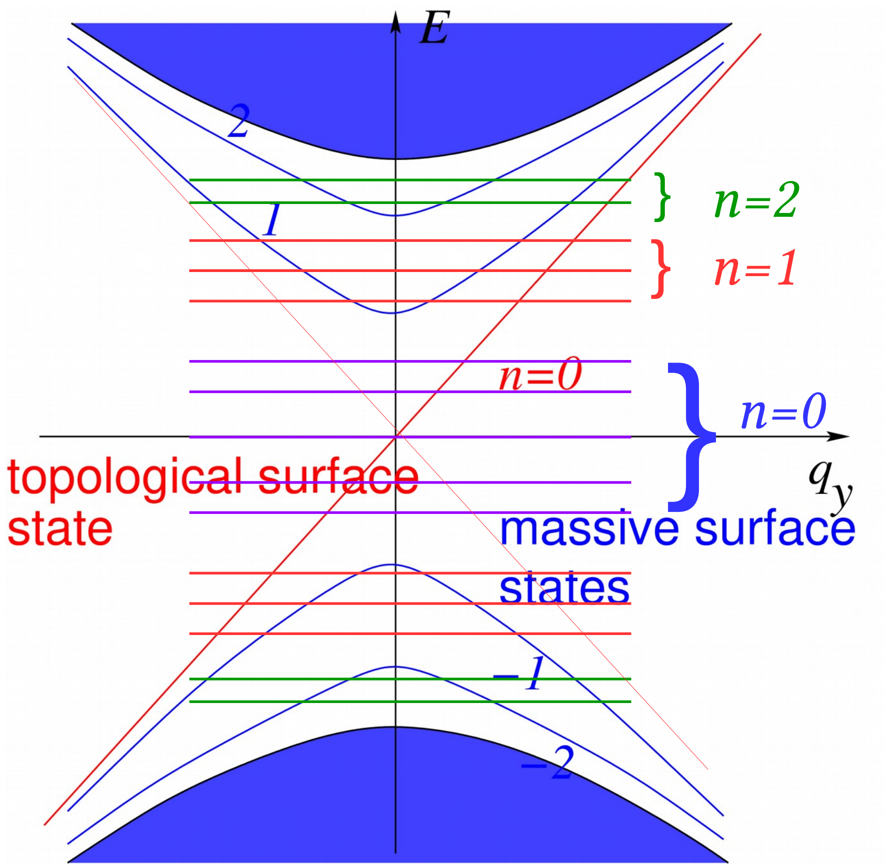
$$E_{n=0} = \hbar v q_{\parallel,\theta}$$

