Tilted Dirac cones in 2D and 3D Weyl semimetals – implications of pseudo-relativistic covariance –

Mark O. Goerbig

J. Sári, C. Tőke

(Pécs, Budapest);

J.-N. Fuchs, G. Montambaux,

F. Piéchon ;

S. Tchoumakov, M. Civelli

Le Studium Workshop – Tours, 13-15/06/2016

Outline

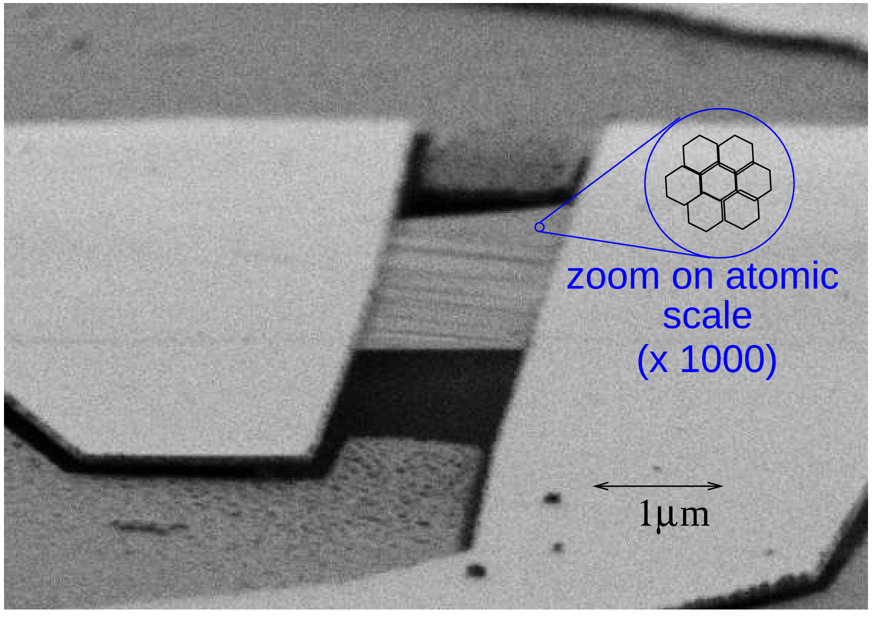
- Massless Dirac fermions in 2D materials: from graphene to α-(BEDT-TTF)$_2$I$_3$
- Tilted Dirac cones – theoretical description
- Pseudo-relativity in α-(BEDT-TTF)$_2$I$_3$ in a magnetic fields

$\Rightarrow$ 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

Interest for fundamental research:

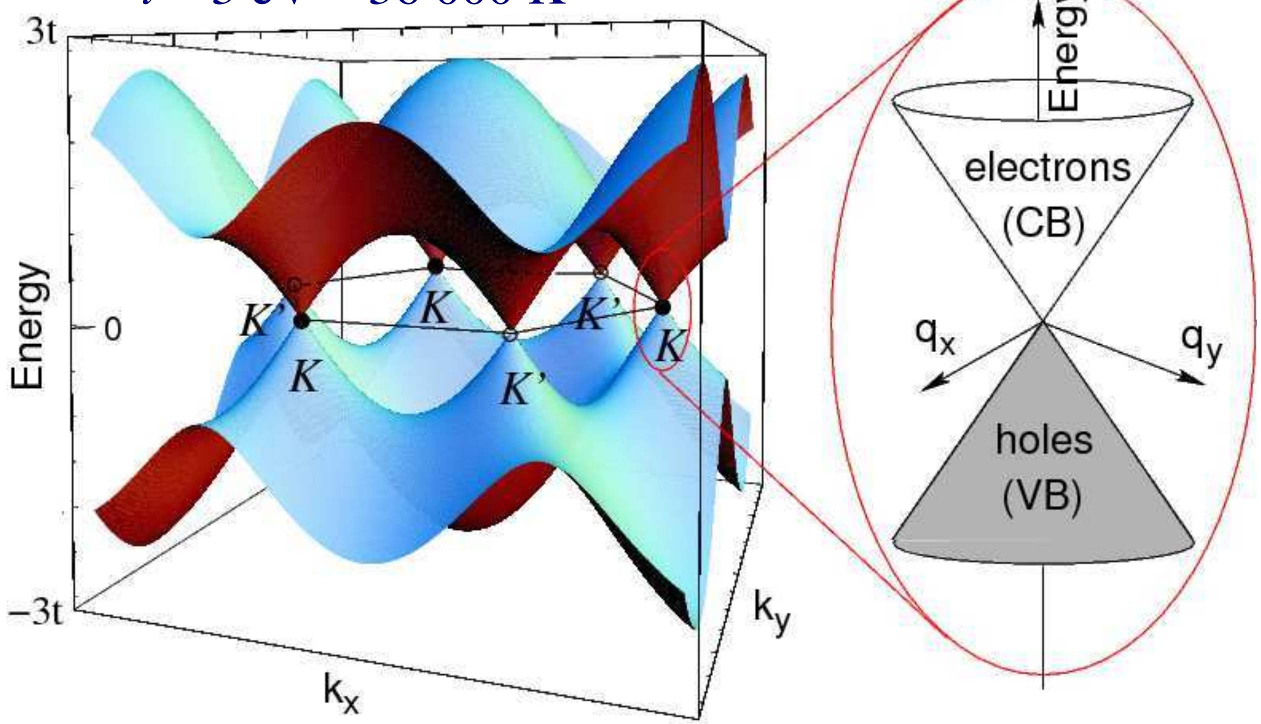
"Quantum mechanics meets relativity in condensed matter"
(electrons behave as 2D massless Dirac fermions)

Band structure of graphene

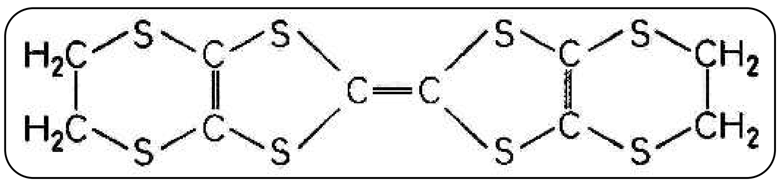
Dirac Hamiltonian (two *valleys* $\xi = \pm \sim$ fermion doubling)

