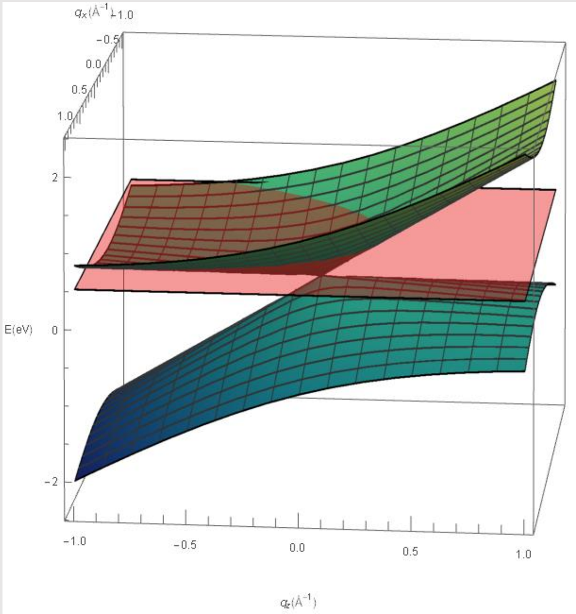
Relativistic properties of Weyl quasiparticles

TOPOLyon

S.Tchoumakov, M. Civelli and M.O.Goerbig



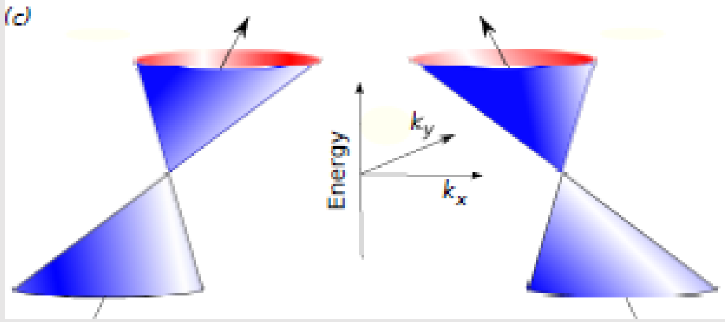
Phys. Rev. Lett. **117**, 086402 (2016)

Short outline

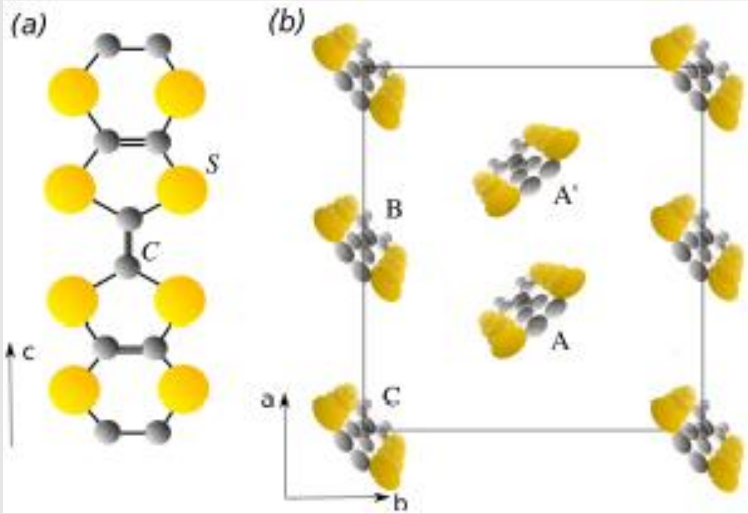
1. Massless Dirac quasiparticles in condensed matter.
2. Relativistic analogy in presence of a magnetic field.
3. Observable effects in infrared spectroscopy.

Massless Dirac fermions can be tilted

- **2D** : Organic compound $\alpha-(BEDT-TTF)_2I_3$

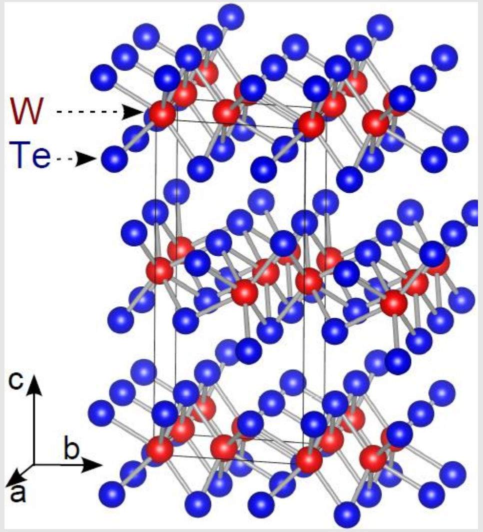


➢ Quasi-2D behavior,
➢ **Under pressure** : low-energy tilted Dirac cones,
➢ A.Kobayashi et al.,
J. Phys. Soc. Jpn. 76, 034711 (2007)



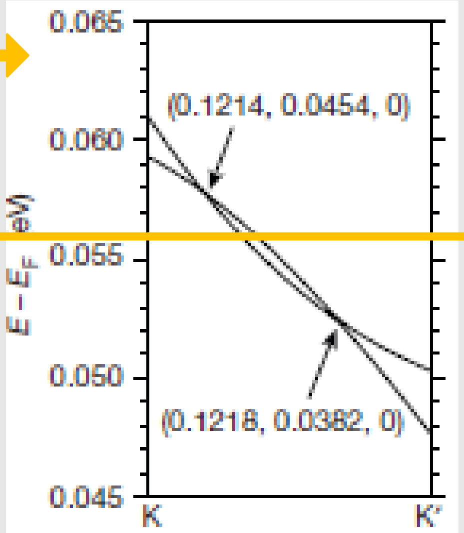
BEDT-TTF = bis(ethylenedithio)tetrathiafulvalene

