Signatures of Relativistic Covariance in 2D and 3D Weyl Semimetals

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Frontiers in Topological Quantum Matter – Nordita, 05/05/2017

Outline

- Massless Dirac fermions in 2D materials: from graphene to α-(BEDT-TTF)$_2$I$_3$

- Tilted Dirac cones – theoretical description

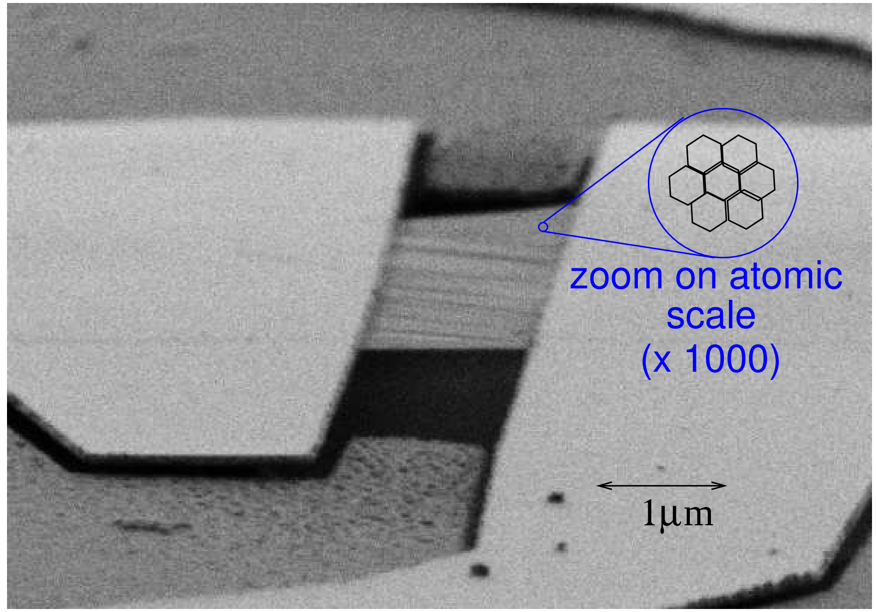
- Pseudo-relativity in α-(BEDT-TTF)$_2$I$_3$ in a magnetic fields

$\Rightarrow$ Effects on magneto-optics

- Weyl fermions in 3D materials

It all started with graphene

- one-atom thick layer of graphite, isolated in 2004
- electronic conductor
- flexible membrane of exceptional mechanical stability
- Nobel Prize in Physics, 2010



Chuan Li, physique mésoscopique, LPS, Orsay

<u>Interest for fundamental research:</u>

"Quantum mechanics meets relativity in condensed matter"

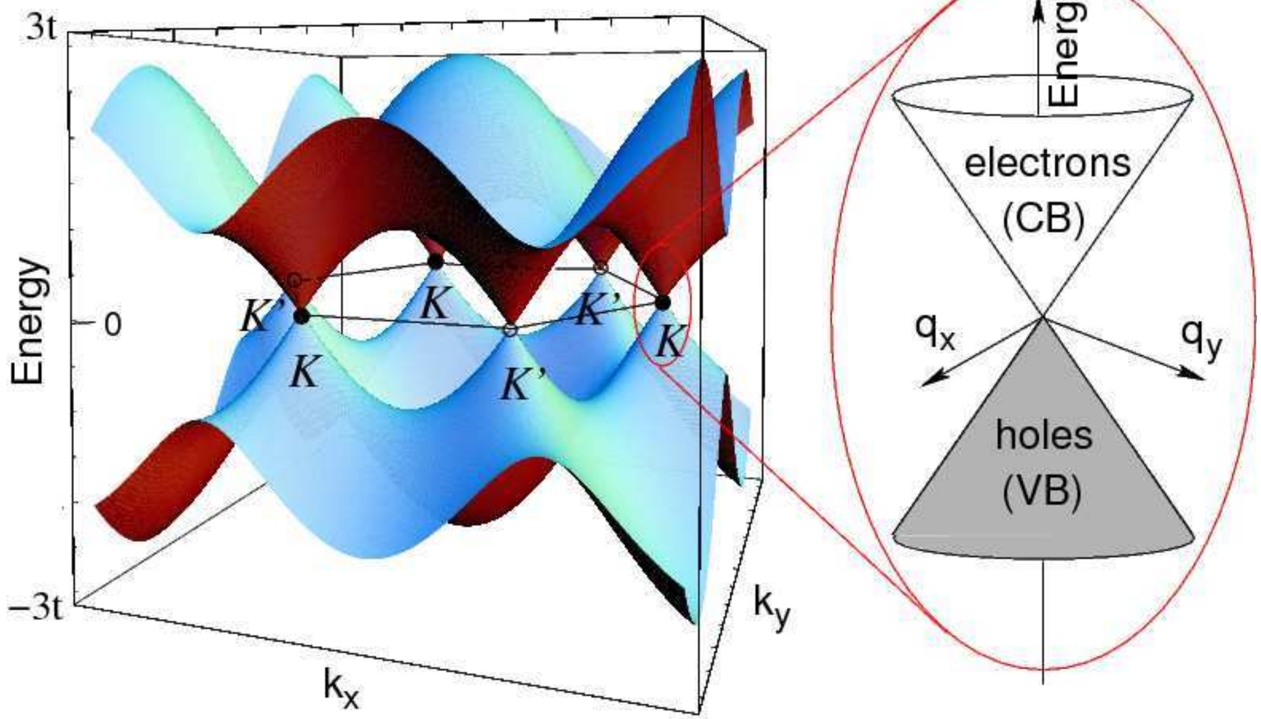
(electrons behave as 2D massless Dirac fermions)

Band structure of graphene

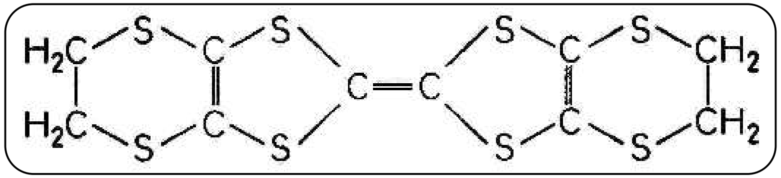
Dirac Hamiltonian (two *valleys* $\xi = \pm$ $\sim$ fermion doubling)

$$\mathcal{H}_{\mathbf{q}}^{\xi} \simeq \hbar v_F \begin{pmatrix} 0 & \xi q_x - i q_y \\ \xi q_x + i q_y & 0 \end{pmatrix}$$

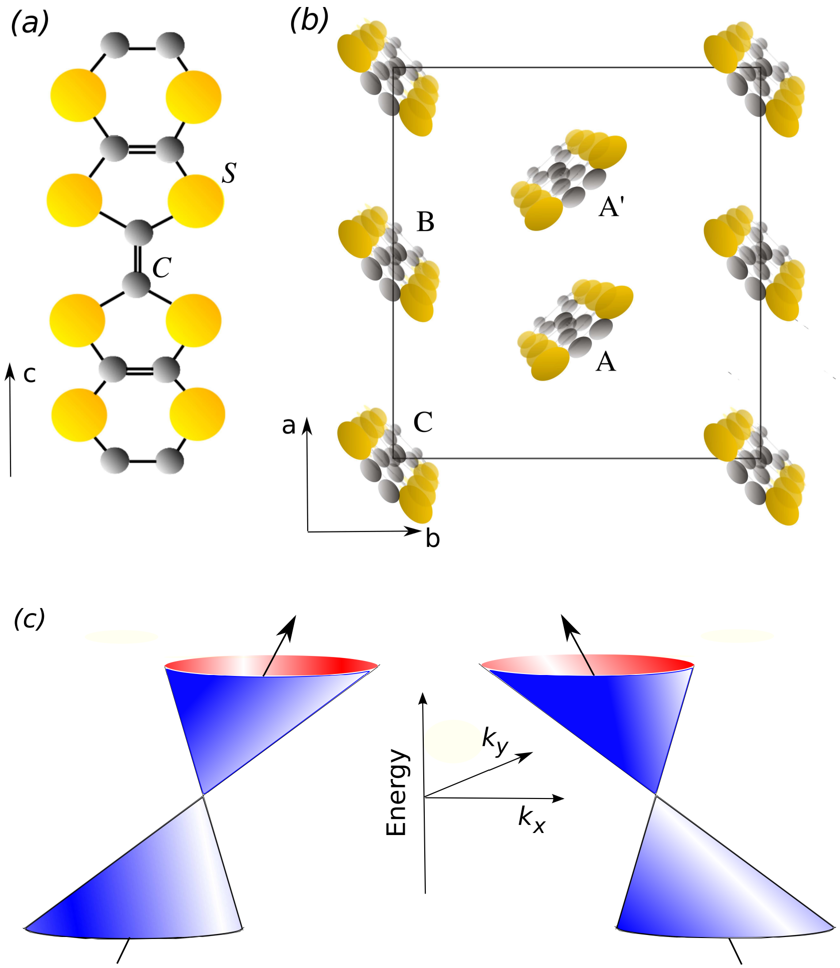
t ~ 3 eV ~ 36 000 K



α-(BEDT-TTF)$_2$I$_3$: another 2D Dirac material



BEDT-TTF
=bis(ethylenedithio)tetrathiafulvalene

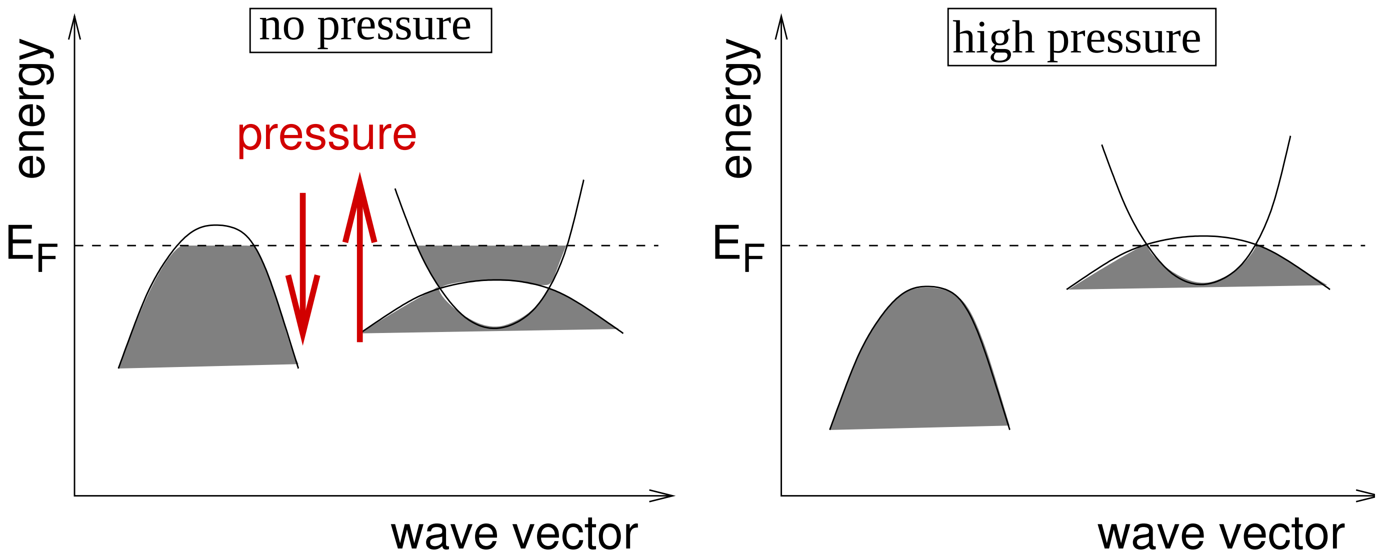


- quasi-2D (stacked layers)
- 4 molecules/unit cell $\rightarrow$ 4 bands
- electronic filling 3/4
- $t_i \sim 20...140$ meV

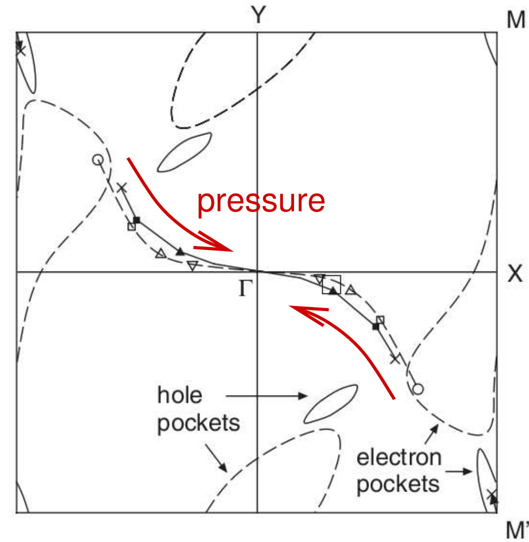
under pressure: low-energy tilted Dirac cones