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



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

X. Lu, MOG, EPL 126, 67004 (2019)

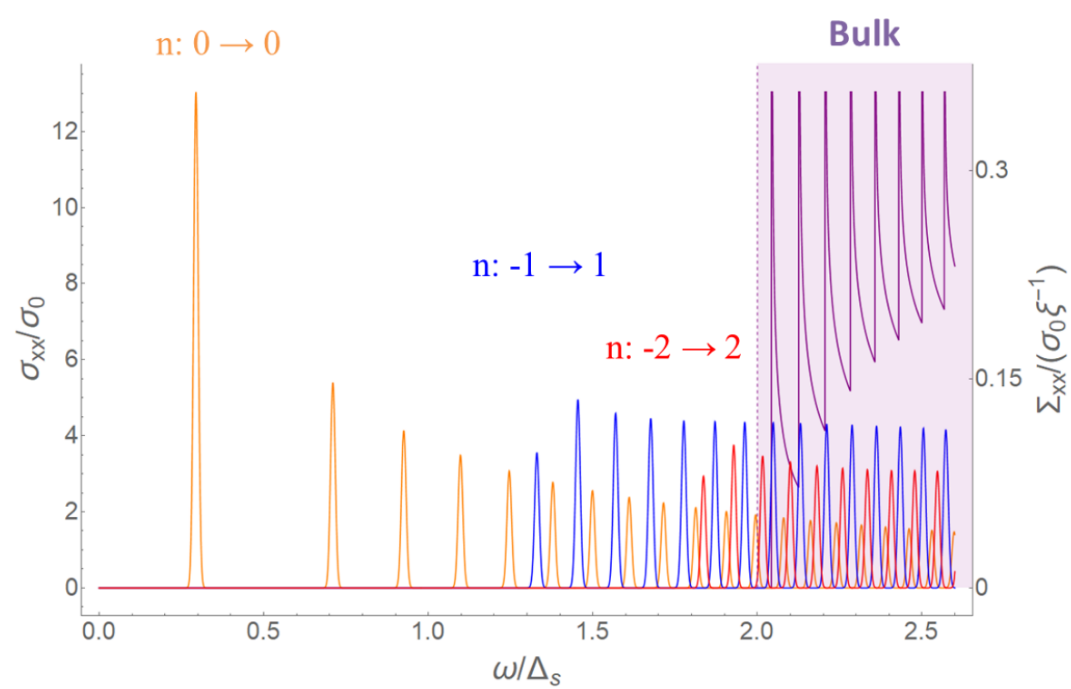


selection rules:

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

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

(polarisation in surface)

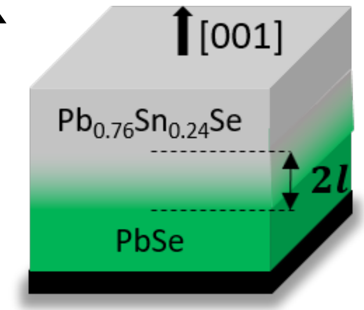


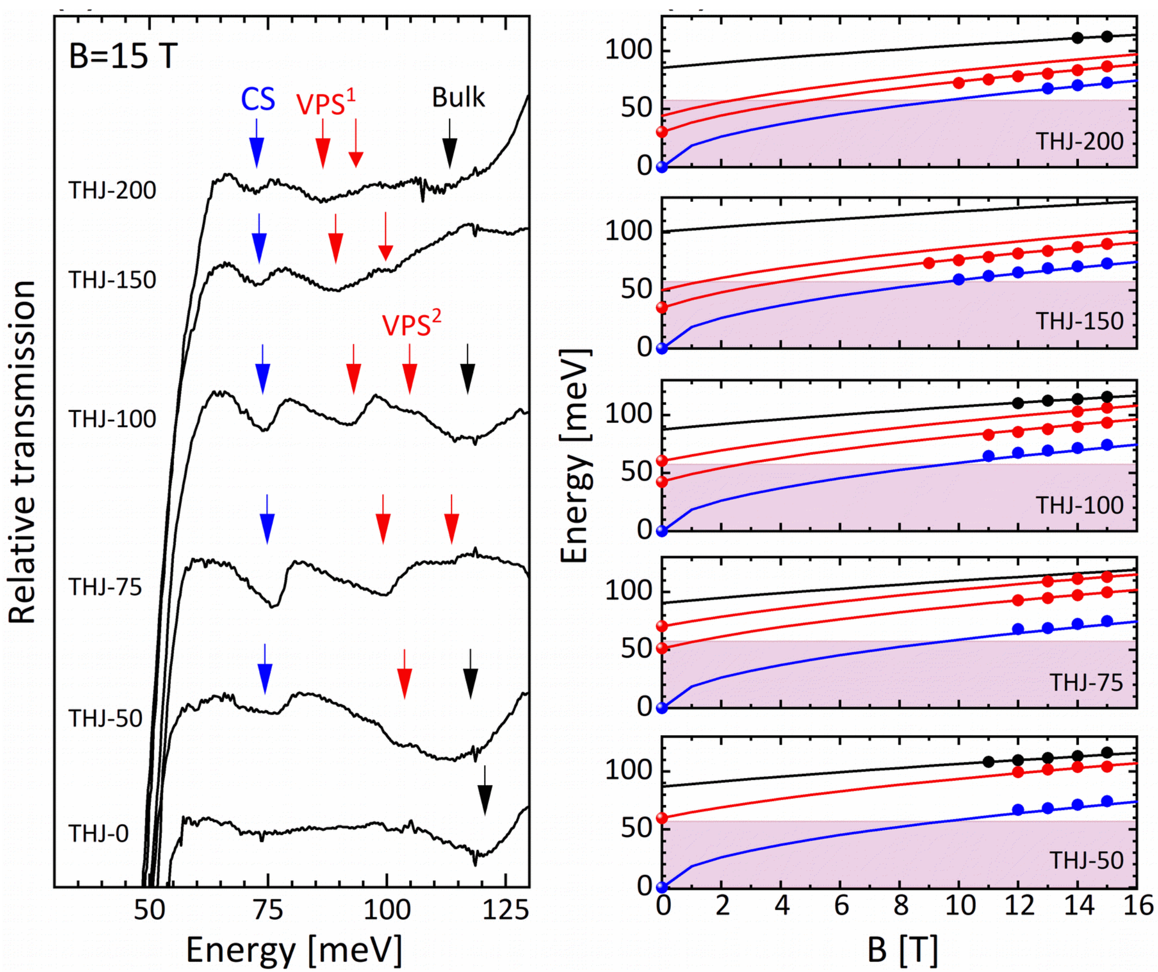
$$E_{\lambda,m,n} = \lambda\hbar v\sqrt{2m/l_B^2 + 2n/\ell_S^2}$$