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

$t \sim 3$ eV $\sim 36\,000$ K

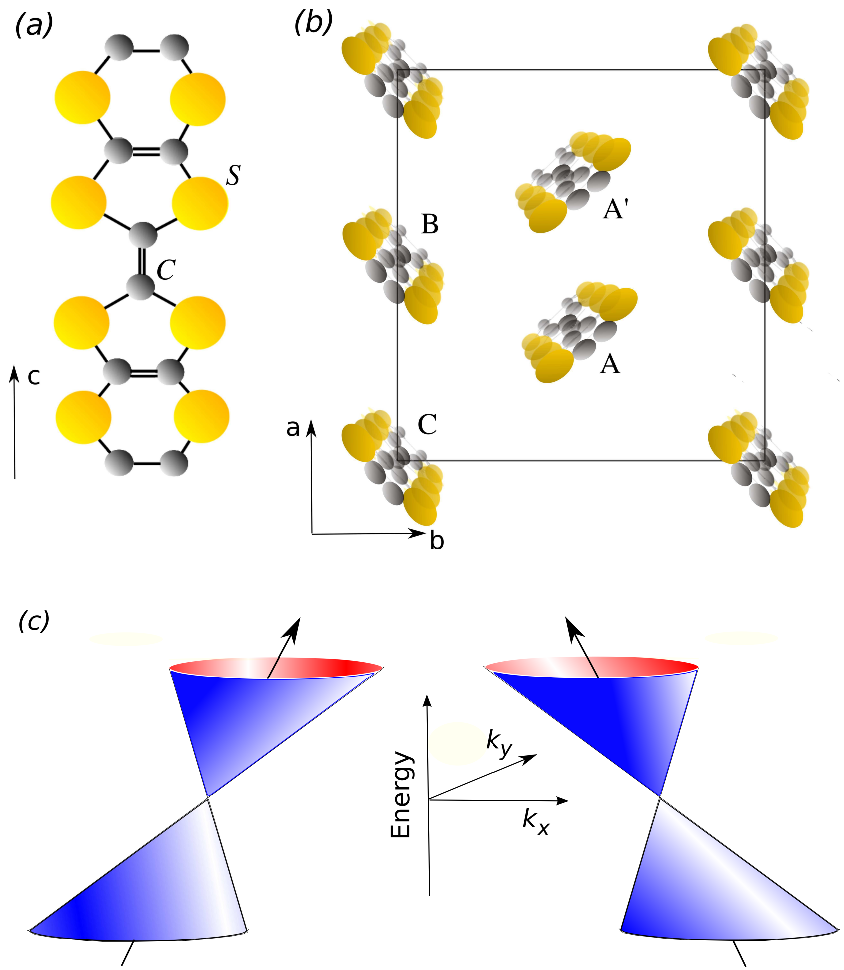


α-(BEDT-TTF)$_2$I$_3$: another 2D Dirac material



BEDT-TTF
=bis(ethylenedithio)tetrathiafulvalene

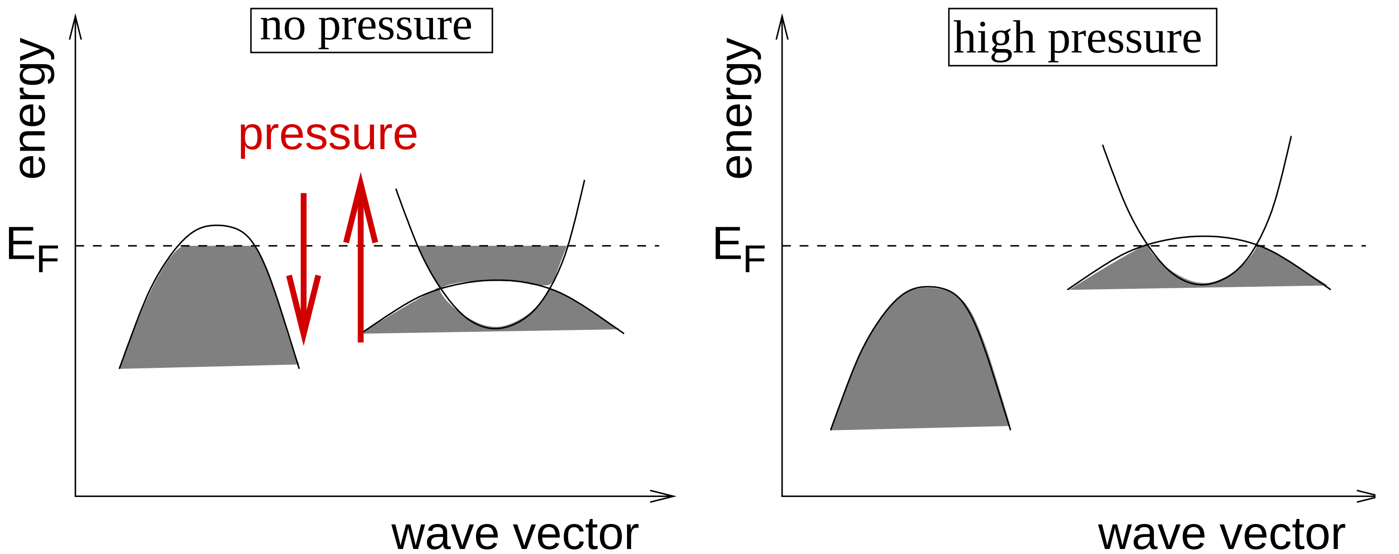
- quasi-2D (stacked layers)
- 4 molecules/unit cell $\rightarrow$ 4 bands
- electronic filling 3/4
- $t_i \sim 20...140$ meV



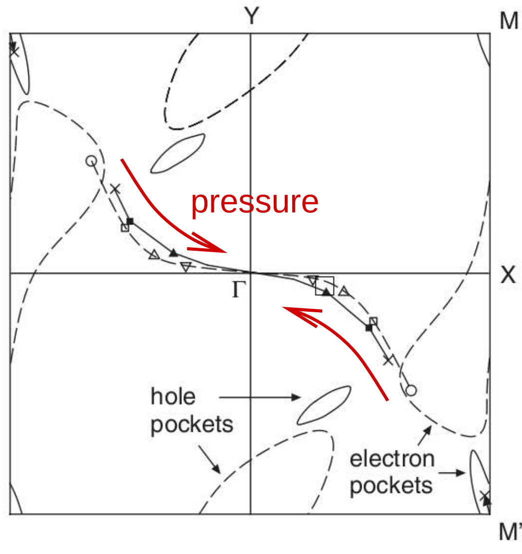
under pressure: low-energy tilted Dirac cones

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

schematic view on upper two bands



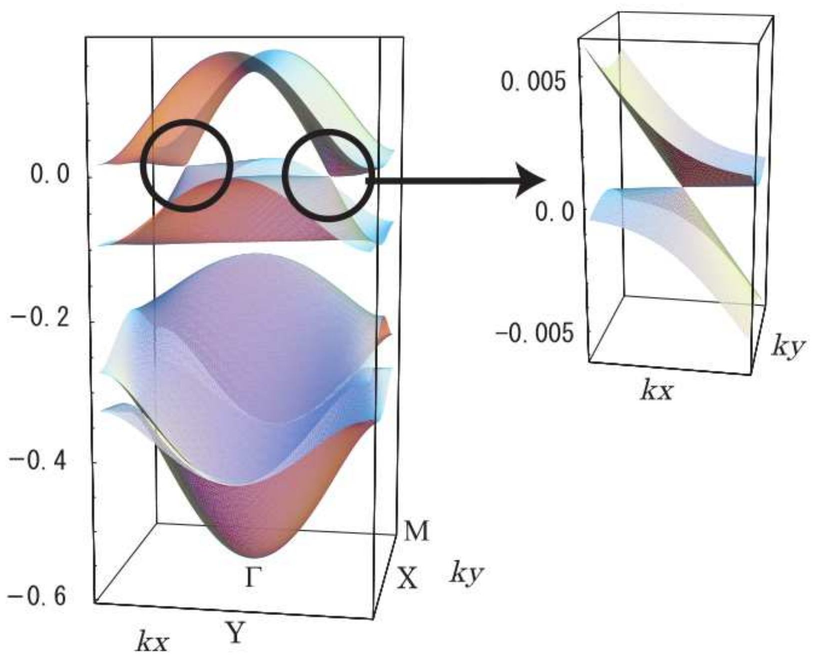
Brillouin zone



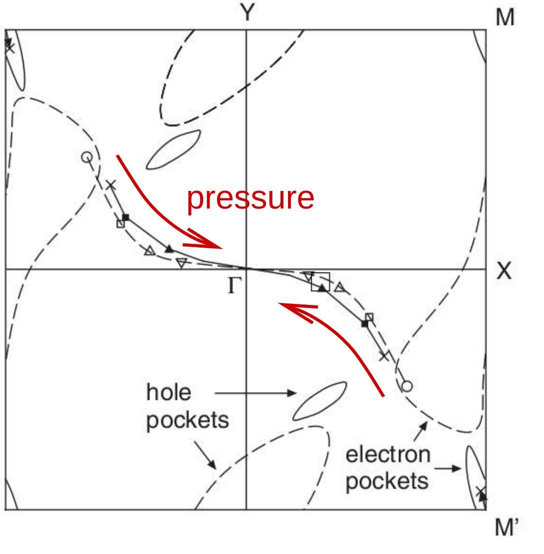
Katayama, Kobayashi, Suzumura, J. Phys. Soc. Japan **75**, 054705 (2006)