α-(BEDT-TTF)$_2$I$_3$: electronic band structure

schematic view on upper two bands



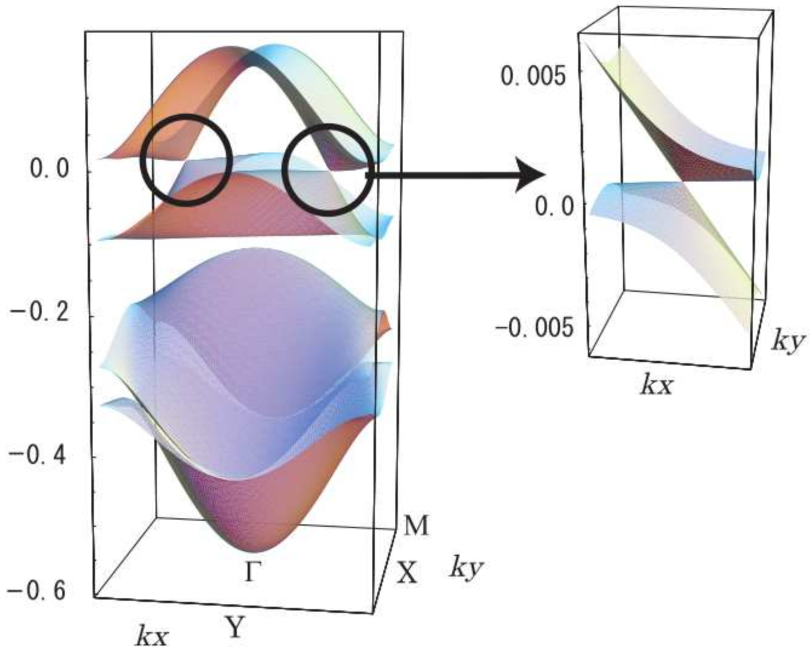
Brillouin zone



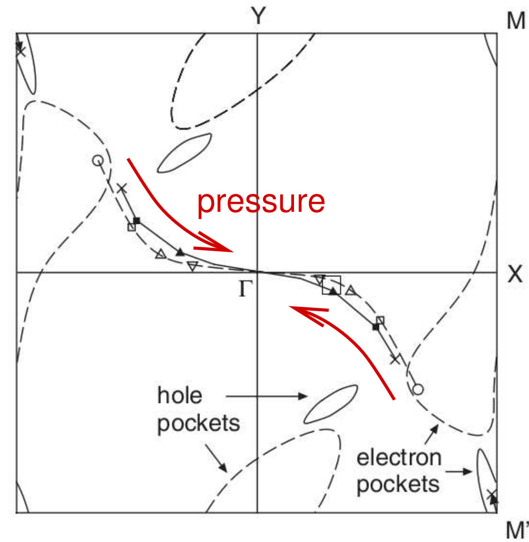
Katayama, Kobayashi, Suzumura, J. Phys. Soc. Japan **75**, 054705 (2006)

α-(BEDT-TTF)$_2$I$_3$: electronic band structure

energy bands under pressure



Brillouin zone



Katayama, Kobayashi, Suzumura, J. Phys. Soc. Japan **75**, 054705 (2006)

Theoretical description of tilted 2D Dirac cones

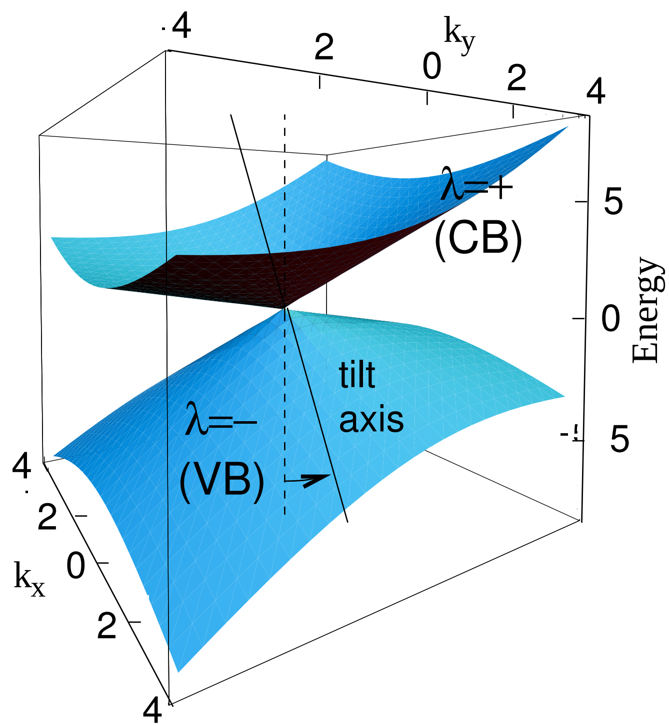
Most general 2D Hamiltonian (2×2 matrix) with linear dispersion (generalised Weyl Hamiltonian):

$$H = \sum_{\mu=0}^{3} \hbar \mathbf{v}_\mu \cdot \mathbf{q}\, \sigma^\mu \qquad (\sigma^0 = \mathbb{1},\ \sigma^1 = \sigma^x,\ \sigma^2 = \sigma^y,\ \sigma^3 = \sigma^z)$$

$$\hat{=}\ \hbar\left(\mathbf{w}_0 \cdot \mathbf{q}\, \mathbb{1} + w_x q_x \sigma^x + w_y q_y \sigma^y\right)$$

Energy dispersion ($\hbar \equiv 1,\ \lambda = \pm$):

$$\epsilon_\lambda(\mathbf{q}) = \mathbf{w}_0 \cdot \mathbf{q} + \lambda\sqrt{w_x^2 q_x^2 + w_y^2 q_y^2}$$

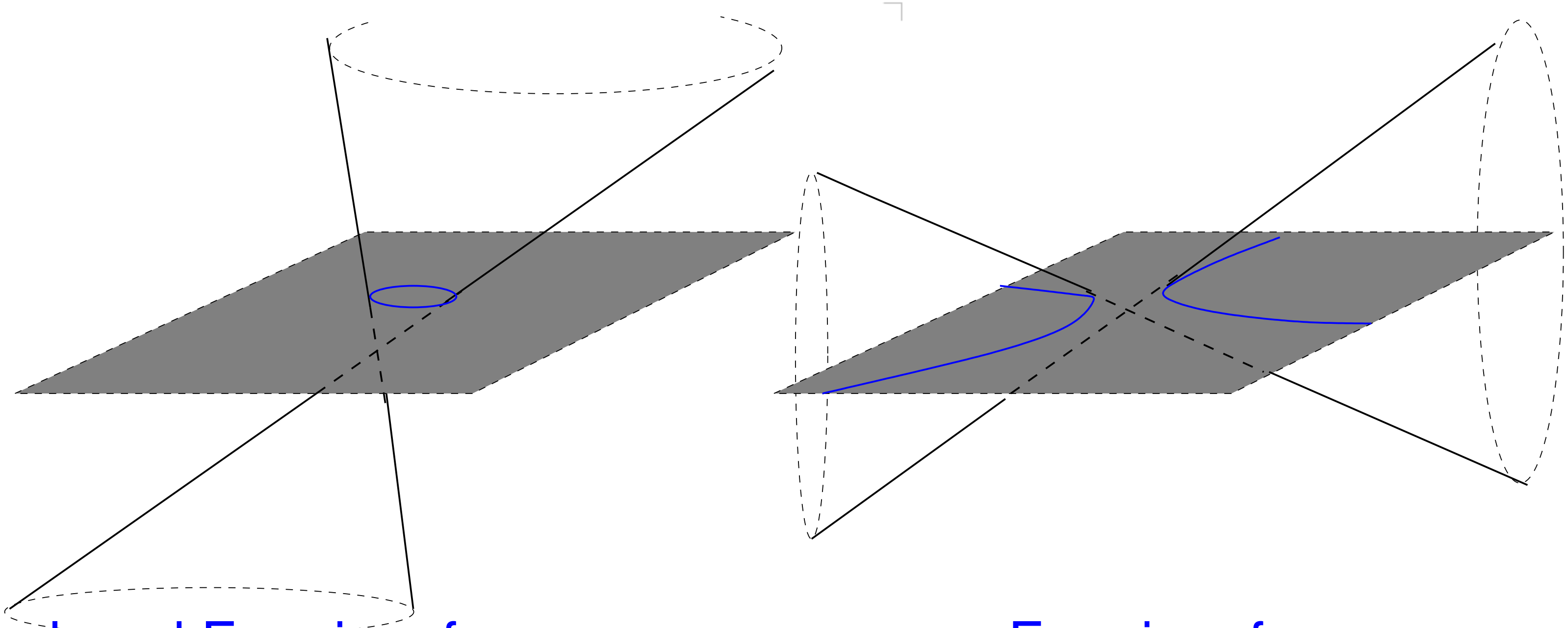


$\mathbf{w}_0$: "tilt velocity"

Graphene: $\mathbf{w}_0 = 0,\ w_x = w_y = v_F$

Criterion for maximal tilt

$$\left(\frac{w_{0x}}{w_x}\right)^2 + \left(\frac{w_{0y}}{w_y}\right)^2 < 1 \qquad \left(\frac{w_{0x}}{w_x}\right)^2 + \left(\frac{w_{0y}}{w_y}\right)^2 > 1$$



closed Fermi surface (ellipse) | open Fermi surface (hyperbolas)

MOG, J.-N. Fuchs, G. Montambaux, F. Piéchon, PRB (2008)

Criterion for maximal tilt

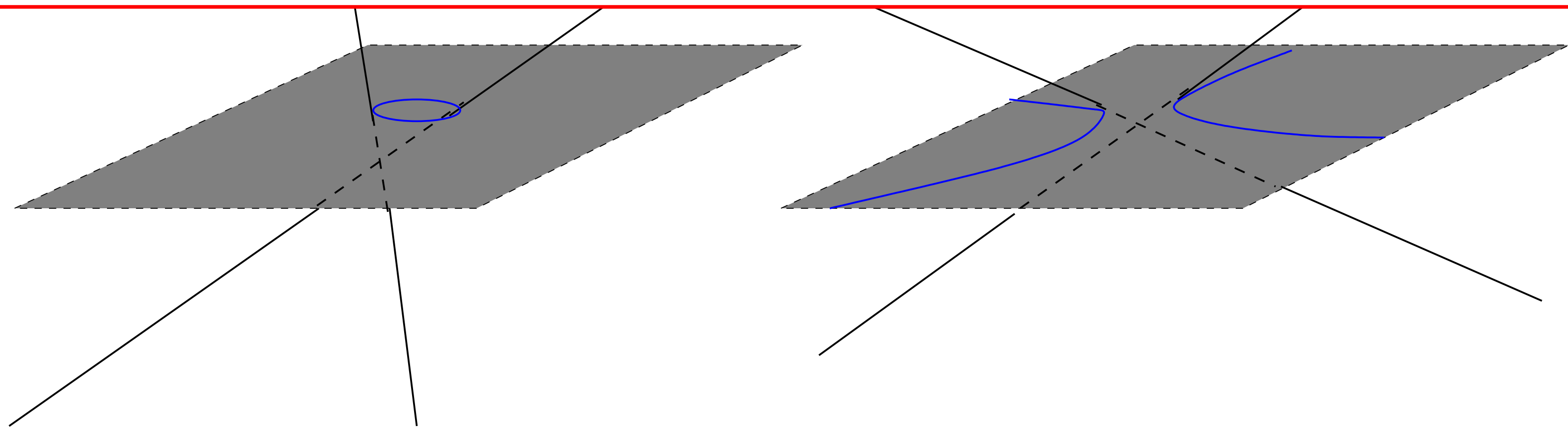
in 3D :

A New Type of Weyl Semimetals

Alexey A. Soluyanov[1], Dominik Gresch[1], Zhijun Wang[3], QuanSheng Wu[1], Matthias Troyer[1], Xi Dai[2], and B. Andrei Bernevig[3]
[1] *Institute for Theoretical Physics, ETH Zürich, 8093 Zürich, Switzerland*
[2] *Institute of Physics, Chinese Academy of Sciences, Beijin 100190, China and*
[3] *Department of Physics, Princeton University, New Jersey 08544, USA*
(Dated: July 8, 2015)

arXiv:1507.01603

Nature (2015)



closed Fermi surface
(ellipse)

open Fermi surface
(hyperbolas)

MOG, J.-N. Fuchs, G. Montambaux, F. Piéchon, PRB (2008)

Tilted cones in a strong magnetic field

How is the Landau level spectrum affected by the tilt?