Spectroscopic evidence for Volkov-Pankratov states in $Pb_{1-x}Sn_xSe$

*J. Bermejo-Ortiz et al., PRB **107**, 075129 (2023)*

MBE pseudoalloy growth

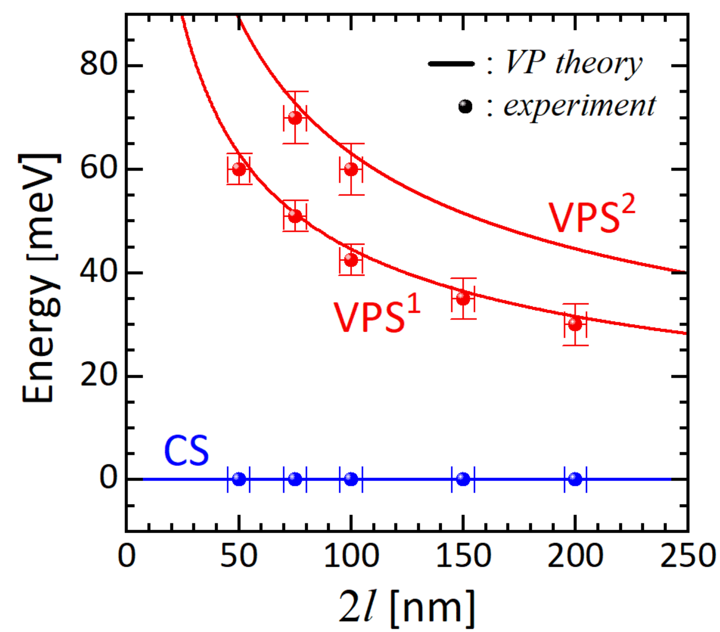




Faraday geometry

B→0 limit: fit with

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



Summary

– Relativistic renormalization of LL spectrum due to *Lorentz boosts* (in crossed magnetic and electric fields)

– *Tilt* in materials with tilted Dirac cones analogous to an *effective electric field* if material submitted to a magnetic field

- in 2D Dirac materials (organics)
- in type-I and type-II Weyl semimetals

Goerbig et al., EPL (2009)
Sári et al., PRB (2015)
Tchoumakov et al., PRL (2017)

– *Experimental evidence* for relativistic renormalization in (gapped) nodal-line semimetals → tilt depends on orientation of B-field

Wyzula et al., Adv. Sci. (2022)

– *Bulk-edge/surface correspondence* in topological matter
→ *Volkov-Pankratov states* in smooth interfaces

(a) in transport

*Tchoumakov et al., PRB **96**, 201302 (2017)*
Exp: Inhofer et al., PRB 96, 195104 (2017)

(b) in MO spectroscopy

*Lu, MOG, EPL **126**, 67004 (2019)*
Exp: Bermejo-Ortiz et al., PRB 107, 075129 (2023)