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

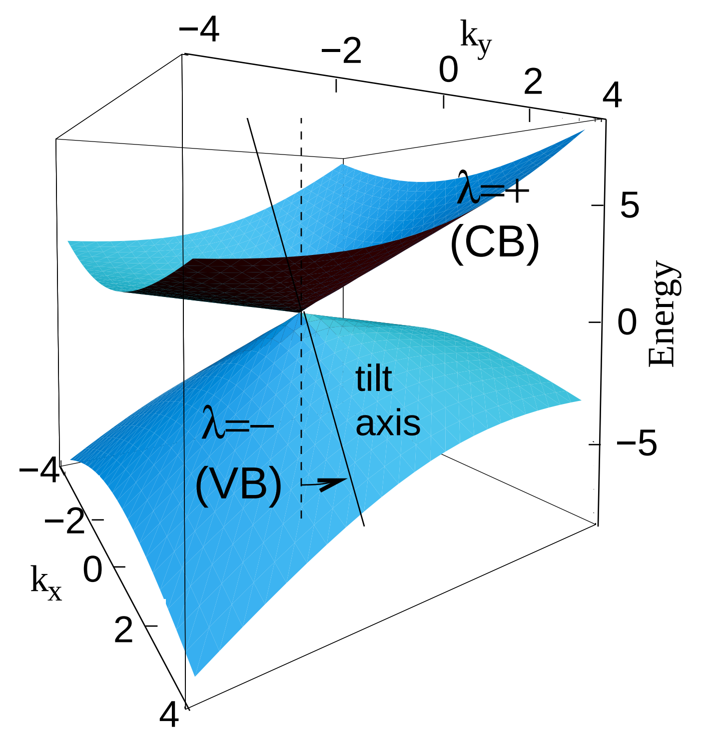
Most general 2D Hamiltonian (2×2 matrix) with linear dispersion (generalised Weyl Hamiltonian):

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

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

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

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:

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

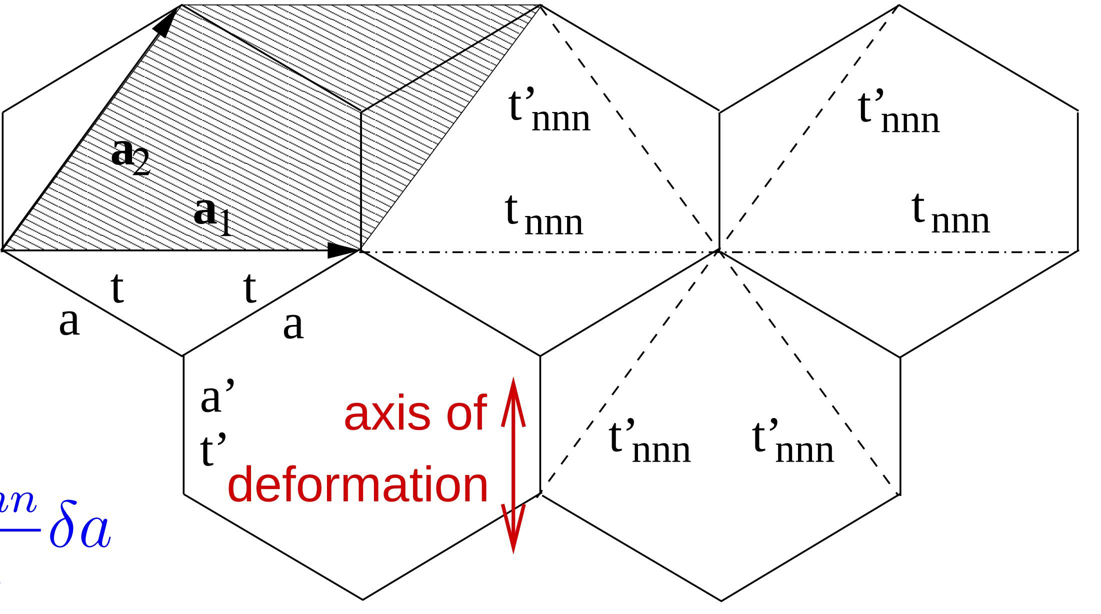
i.e. not linear in $\mathbf{q}$, but quadratic

- 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:



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

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

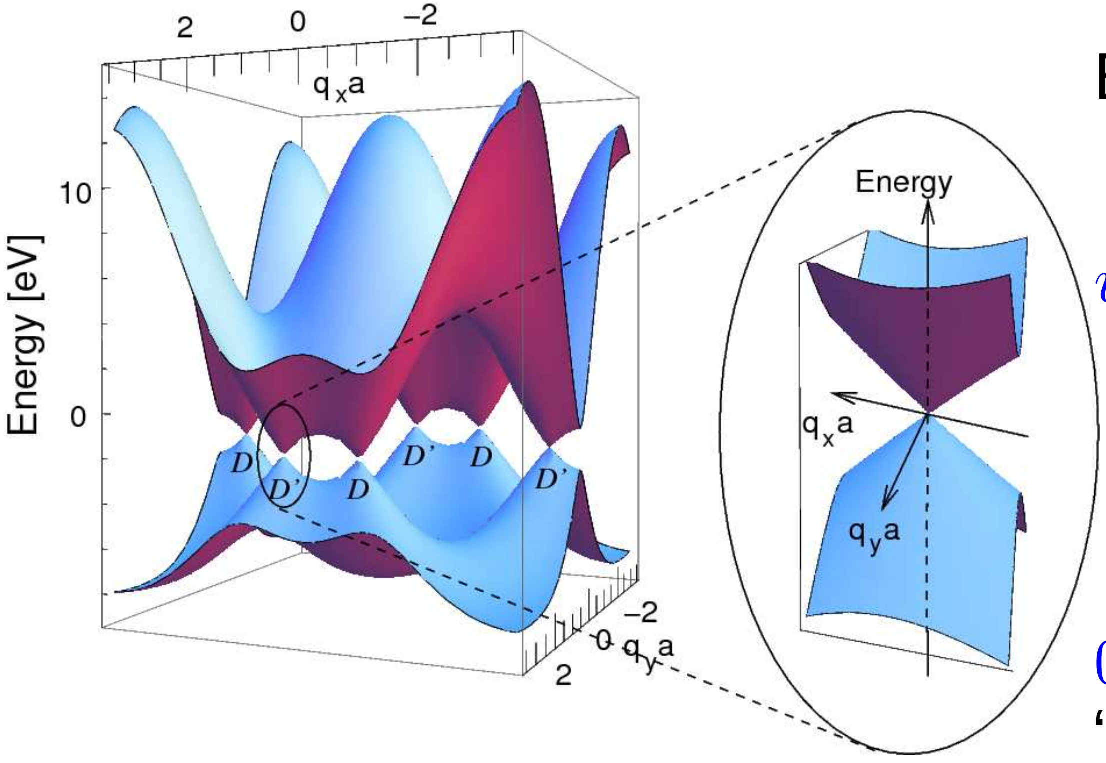
$$t_{nnn} \to t'_{nnn} = t_{nnn} + \frac{\partial t_{nnn}}{\partial a}\delta a$$

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:

$$\tilde{w}_0 \equiv \sqrt{\left(\frac{w_{0x}}{w_x}\right)^2 + \left(\frac{w_{0y}}{w_y}\right)^2} \simeq 0.6\,\frac{\delta a}{a}$$