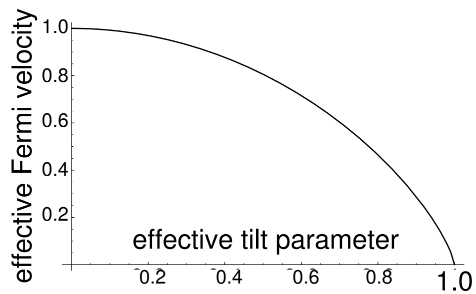
$$H_\xi = \xi \left(\mathbf{w}_0 \cdot \mathbf{q}\, \mathbb{1} + w_x q_x \sigma^x + w_y q_y \sigma^y \right) \qquad \tilde{w}_0 = \sqrt{\left(\frac{w_{0x}}{w_x}\right)^2 + \left(\frac{w_{0y}}{w_y}\right)^2}$$

⊕ Peierls substitution: $\mathbf{q} \to \mathbf{q} + e\mathbf{A}(\mathbf{r})$

- semiclassics: $q \sim \sqrt{2n}/l_B$, ($l_B = 1/\sqrt{eB}$: magnetic length)

⇒ energy spectrum (as for graphene):

$$\epsilon_{\lambda,n} = \lambda \frac{v_F^*}{l_B}\sqrt{2n}$$



- effect of the tilt: renormalisation $v_F^* = \sqrt{w_x w_y}\,(1 - \tilde{w}_0^2)^{3/4}$

MOG, J.-N. Fuchs, F. Piéchon, G. Montambaux, PRB **78**, 045415 (2008)

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

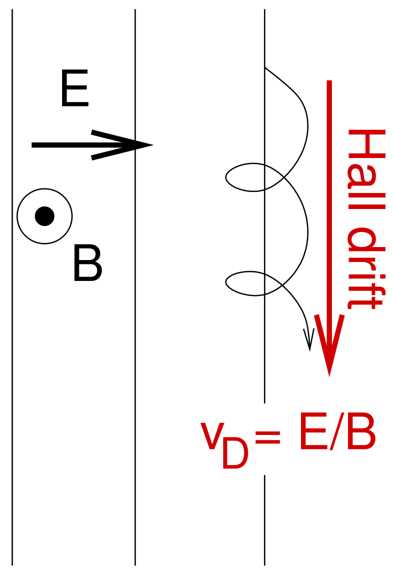
$$H_0(\hbar\mathbf{q}) \qquad \rightarrow \qquad H_0(\mathbf{p} + e\mathbf{A}(\mathbf{r})) - eEy$$

- (non-relativistic) Schrödinger fermions

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

- Landau levels

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



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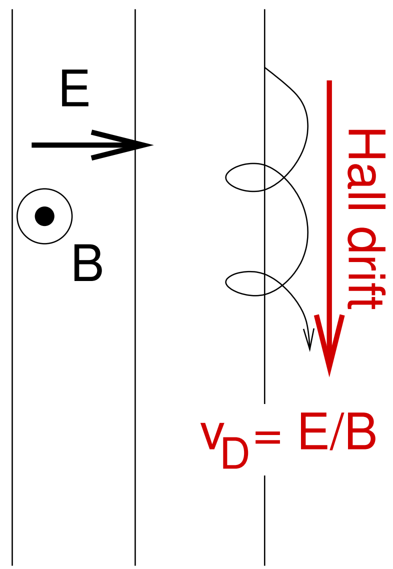
$$H_0(\hbar\mathbf{q}) \qquad \to \qquad H_0(\mathbf{p} + e\mathbf{A}(\mathbf{r})) - eEy$$

- relativistic electrons (graphene)

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

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

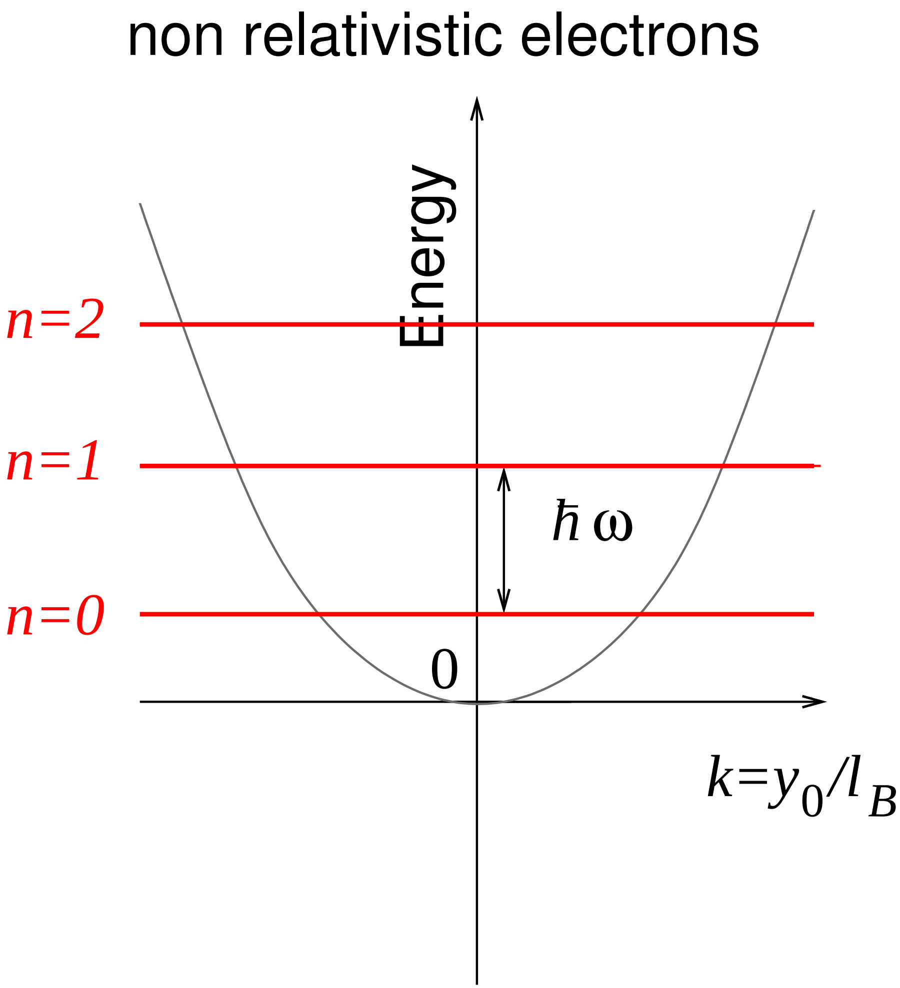
$$\epsilon \quad \to \quad \epsilon' \propto 1/l'_B \propto \sqrt{B'}$$

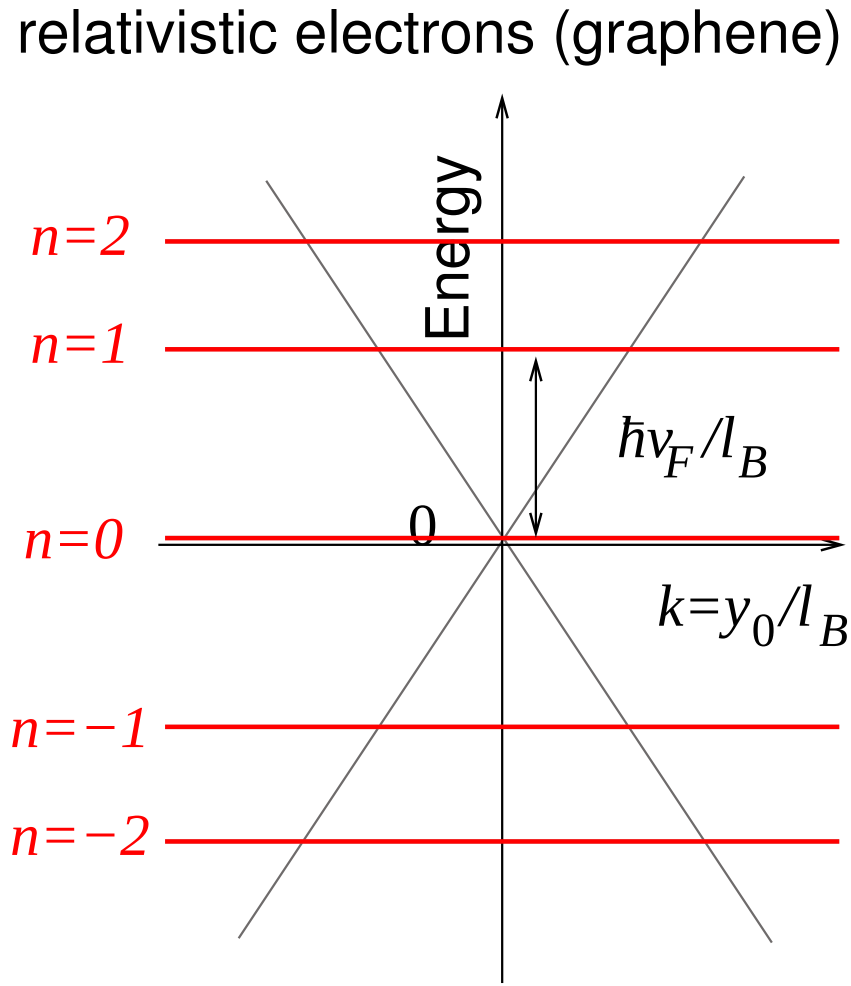


$\to$ energy in lab frame

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

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

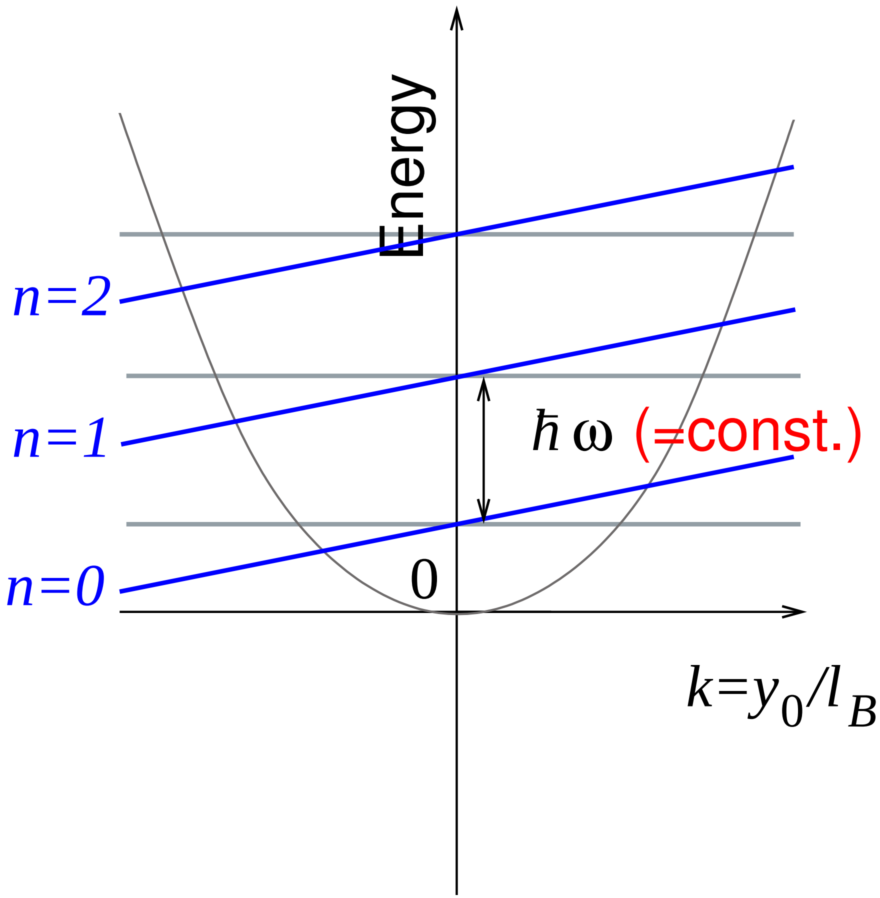




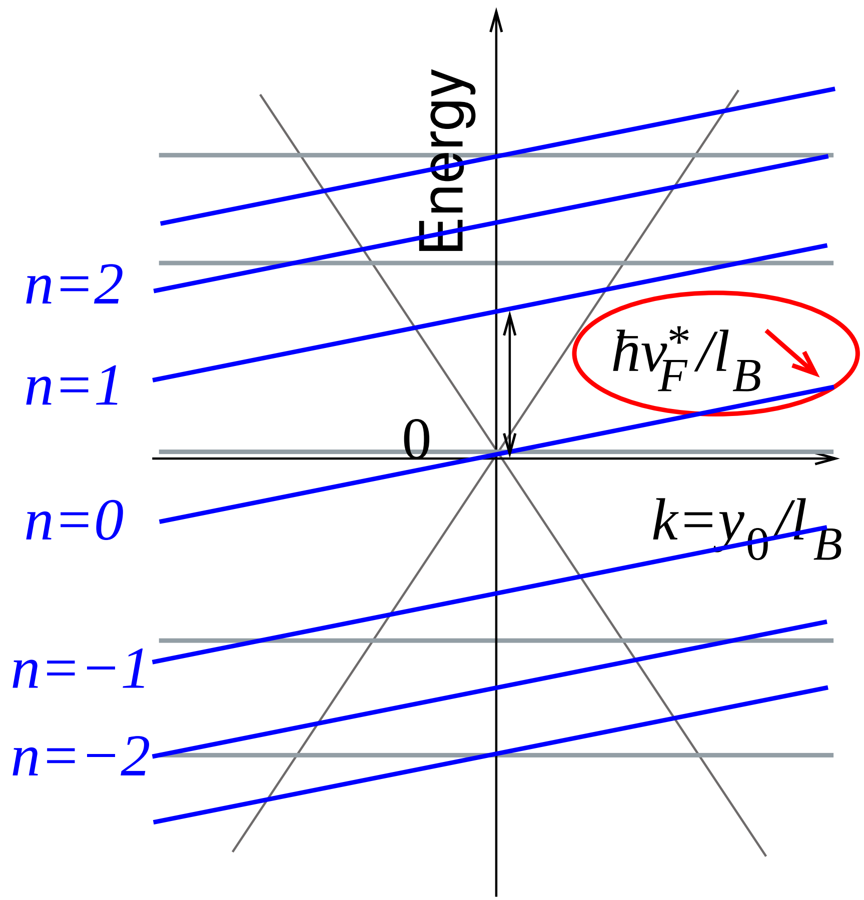
no electric field

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

non relativistic electrons



relativistic electrons (graphene)



in the presence of an electric field

Pseudo-covariance in α-(BEDT-TTF)$_2$I$_3$

- (Weyl) Hamiltonian

$$H_0(\mathbf{q}) = \begin{pmatrix} 0 & \hbar(w_x q_x - i w_y q_y) \\ \hbar(w_x q_x + i w_y q_y) & 0 \end{pmatrix} \rightarrow H_0(\mathbf{q}) + \hbar w_0 q_x \mathbb{1}$$

- tilt term in a magnetic field

$$\hbar w_0 q_x \mathbb{1} \rightarrow w_0(p_x + eA_x(\mathbf{r}))\mathbb{1} = w_0(p_x - eBy)\mathbb{1}$$

$\Rightarrow$ same (relativistic) model as before with $v_D = w_0 = E/B$
[MOG, Fuchs, Montambaux, Piéchon, EPL 2009]

- maximal tilt ($v_D = v_F$) related to maximal velocity for Lorentz boost

Covariance and wave functions

- Lorentz boost in x-direction (with $w_0 = E_{\rm eff}/B$):

$$x'^{\mu} = \Lambda^{\mu}_{\nu} x^{\nu} \qquad (v_F t', x') = (v_D t + \beta x)/\sqrt{1-\beta^2}$$

- transformation of wave function ($\tanh\theta = \beta = v_D/v_F$):

$$\psi'(v_F t', x', y) = S(\Lambda)\psi(v_F t, x, y) \qquad \text{with} \qquad S(\Lambda) = e^{\theta\sigma_x/2}$$

- ...needed in matrix element of light-matter coupling

$$\propto \ \psi'^{\dagger} \mathbf{v} \psi'$$

$\mathbf{v}$: velocity operator

Light-matter coupling

- Peierls substitution $\mathbf{q} \to \mathbf{q} + \frac{e}{\hbar}\left[\mathbf{A}(\mathbf{r}) + \mathbf{A}_{\mathrm{rad}}(t)\right]$
- $\nabla \times \mathbf{A}(\mathbf{r}) = \mathbf{B}$ (magnetic field), $\mathbf{A}_{\mathrm{rad}}(t)$ (radiation field)

$\to$ in Hamiltonian (linear expansion in radiation field)

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

- $\mathcal{H}_B \to$ Landau levels, velocity operator $\mathbf{v} = \nabla_{\mathbf{q}}\mathcal{H}/\hbar$

<u>dipolar selection rules (in comoving frame):</u>

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

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

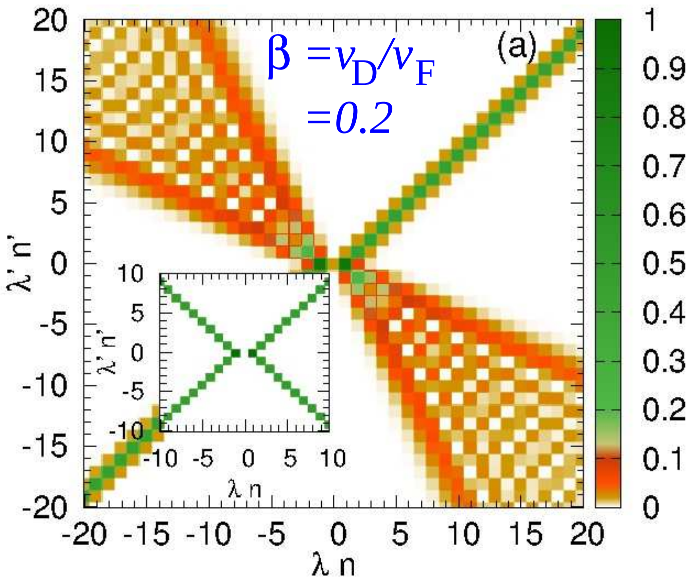
Magnetooptical selection rules

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

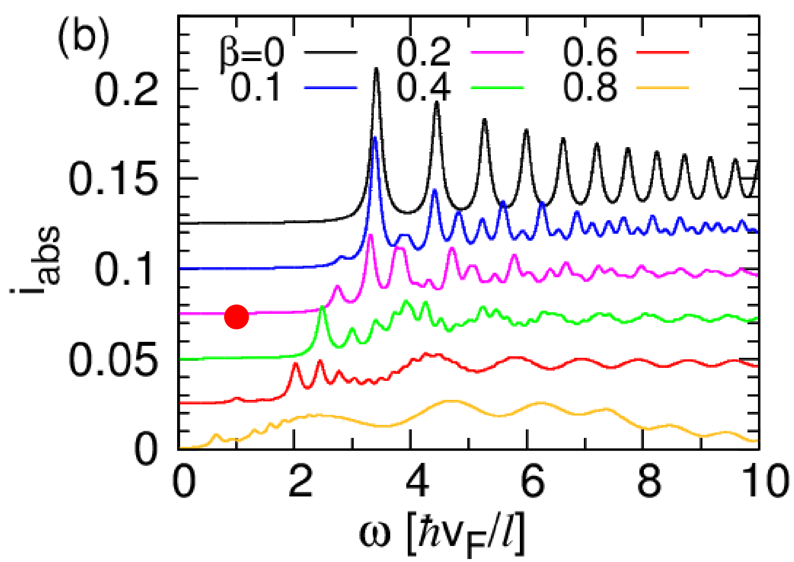
$$\lambda n \to \lambda'(n \pm 1)$$

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

matrix elements



absorption coefficient



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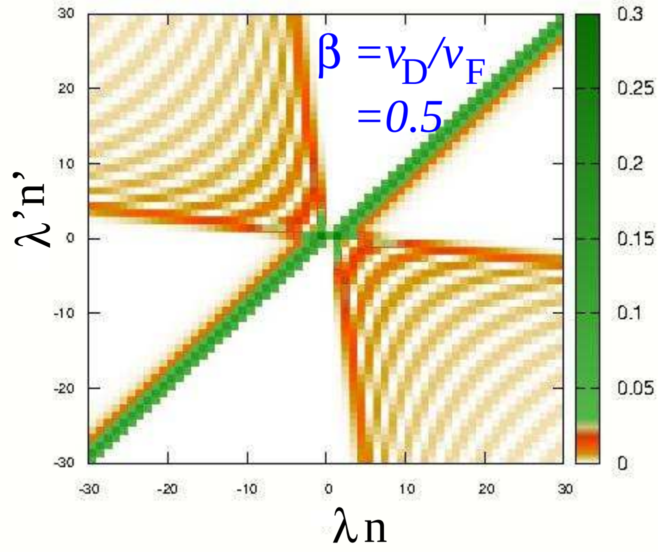
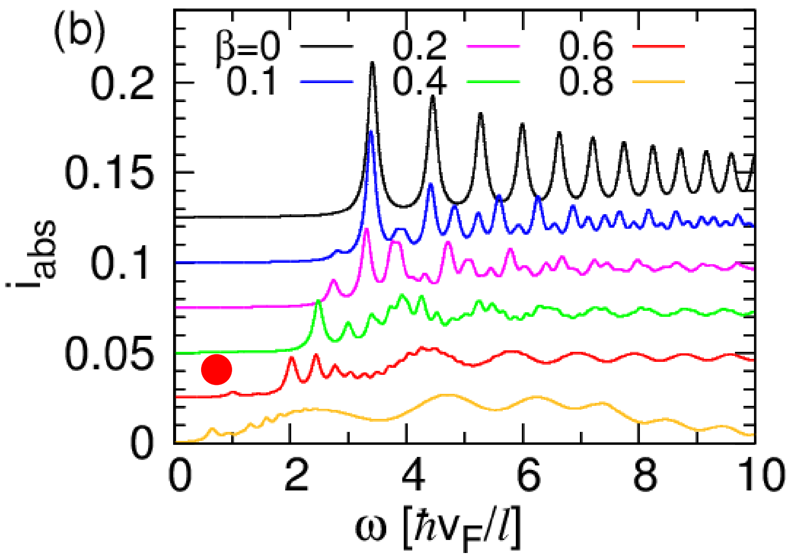


absorption coefficient



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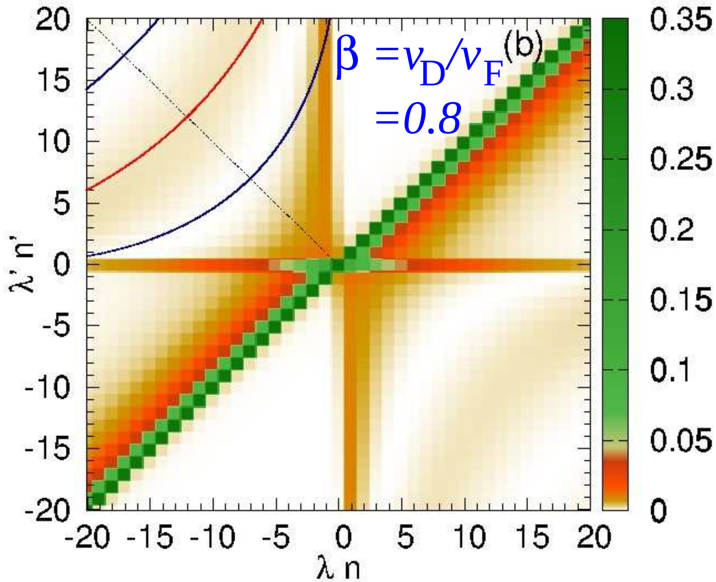
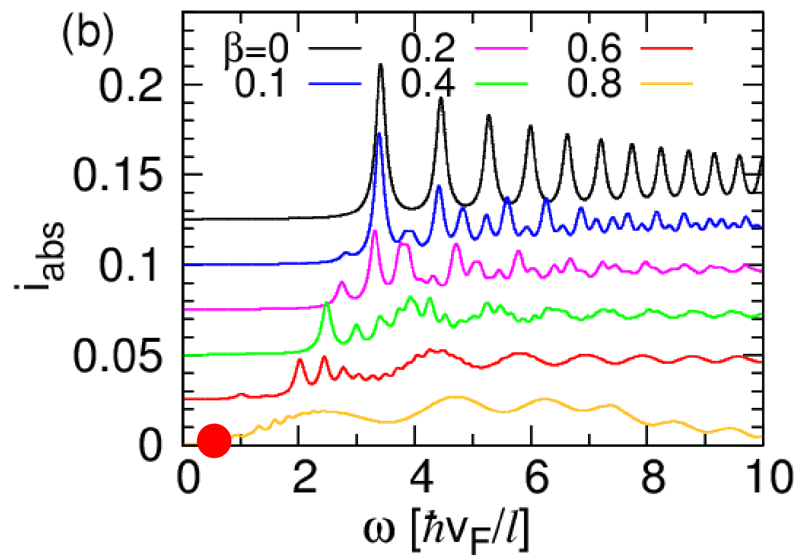


absorption coefficient



selection rules (absorbed frequencies) depend on frame of reference [Sári, MOG, Tőke, PRB 2015]

Tilted Cones in 3D Materials – Weyl Semimetals

in collaboration with :

S. Tchoumakov and M. Civelli

Phys. Rev. Lett. **117**, 086402 (2016)

similar results :

Z.-M. Yu, Y. Yao, S. Yang, PRL **117**, 077202 (2016)
M. Udagawa, E. Bergholtz, PRL **117**, 086401 (2016)

Theory of Weyl fermions with a tilt

2×2 matrix Hamiltonian with linear dispersion in 3D

$$H = \hbar \left(\mathbf{w}_0 \cdot \mathbf{q}\, \mathbb{1} + w_x q_x \sigma^x + w_y q_y \sigma^y + w_z q_z \sigma^z \right)$$

Energy dispersion ($\hbar \equiv 1,\ \lambda = \pm$):

$$\epsilon_\lambda(\mathbf{q}) = \mathbf{w}_0 \cdot \mathbf{q} + \lambda \sqrt{w_x^2 q_x^2 + w_y^2 q_y^2 + w_z^2 q_z^2}$$

$\mathbf{w}_0$: “tilt velocity”

$$\left(\frac{w_0 x}{w_x}\right)^2 + \left(\frac{w_0 y}{w_y}\right)^2 + \left(\frac{w_0 z}{w_z}\right)^2 < 1 \qquad \mathrm{type-I\ WSM}$$

$$\left(\frac{w_0 x}{w_x}\right)^2 + \left(\frac{w_0 y}{w_y}\right)^2 + \left(\frac{w_0 z}{w_z}\right)^2 > 1 \qquad \mathrm{type-II\ WSM}$$