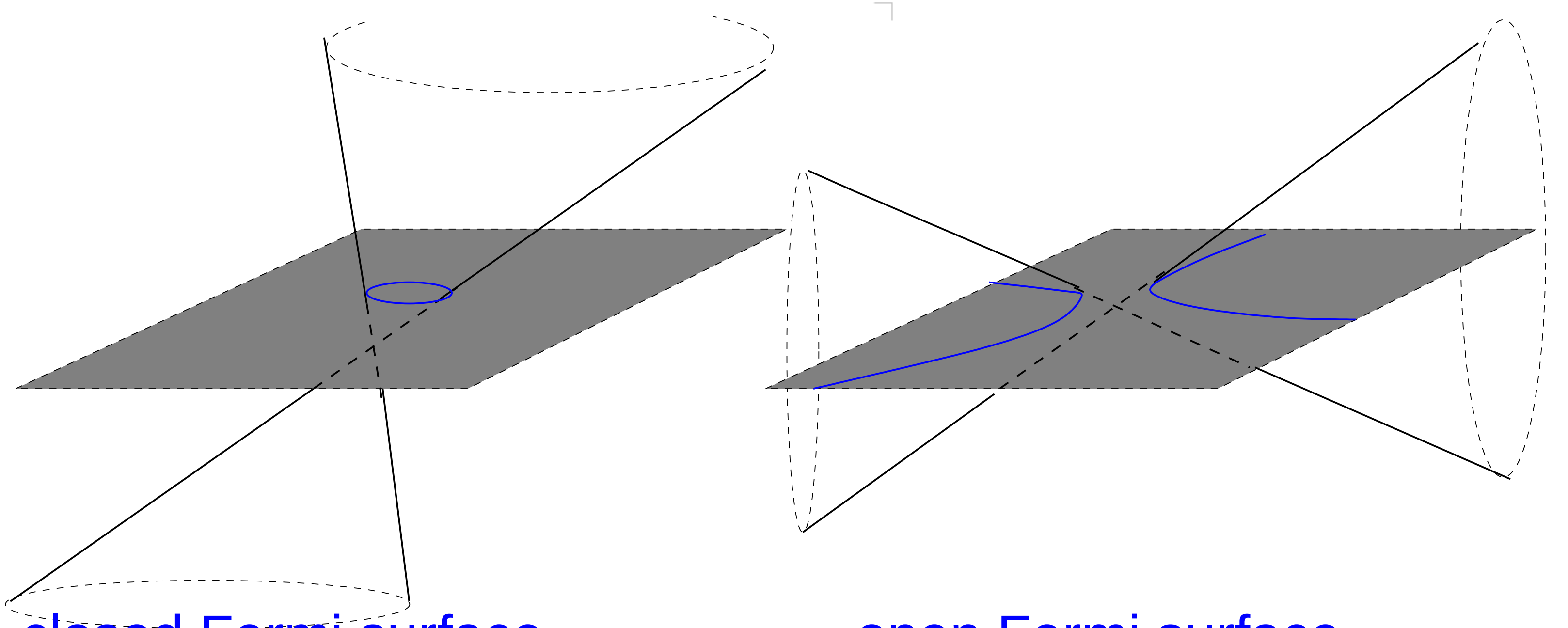
$0 \leq \tilde{w}_0 < 1$:
"tilt parameter"

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

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

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)

see also G. Volovik and M. Zubkov, NPB (2014)

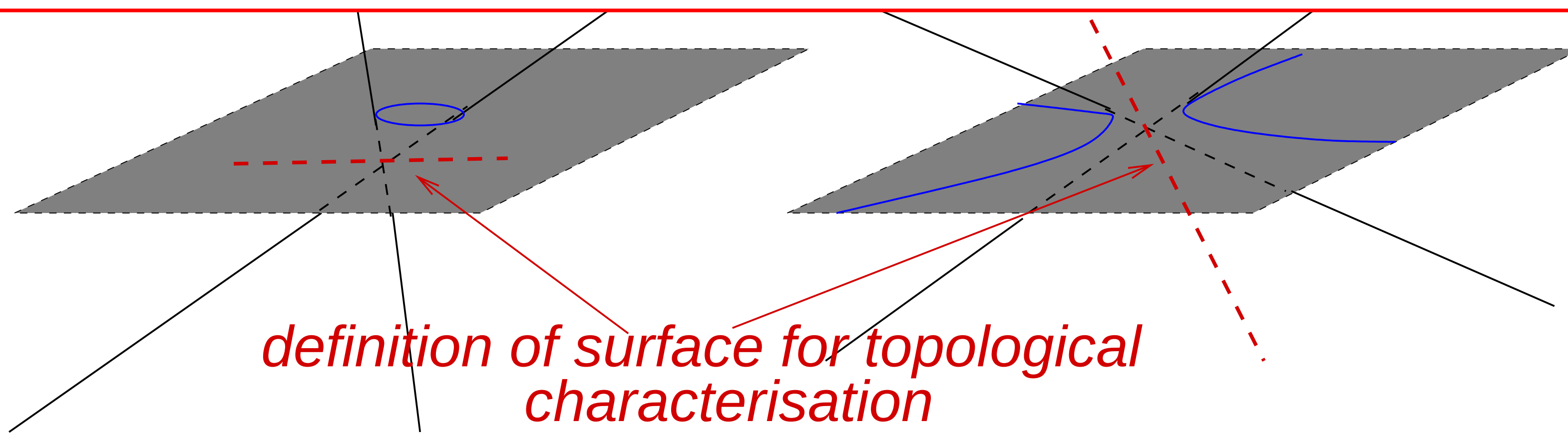
Criterion for maximal tilt

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)



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

see also G. Volovik and M. Zubkov, NPB (2014)

Tilted cones in a strong magnetic field

How is the Landau level spectrum affected by the tilt?

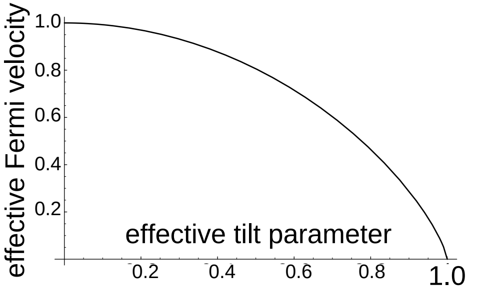
$$H_\xi = \xi \left(\mathbf{w}_0 \cdot \mathbf{q}\, \mathbb{1} + w_x q_x \sigma^x + w_y q_y \sigma^y \right) \qquad \tilde{w}_0 = \sqrt{\left(\frac{w_{0x}}{w_x}\right)^2 + \left(\frac{w_{0y}}{w_y}\right)^2}$$

⊕ 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)

$\Rightarrow$ energy spectrum (as for graphene):

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



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

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

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

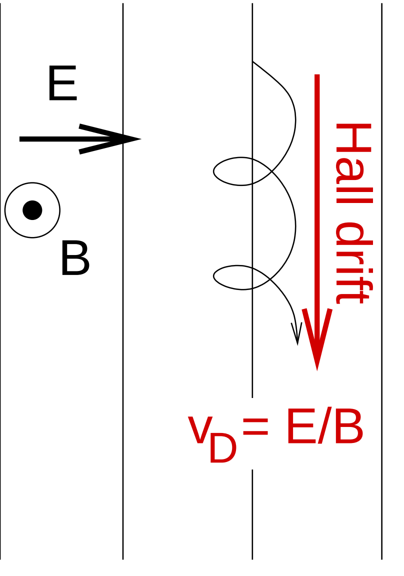
2D electrons in a perpendicular magnetic $\mathbf{B} = \nabla \times \mathbf{A}$ and inplane electric E fields

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

- (non-relativistic) Schrödinger fermions

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

- Landau levels



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

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

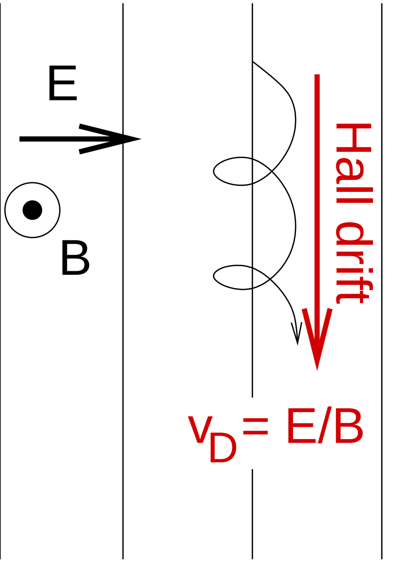
$$H_0(\hbar \mathbf{q}) \quad \rightarrow \quad H_0(\mathbf{p} + e\mathbf{A}(\mathbf{r})) - eEy$$

- relativistic electrons (graphene)