Role of the magnetic field and Landau quantisation

tilt parameter (vector)

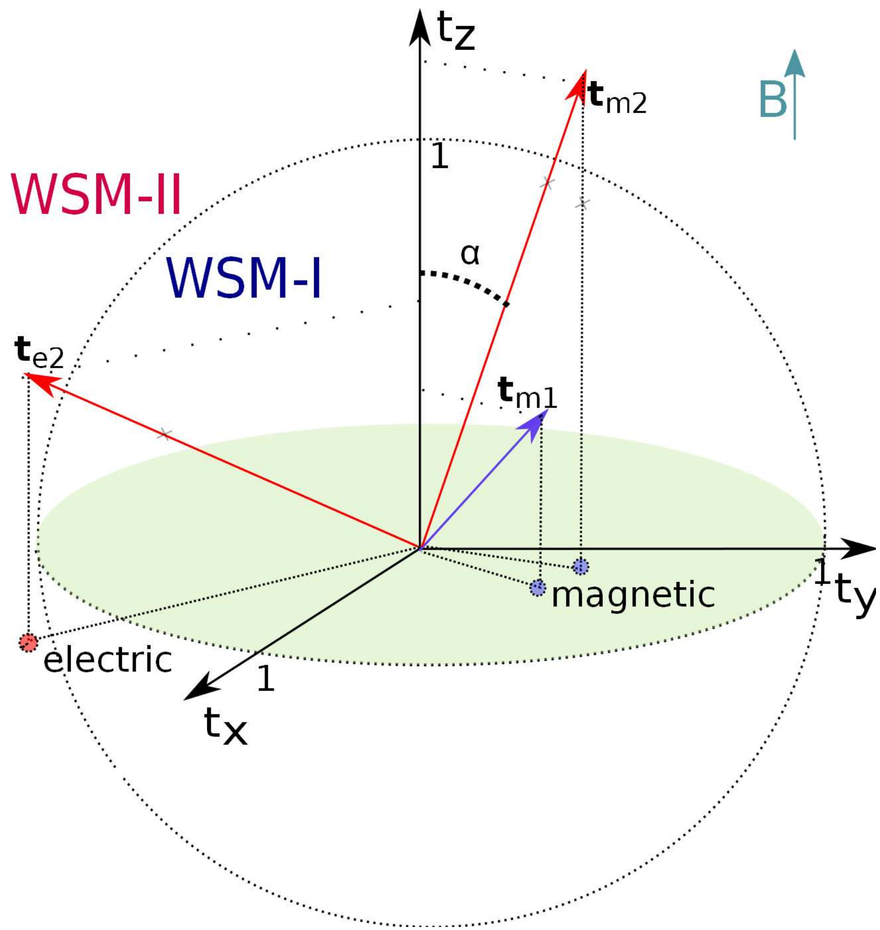
$$\mathbf{t} = \left(\frac{w_{0x}}{w_x}, \frac{w_{0y}}{w_y}, \frac{w_{0z}}{w_z} \right)$$

inplane tilt parameter

$$\mathbf{t}_\perp = \frac{\mathbf{t} \times \mathbf{B}}{B} = \left(\frac{w_{0x}}{w_x}, \frac{w_{0y}}{w_y} \right)$$

$\Rightarrow$ Landau level quantisation if B-field "close" to tilt axis

$$|\sin\alpha| < 1/|\mathbf{t}|$$



Landau quantisation

same recipe as for 2D:
Lorentz boost to a frame of reference, where $\mathbf{t}_\perp$ *vanishes*

1D Landau bands

$$\epsilon_{\lambda,n}(k_z) = w_{0z}k_z + \lambda\sqrt{1-\beta^2}\sqrt{w_z^2k_z^2 + 2\frac{w_x w_y\sqrt{1-\beta^2}}{l_B^2}n}$$

where $\beta = |\mathbf{t}_\perp|$

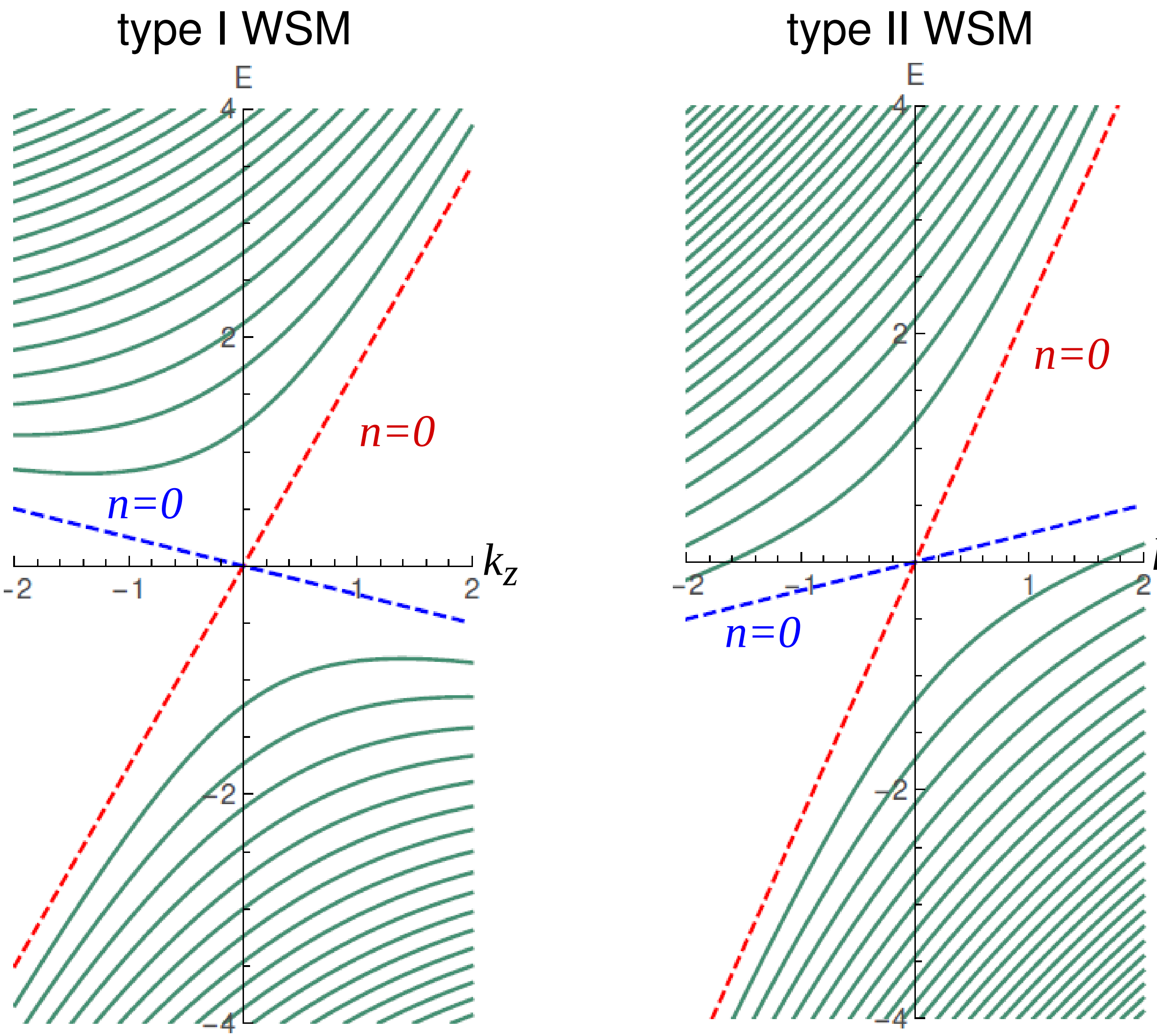
3-dimensional Weyl semimetals	$\lvert\mathbf{t}_\perp\rvert = \beta < 1$	$\lvert\mathbf{t}_\perp\rvert = \beta > 1$
$\lvert\mathbf{t}\rvert < 1$	type-I WSM *magnetic* regime	type-I WSM *electric* regime ?
$\lvert\mathbf{t}\rvert > 1$	type-II WSM *magnetic* regime	type-II WSM *electric* regime

Landau bands in the magnetic regime

WSM type confered to 1D bands

$$t_z = \frac{w_{0z}}{w'_z} = \frac{|\mathbf{t}\cos\alpha|}{\sqrt{1 - t^2 \sin^2\alpha}}$$

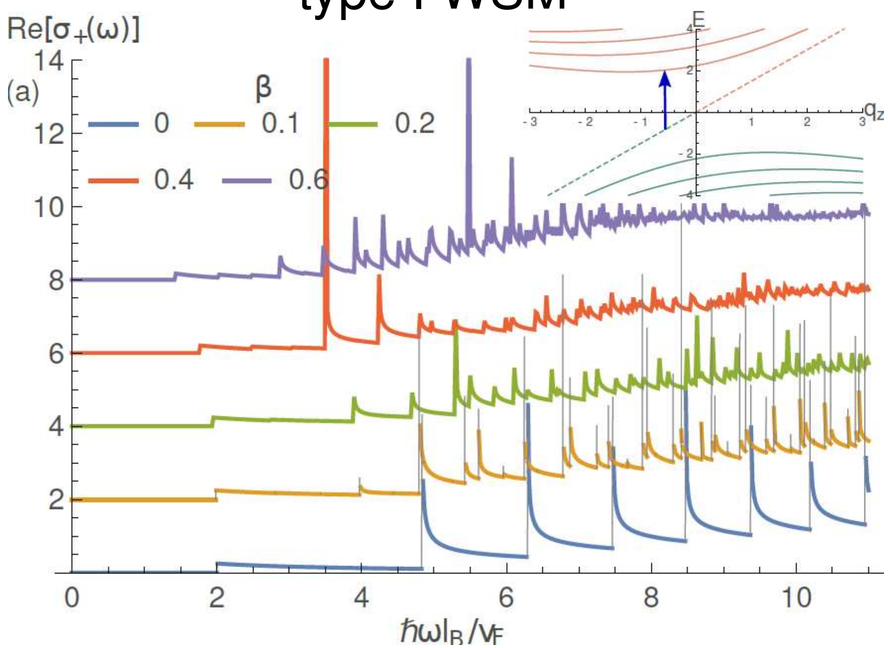
(1D tilt parameter)



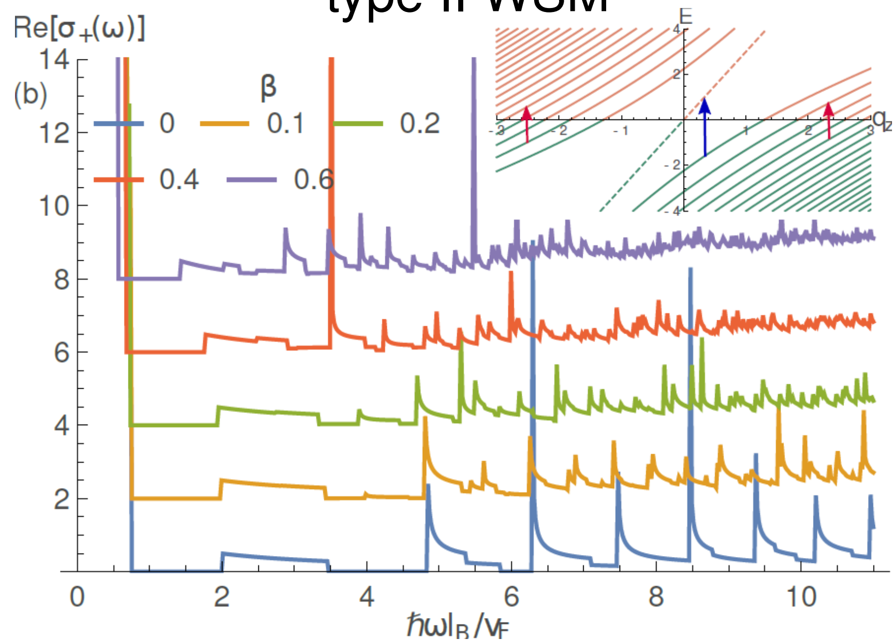
Optical conductivity of a WSM in the magnetic regime

$$\mathrm{Re}\ \sigma_{ll}(\omega) = \frac{\sigma_0}{2\pi l_B^2 \omega} \sum_{j,j'} |\mathbf{u}_l \cdot \mathbf{v}_{j,j'}|^2 \left[f(\epsilon_j) - f(\epsilon_{j'}) \right] \delta(\omega - \omega_{j,j'})$$

type I WSM



type II WSM



again: *violation of dipolar selection rules*

Conclusions

- massless fermions in 2D and 3D *tilted cones*
  - quasi-2D organic material α-(BEDT-TTF)$_2$I$_3$
  - 3D Weyl semimetals (Cd_3As_2, $MoTe_2$, WTe_2, ...)
- intimite relation with Lorentz boosts
  - 2D: magnetic regime = type-I (massless) Dirac semimetal
    electric regime = type-II (massless) Dirac semimetal

3-dimensional Weyl semimetals	$\|\mathbf{t}_\perp\| = \beta < 1$	$\|\mathbf{t}_\perp\| = \beta > 1$
$\|\mathbf{t}\| < 1$	type-I WSM *magnetic* regime	type-I WSM *electric* regime ?
$\|\mathbf{t}\| > 1$	type-II WSM *magnetic* regime	type-II WSM *electric* regime

- signatures expected in magneto-optical meaurements (violation of dipolar selection rules, $n \to n \pm 1$)

3D Topological Materials with Smooth Interfaces – Fermi Arcs and Surface States Obtained From Landau Quantisation

in collaboration with :

S. Tchoumakov and M. Civelli

`arXiv:1612.07693 (PRB in press)`

A. Inhofer, E. Bocquillon, B. Plaçais (groupe méso, LPA-ENS) ;
V. Jouffrey, D. Carpentier (ENS Lyon) ; Würzburg group

How to obtain surface states in topo. materials?

- 2D massive Dirac model

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

- gap inversion triggered by $\Delta x/\ell$ (interface of size ℓ)

How to obtain surface states in topo. materials?

- 2D massive Dirac model $\oplus$ interchange $\sigma_y \leftrightarrow \sigma_z$

$$H = \begin{pmatrix} vq_y & vq_x + i\Delta\frac{x}{\ell} \\ vq_x - i\Delta\frac{x}{\ell} & -vq_y \end{pmatrix}$$

- gap inversion triggered by $\Delta x/\ell$ (interface of size ℓ)

How to obtain surface states in topo. materials?

- 2D massive Dirac model $\oplus$ interchange $\sigma_y \leftrightarrow \sigma_z$

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

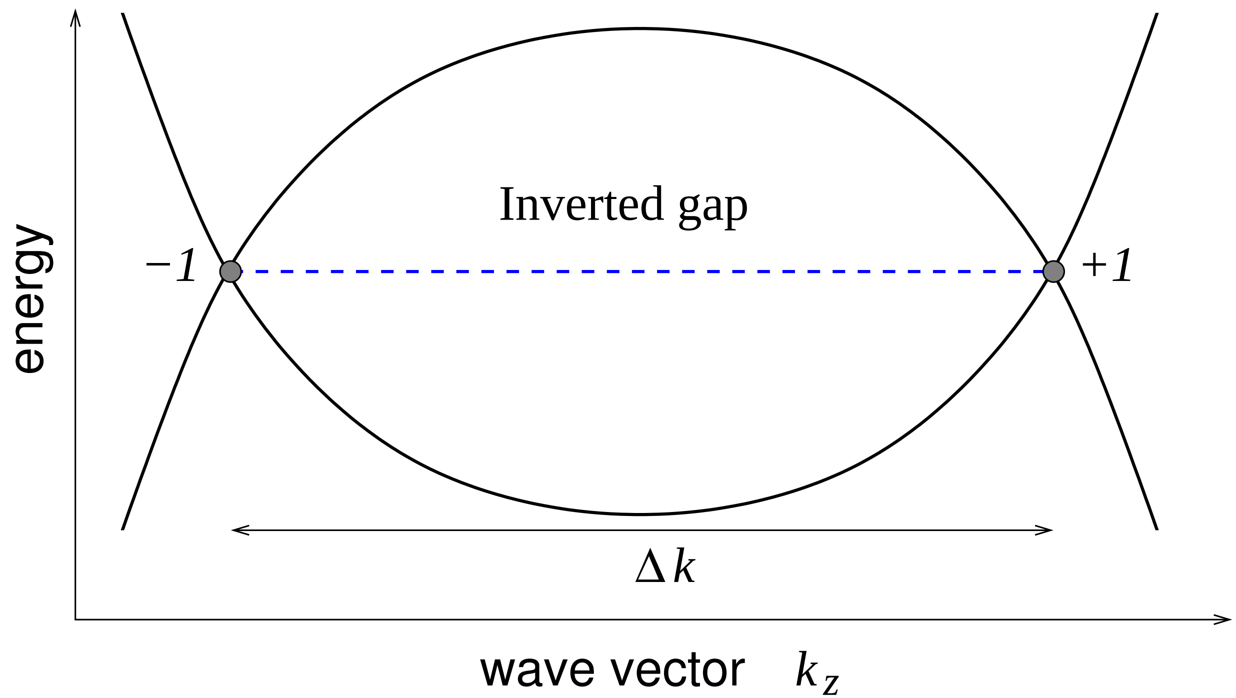
- gap inversion triggered by $\Delta x/\ell$ (interface of size ℓ)
- size of surface state given by "magnetic length" $\ell_S = \sqrt{\ell v/\Delta}$
- spectrum (in the interface)

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

- Complication in generalisation to 3D: minimal models are generically four-band models

Fermi arcs of 3D Weyl semimetals (I)

- Fermi arc connecting Weyl nodes at surface



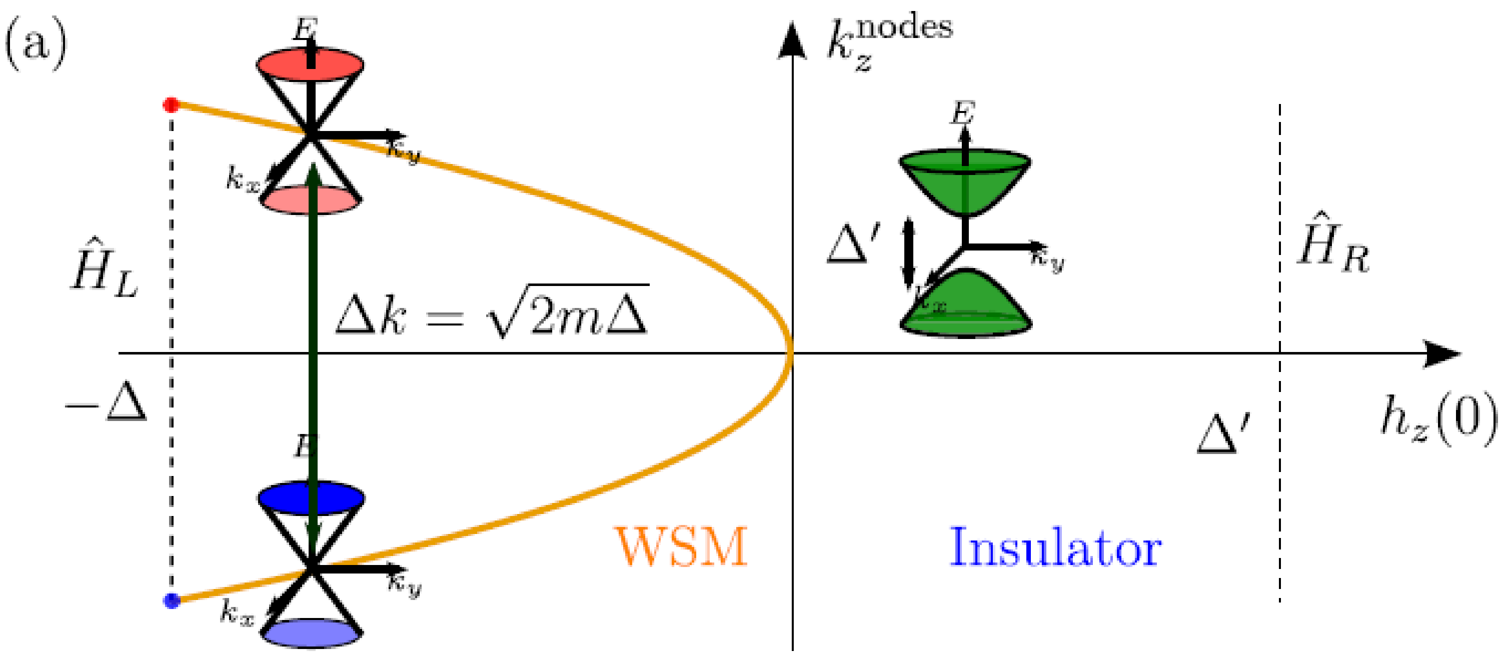
- at any value of k_z, system is either a 2D TI (inverted region) or a 2D trivial insulator

→ Fermi arc = k_z connection of all edge channels of the 2D TI

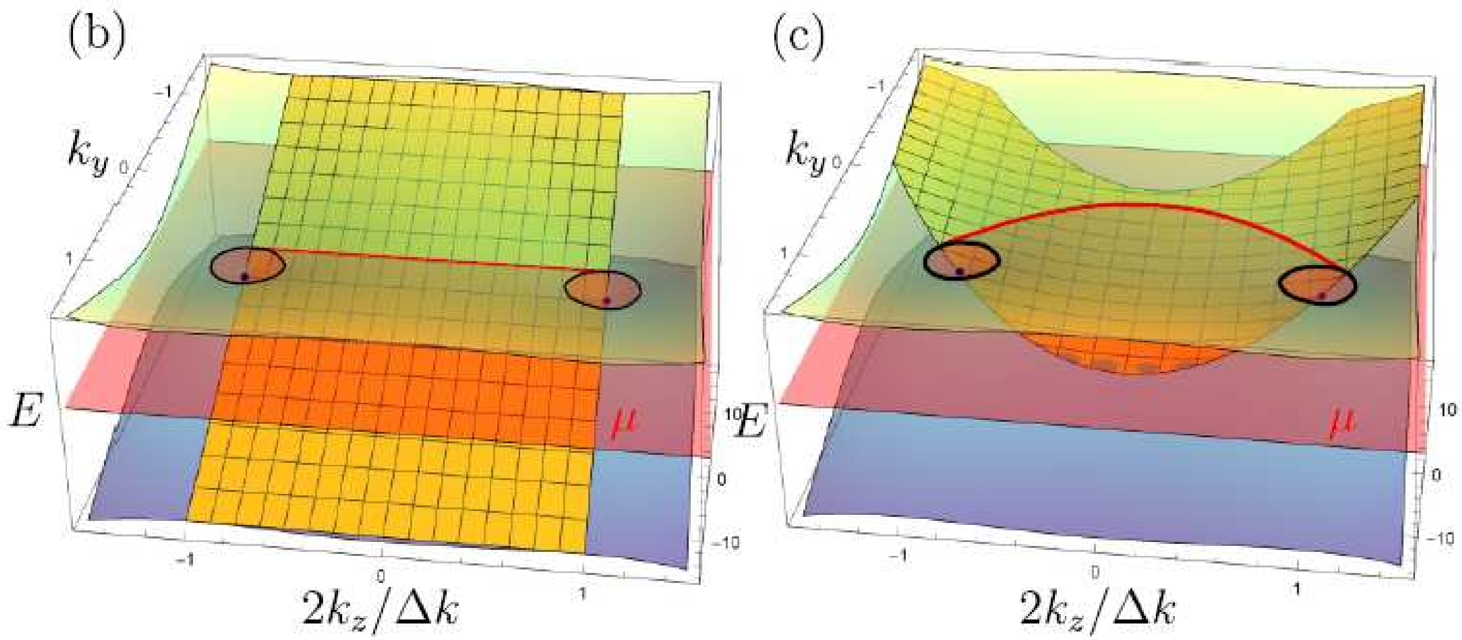
Fermi arcs of 3D Weyl semimetals (II)

Effective interface model for Weyl semimetals (node merging)
[generalisation from 2D, Montambaux, Piéchon, Fuchs, MOG (2009)]

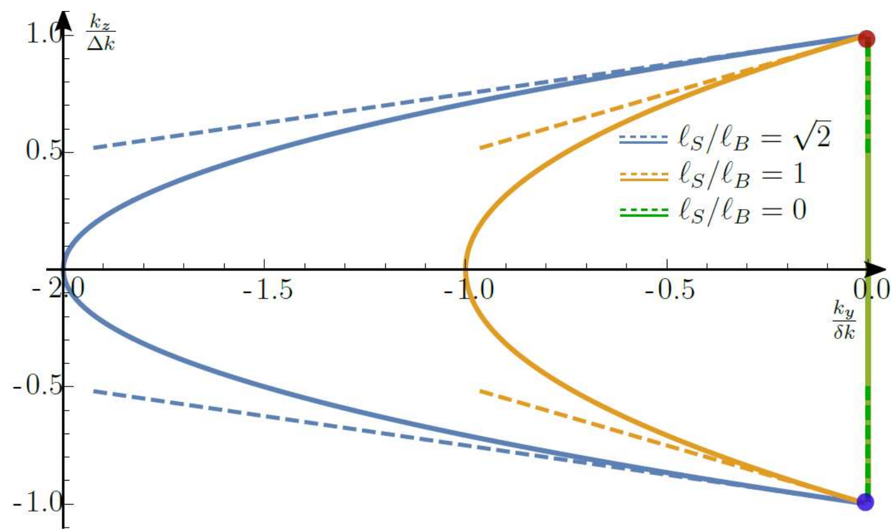
$$H = v(q_x\sigma_x + q_y\sigma_y) + \left(\frac{k_z^2}{2m} - \Delta + \bar{\Delta}\frac{x}{\ell}\right)\sigma_z$$