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

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

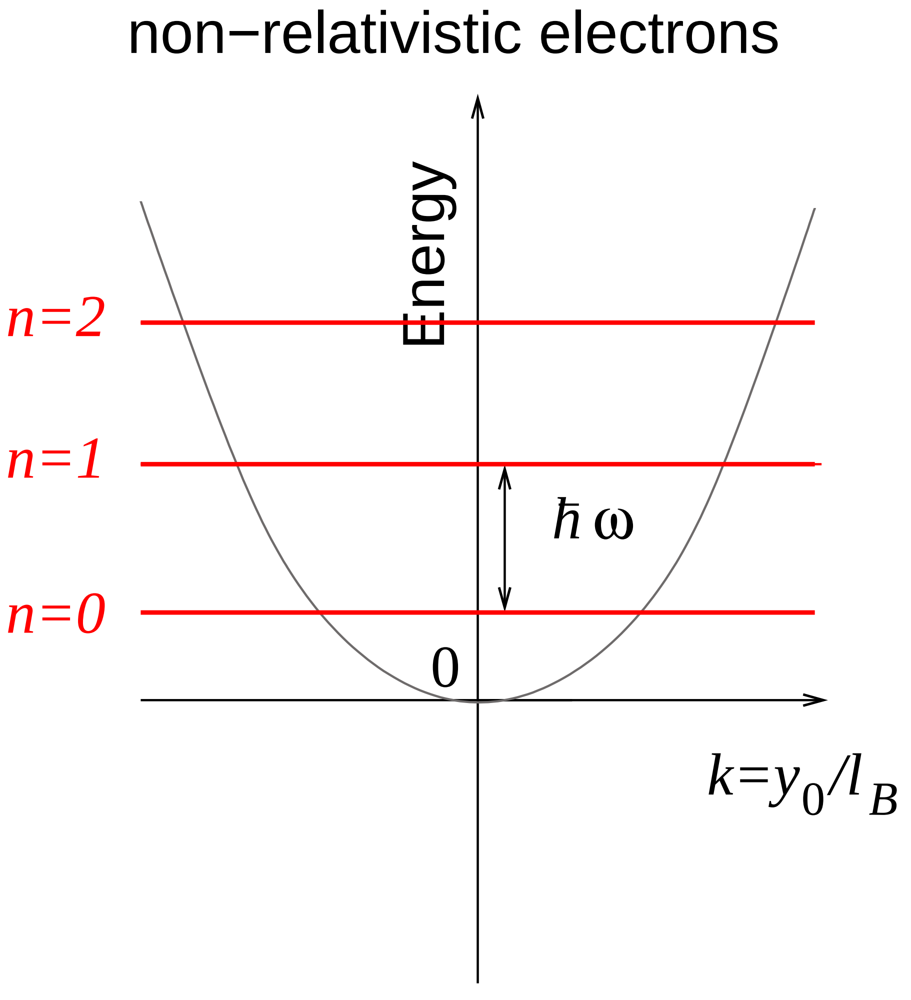
$$\epsilon \rightarrow \epsilon' \propto 1/l'_B \propto \sqrt{B'}$$

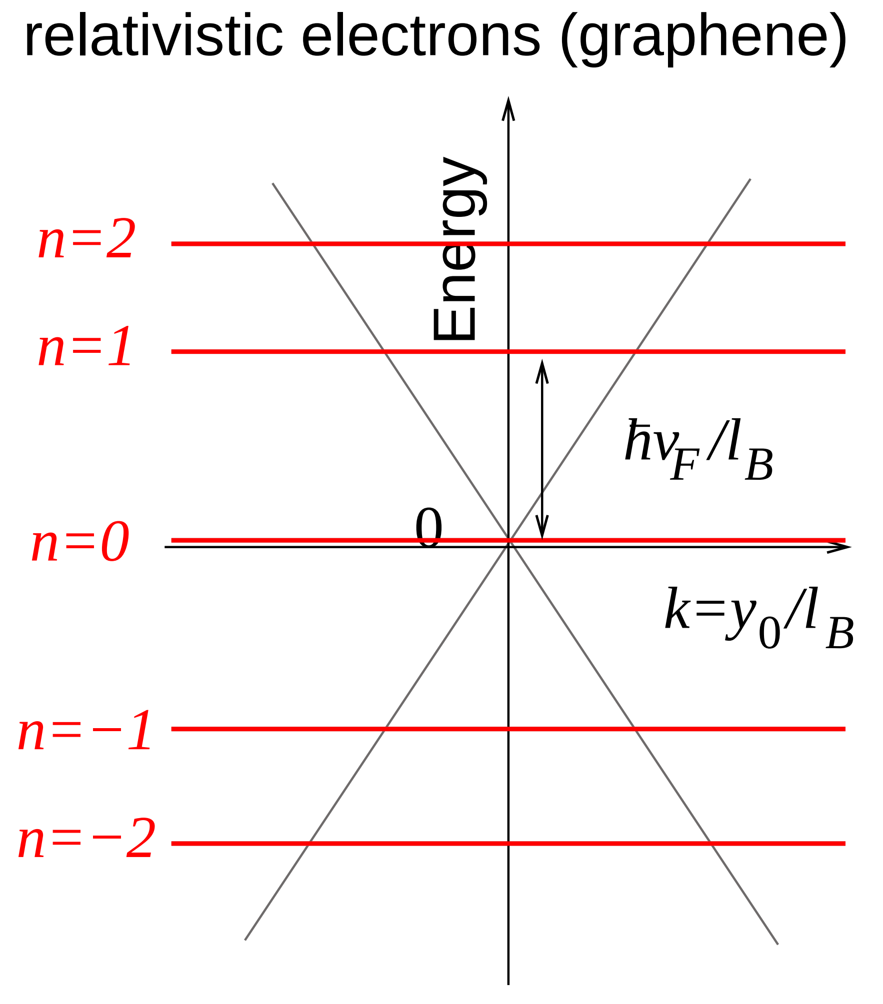


$\rightarrow$ energy in lab frame

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

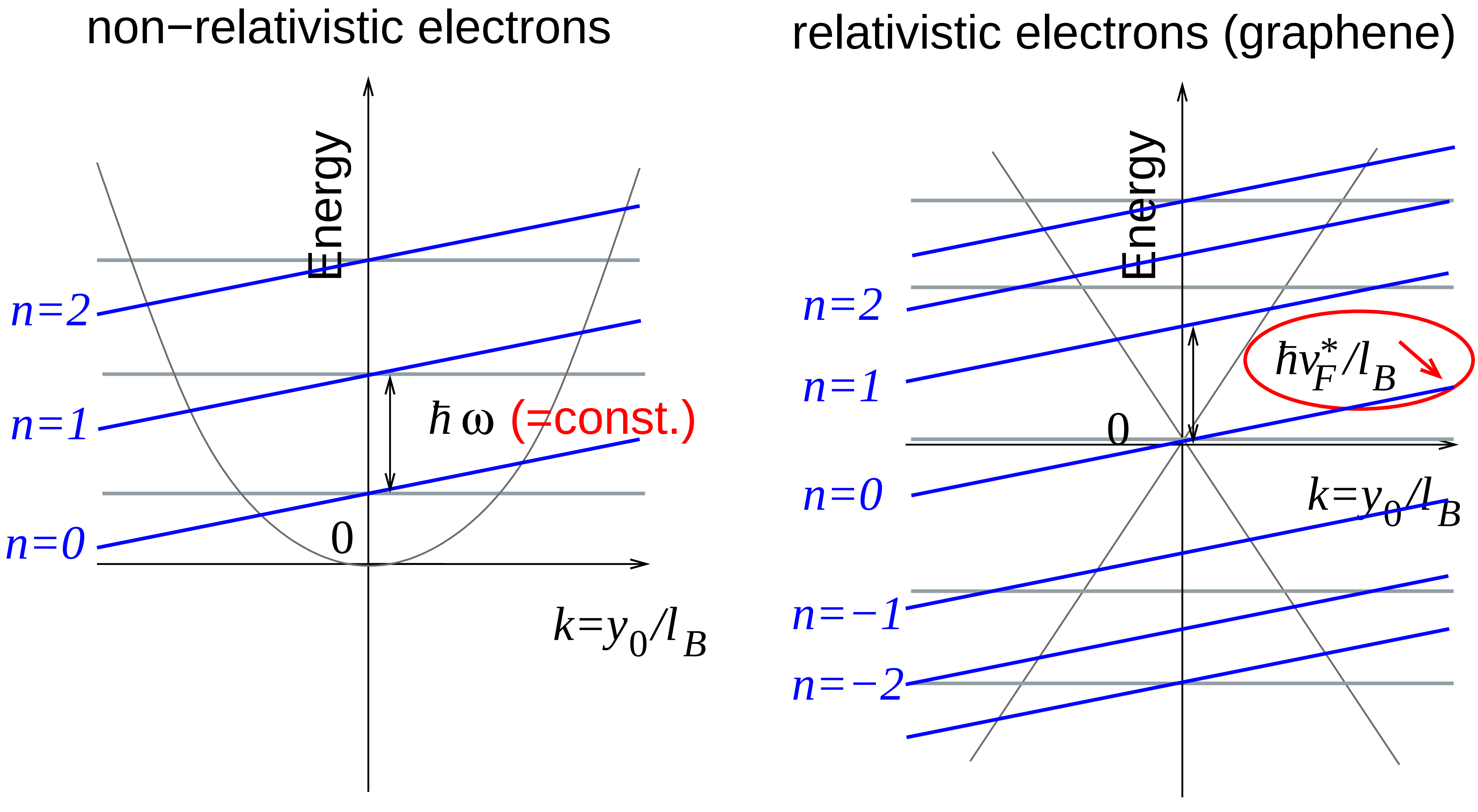
Intermezzo: electrons in crossed B and E fields (II)