Manipulating Fermi arcs with a B-field

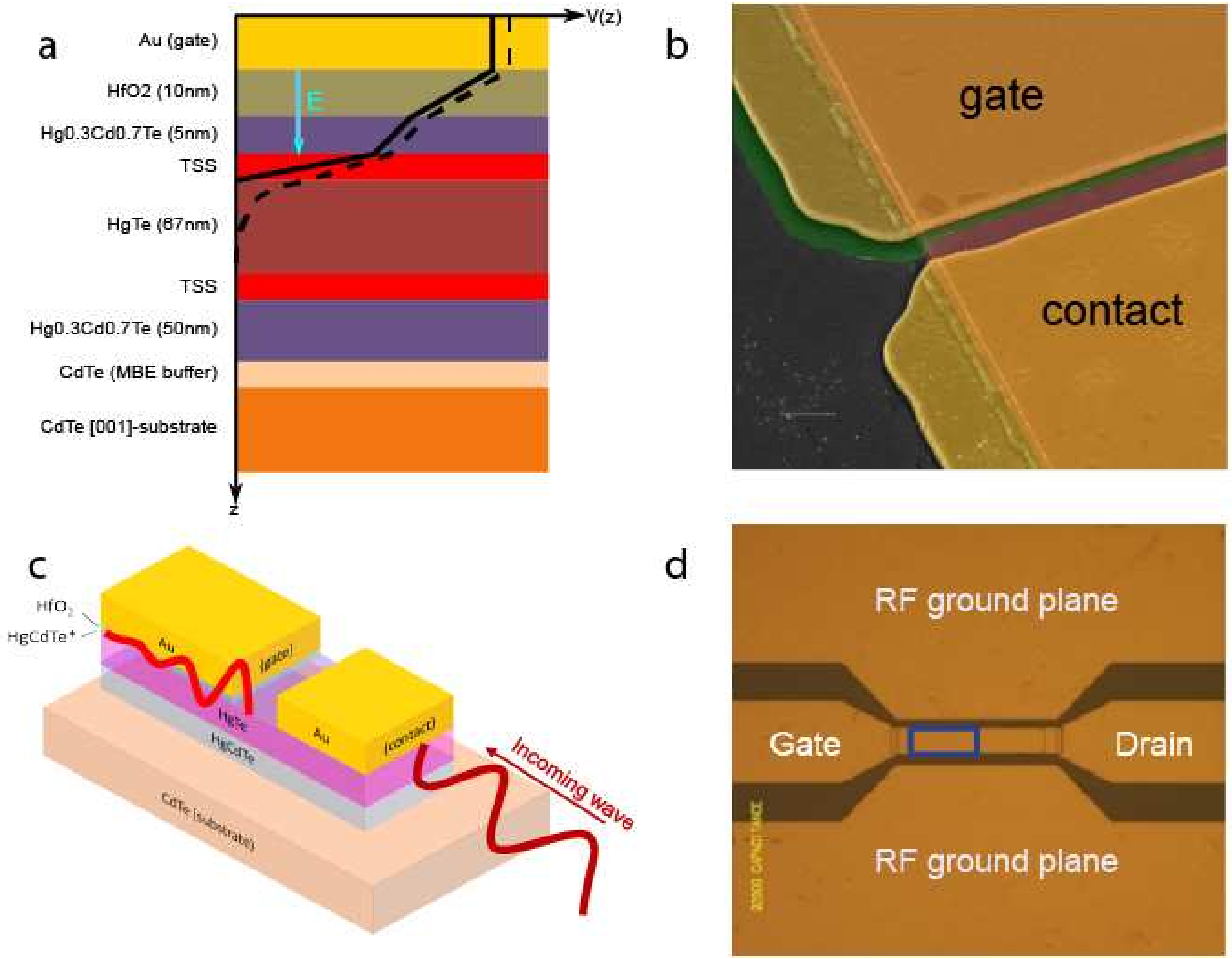


B-field parallel to surface conspires with "confinement field"
$\rightarrow$ Fermi arcs acquires dispersion in k_x

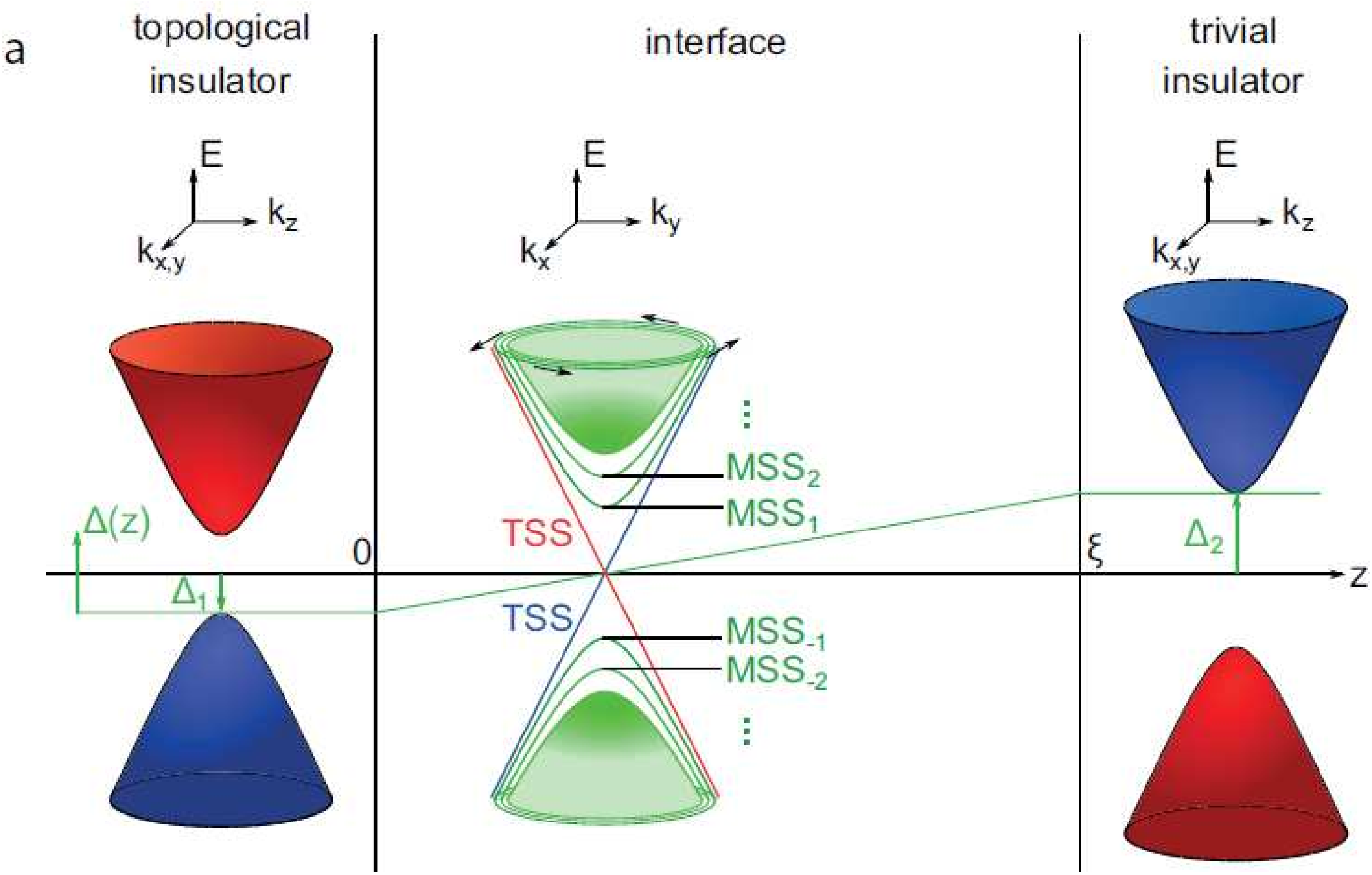


THz experiments in strained HgTe

Strained HgTe = 3D topological insulator (TI)



Topological and massive surface states in 3D TIs



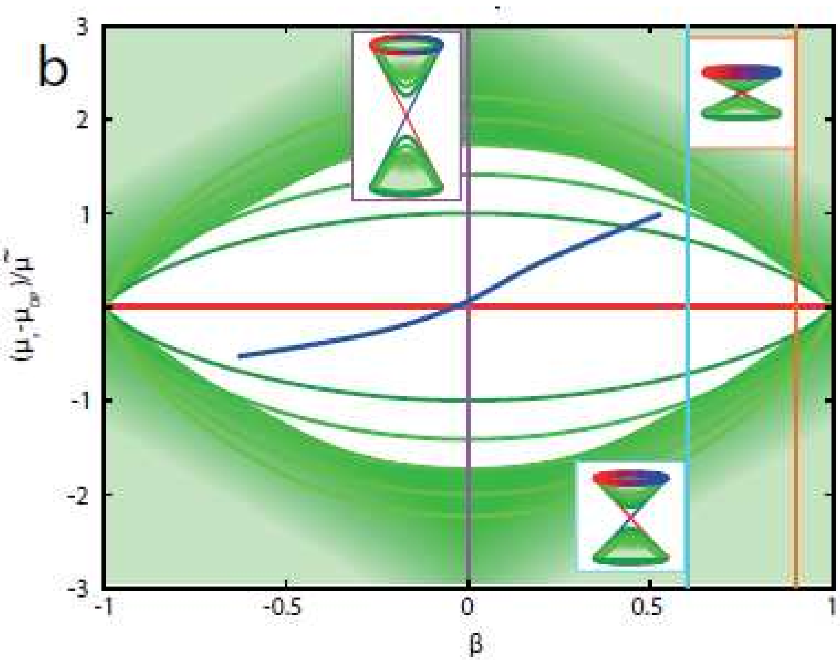
Surface states ressemble relativistic Landau bands

$\rightarrow$ can one probe relativistic properties of these surface states ?

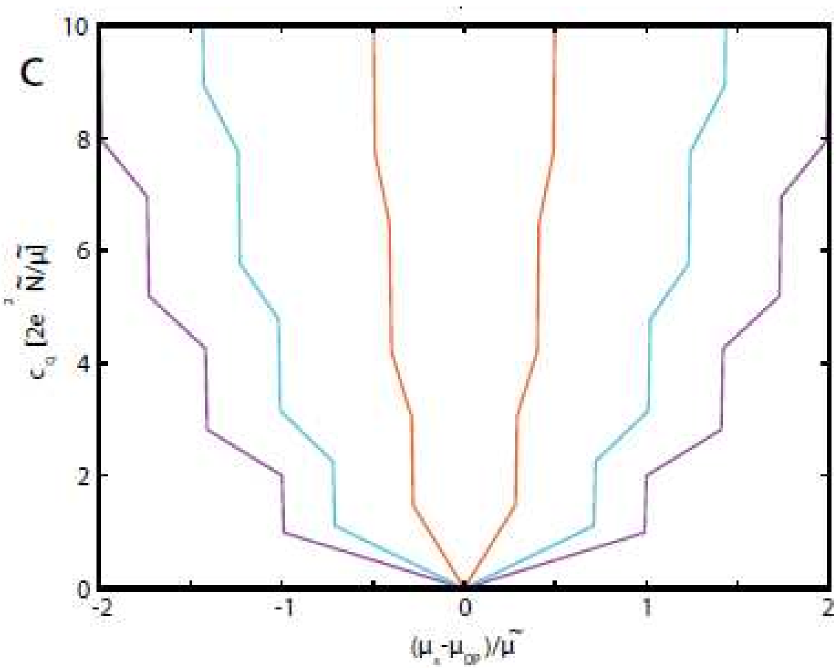
Surface states in a strong electric field $\mathcal{E}$

"Relativisitic" Landau bands (with $\beta = e\mathcal{E}\ell_S^2/v$) :

$$E_{\lambda,b} = \lambda v\sqrt{(1-\beta^2)(k_x^2+k_y^2)+2(1-\beta^2)^{3/2}n/\ell_S^2}$$

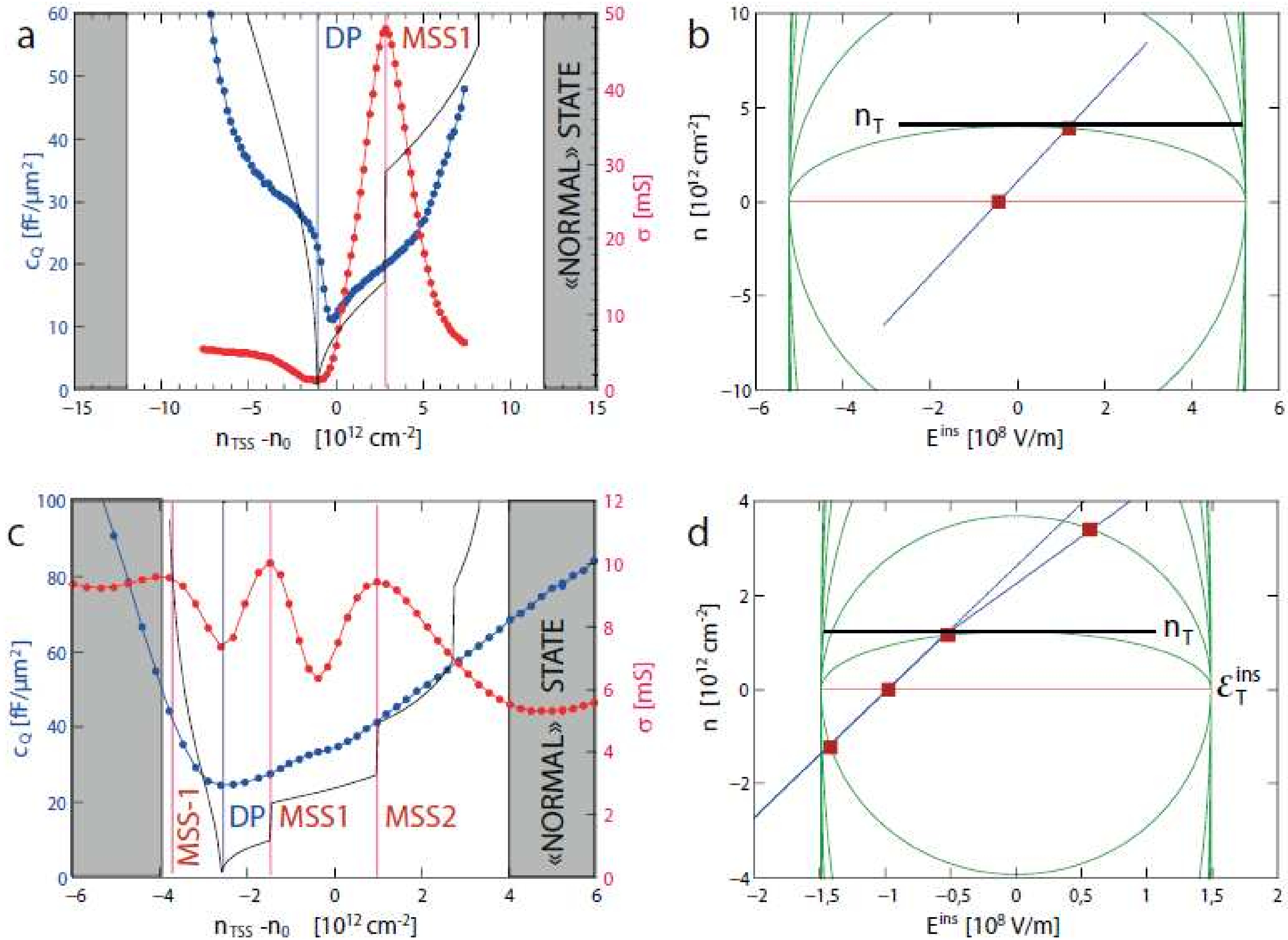


energy spectrum



quantum capacitance (DOS)

Experimental results (LPA-ENS, Paris)



Conclusions (II)

- Confinement of topological materials in smooth interfaces $\rightarrow$ Landau bands
- Topological surface states correspond to $n = 0$ Landau bands
- Massive surface states $(n \neq 0)$ arise in addition

$\rightarrow$ play a role in transport in strained HgTe systems (3D TIs)

- Manipulation via electro-magnetic fields

How to obtain tilted Dirac cones?

- In graphene: $\boldsymbol{\sigma}$ denotes $A - B$ sublattice isospin
- Term proportional to $\mathbb{1}$: nnn hopping ($A \leftrightarrow A$, $B \leftrightarrow B$)

$\Rightarrow$ In continuum limit:

$$H_{\rm diag} = \frac{9}{4} t_{nnn} |\mathbf{q}|^2 a^2 \, \mathbb{1}$$

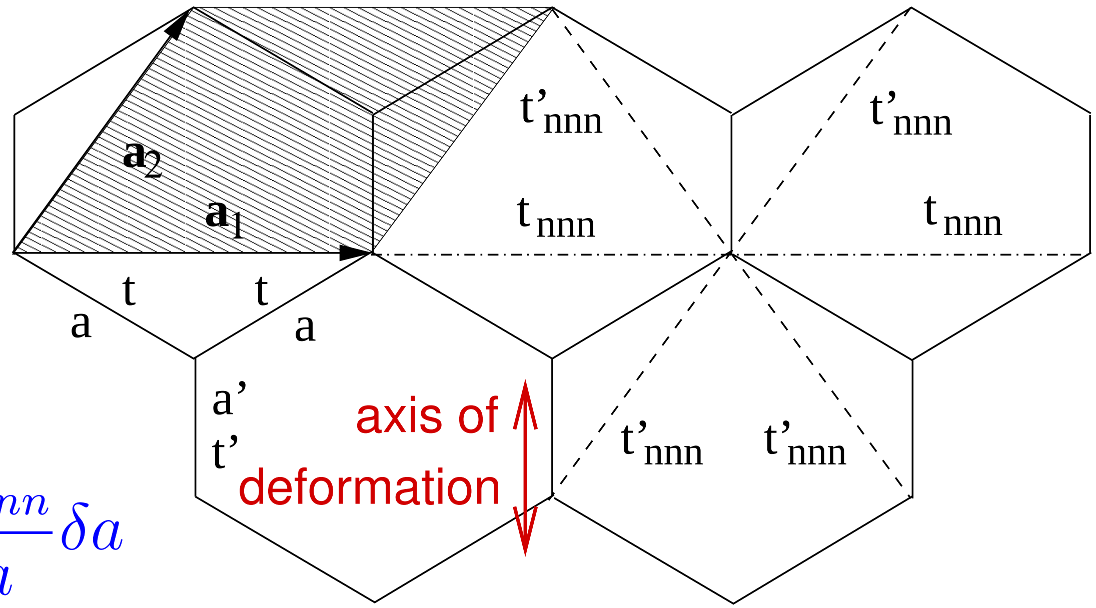
i.e. not linear in $\mathbf{q}$, but quadratic

- Reason: Dirac points [$\epsilon(\mathbf{q}_D) = 0$] coincide with K, K' (points of high crystallographic symmetry)

$\Rightarrow$ Drag Dirac points away from K, K' !

Graphene under strain (I)

Distortion:



$$a \to a' = a + \delta a$$

$$t \to t' = t + \frac{\partial t}{\partial a} \delta a$$

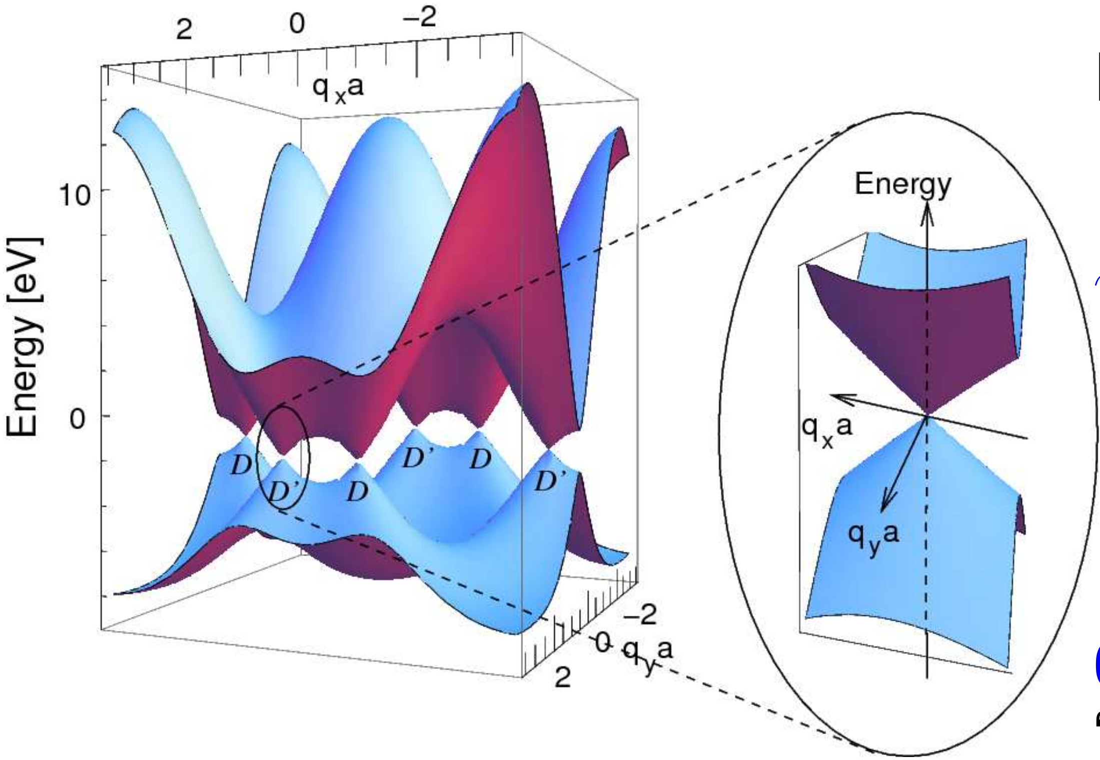
$$t_{nnn} \to t'_{nnn} = t_{nnn} + \frac{\partial t_{nnn}}{\partial a} \delta a$$

Dirac points move from K, K' to:

$$q_y^D = 0, \qquad q_x^D a = \xi \frac{2}{\sqrt{3}} \arccos\left(-\frac{t'}{2t}\right)$$

ξ: valley index

Graphene under strain (II)



Estimation of tilt:

$$\tilde{w}_0 \equiv \sqrt{\left(\frac{w_{0x}}{w_x}\right)^2 + \left(\frac{w_{0y}}{w_y}\right)^2}$$

$$\simeq 0.6\,\frac{\delta a}{a}$$

$0 \leq \tilde{w}_0 < 1$:
"tilt parameter"

$\Rightarrow$ Effect linear in $\delta a/a$!

MOG, J.-N. Fuchs, F. Piéchon, G. Montambaux, PRB **78**, 045415 (2008)

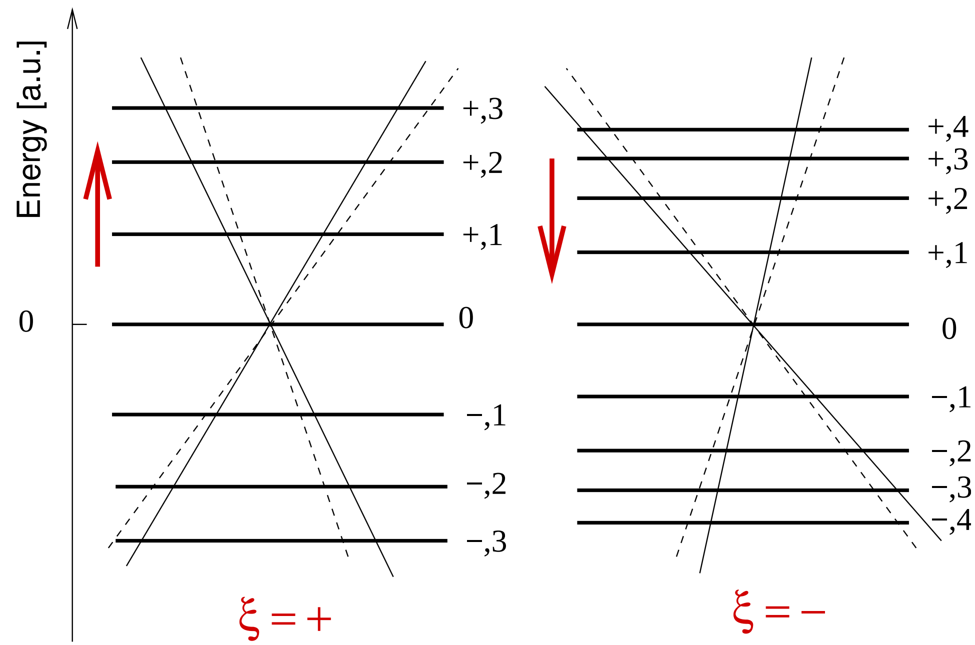
Electric regime in a type-I WSM ?

- $\rightarrow$ add a true electric field to the effective one:

$$\mathbf{w}_0 \rightarrow \mathbf{w}_\xi = \mathbf{w}_0 - \xi \frac{\mathbf{E}\times\mathbf{B}}{B^2}$$

$\Rightarrow$ new tilt parameter

$$\tilde{w}_\xi(E) = \sqrt{\frac{w_{\xi x}^2}{w_x^2} + \frac{w_{\xi y}^2}{w_y^2} + \frac{w_{\xi z}^2}{w_z^2}}$$



Landau level spectrum depends on valley index ξ :

$$\epsilon^{\xi}_{\lambda,n;k}(E) = \lambda \frac{\sqrt{w_x w_y}}{l_B}\left[1 - \tilde{w}_\xi(E)^2\right]^{3/4}\sqrt{2n} + \frac{E}{B}k$$

MOG, J.-N. Fuchs, G. Montambaux, F. Piéchon, EPL **85**, 57005 (2009)