no electric field

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



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

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

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

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

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

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

dipolar selection rules (in comoving frame):

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

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

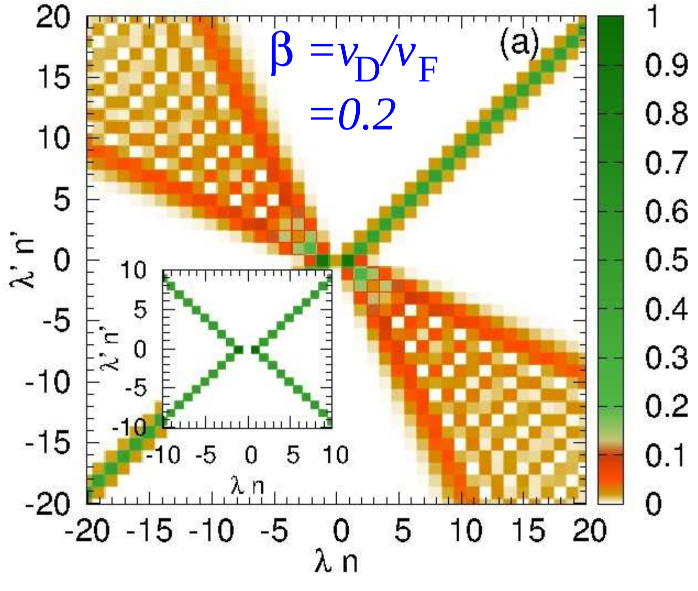
Magnetooptical selection rules

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

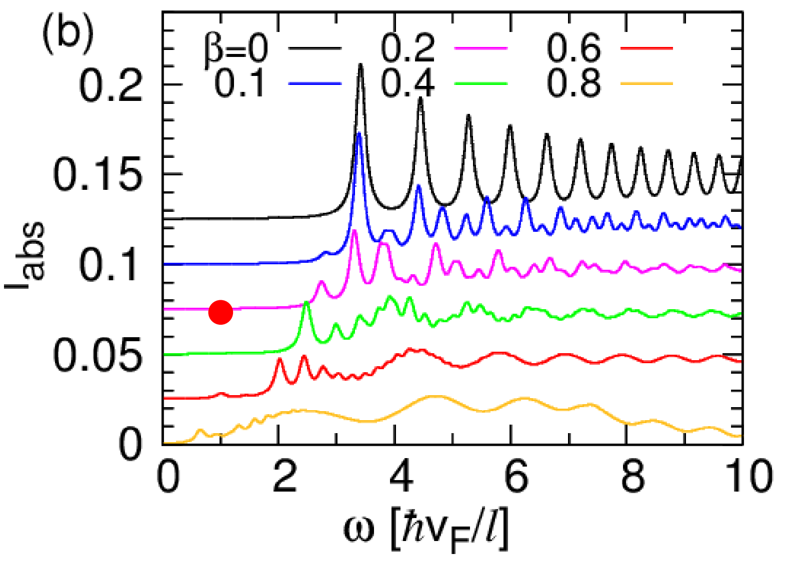
$$\lambda n \to \lambda'(n \pm 1)$$

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

matrix elements



absorption coefficient



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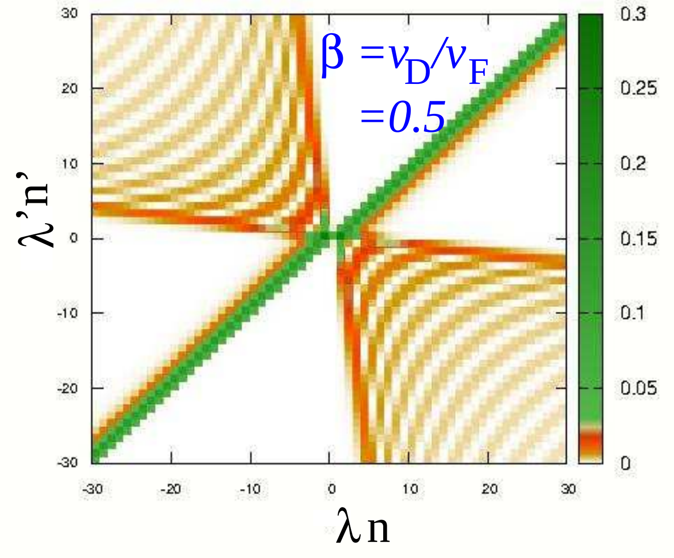

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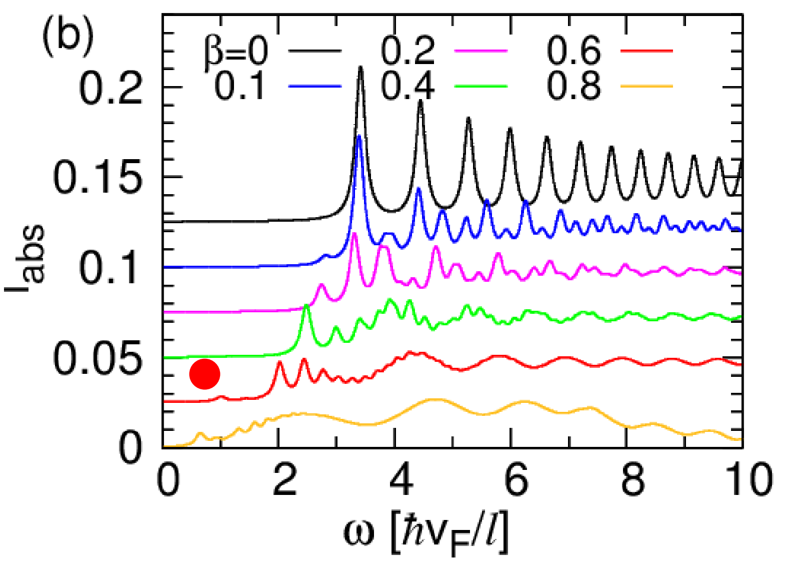

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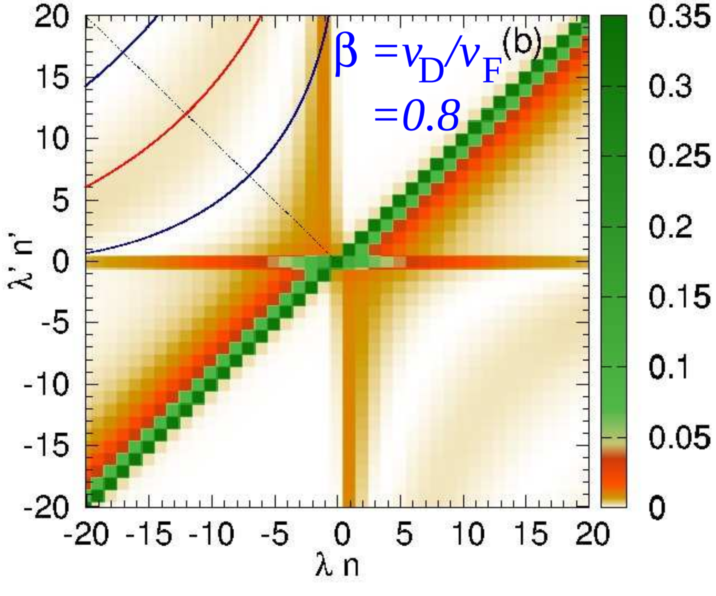
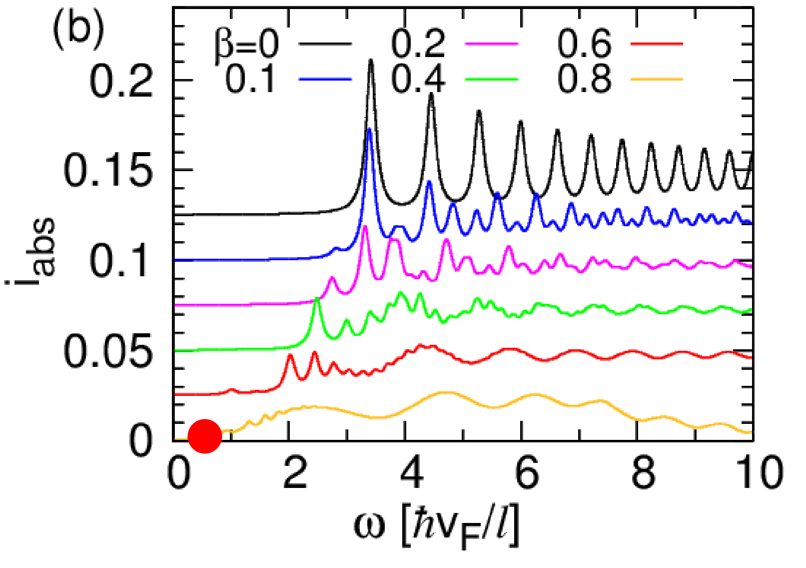


absorption coefficient



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

arXiv:1605.00994

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

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

$\mathbf{w}_0$: “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)

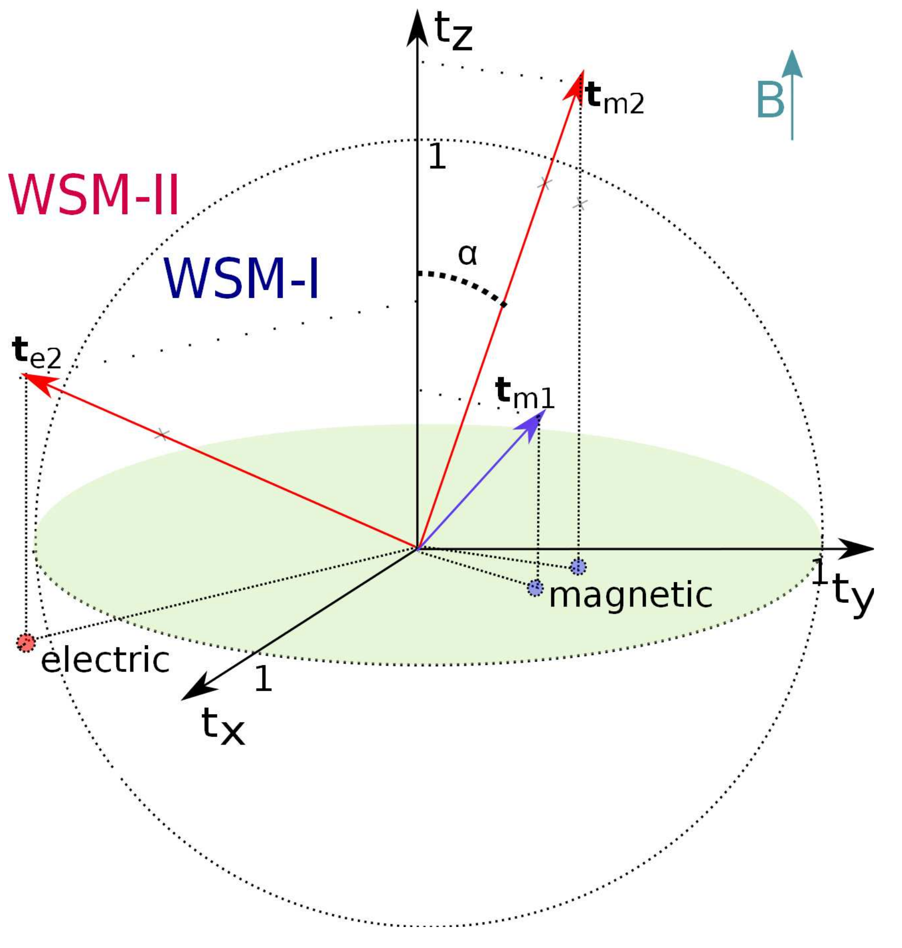
$$\mathbf{t} = \left(\frac{w_{0x}}{w_x}, \frac{w_{0z}}{w_z}, \frac{w_{0z}}{w_z} \right)$$

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

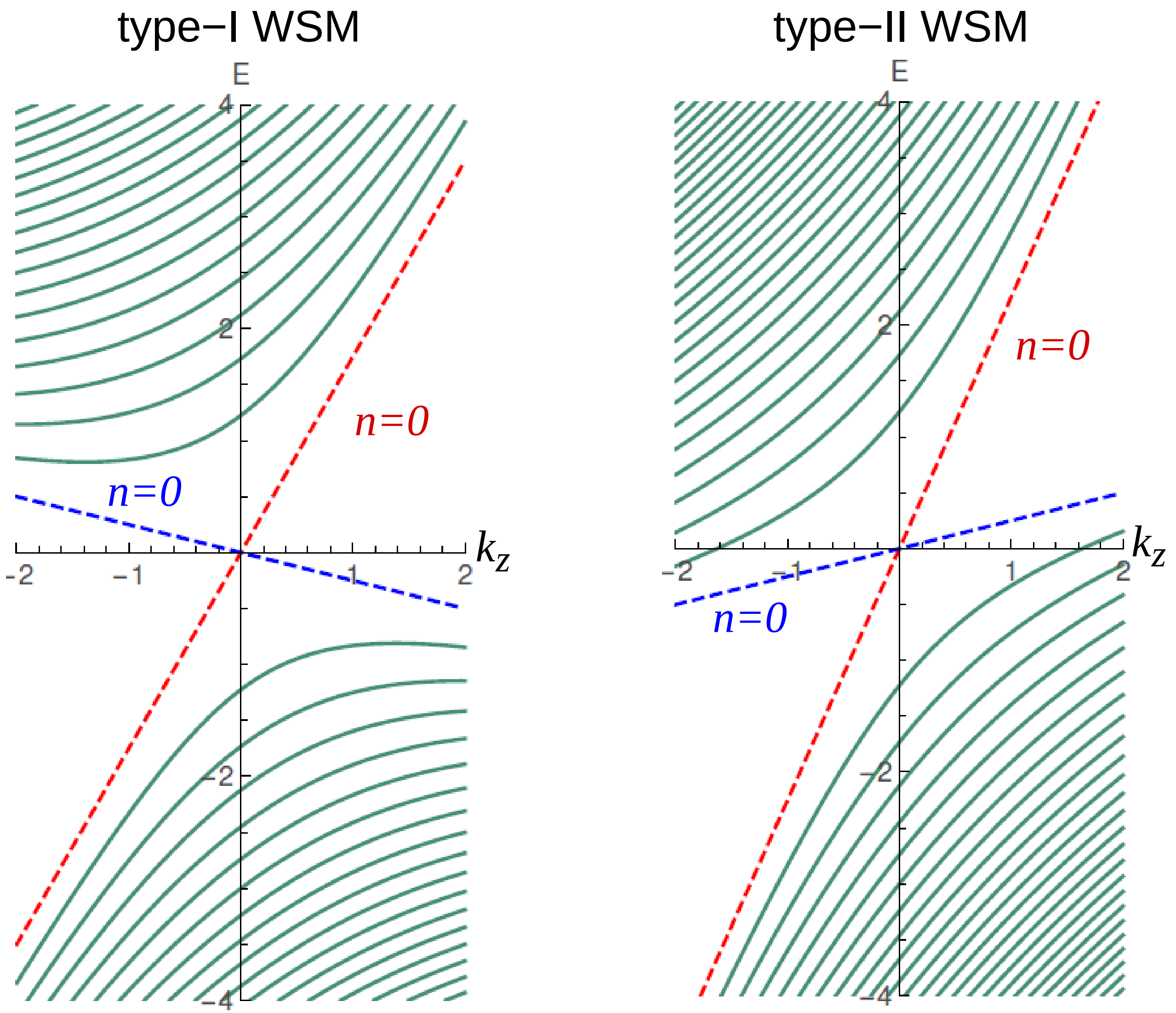
3-dimensional Weyl semimetals	$\lvert\mathbf{t}_\perp\rvert = \beta < 1$	$\lvert\mathbf{t}_\perp\rvert = \beta > 1$
$\lvert\mathbf{t}\rvert < 1$	type-I WSM *magnetic* regime	type-I WSM *electric* regime ?
$\lvert\mathbf{t}\rvert > 1$	type-II WSM *magnetic* regime	type-II WSM *electric* regime

Landau bands in the magnetic regime

WSM type confered to 1D bands

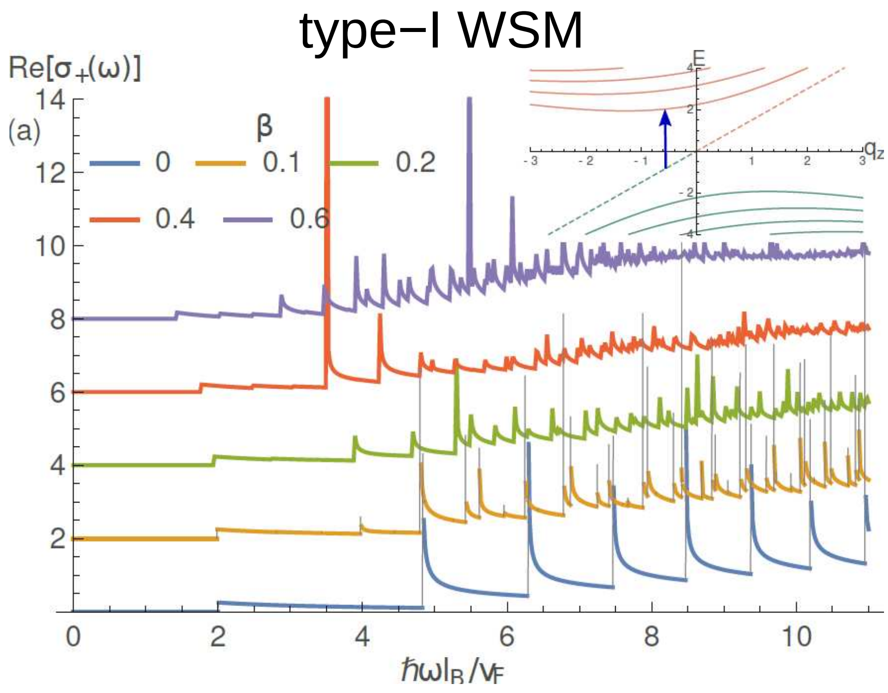
$$t_z = \frac{w_{0z}}{w'_z} = \frac{|\mathbf{t}\cos\alpha|}{\sqrt{1 - t^2\sin^2\alpha}}$$

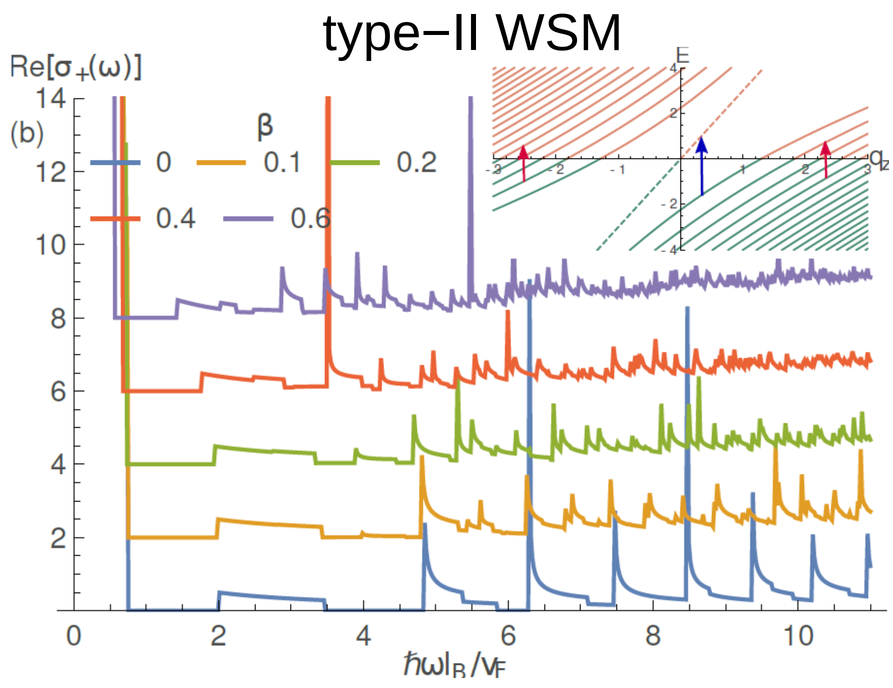
(1D tilt parameter)



Optical conductivity of a WSM in the magnetic regime

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





again: *violation of dipolar selection rules*

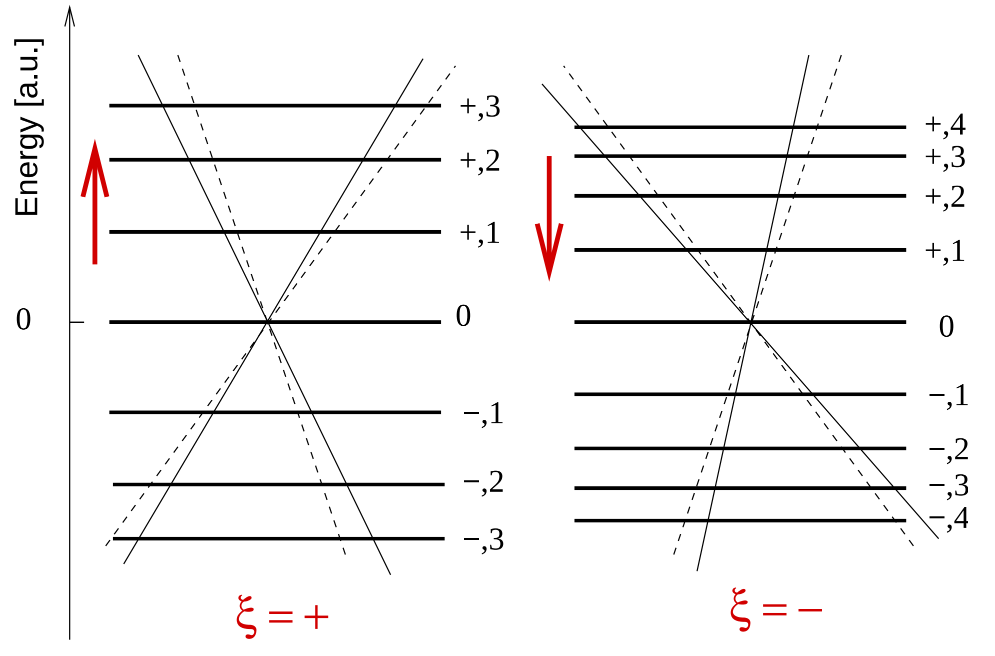
Electric regime in a type-I WSM ?

- $\rightarrow$ 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)

Conclusions

- massless fermions in 2D and 3D *tilted cones*
  - quasi-2D organic material α-(BEDT-TTF)$_2$I$_3$
  - 3D Weyl semimetals (Cd$_3$As$_2$, 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, $n \to n \pm 1$)