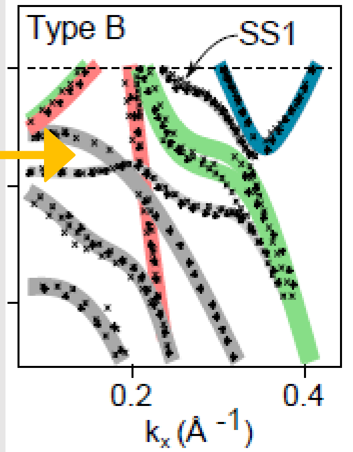
- **3D** : type-I and type-II Weyl semimetals



➢ WTe_2 overtilted Weyl cones,
➢ **Ab-initio and ARPES evidencies :**

➢ A. Soluyanov et al.,
Nature 527, 495-498 (2015)





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Theoretical description of tilted Weyl cones

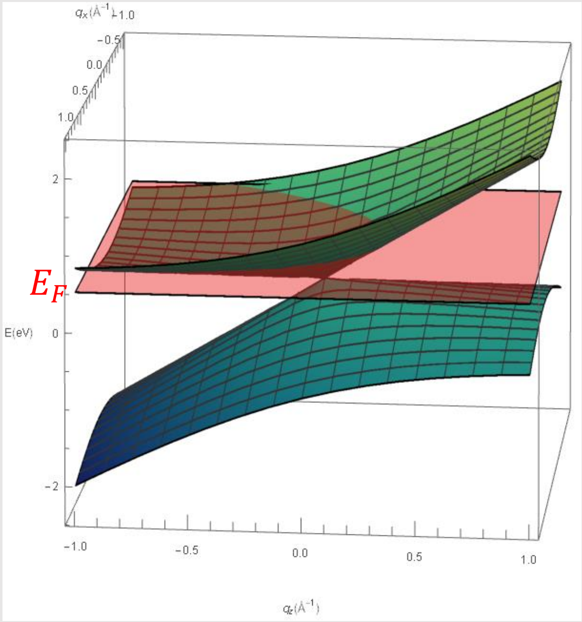
The most general 3D Hamiltonian with linear dispersion and 2x2 matrix is

$$H_0(\boldsymbol{k}) = \sum_{i=x,y,z} v_i k_i (\sigma_i + t_i I)$$

Energy dispersion ($\hbar \equiv 1$):

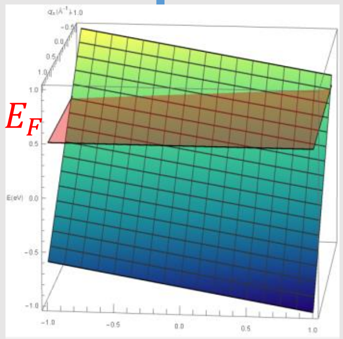
tilt velocity

$$E_{n,\pm} = \sum_{i=x,y,z} t_i v_i k_i \pm \sqrt{\sum_{i=x,y,z} (v_i k_i)^2}$$

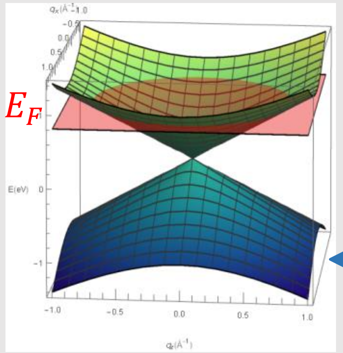


where **t** is the tilt vector.

Large density of states, metallic



$|\boldsymbol{t}| \gg 1$



$|\boldsymbol{t}| \ll 1$

Finite density of states ($\sim E^2$), semi-metallic

Critical regimes separated by $|t_c| = 1$

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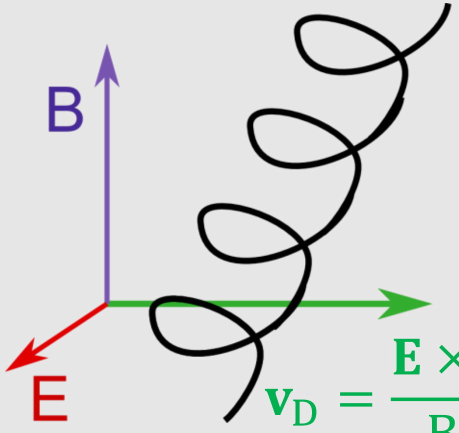
Electric analogy for the tilt

Weyl quasiparticles in an electromagnetic field $(V(\boldsymbol{r}), \boldsymbol{A}(\boldsymbol{r}))$ have

$$H(\boldsymbol{k}) = v_F(\boldsymbol{k} \underbrace{+ e\boldsymbol{A})\boldsymbol{\sigma}}_{\text{magnetic}} + \underbrace{[eV + v_F\boldsymbol{t}\cdot(\boldsymbol{k} + e\boldsymbol{A})]I}_{\text{electric}}$$



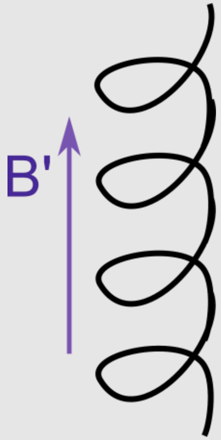
$\mathbf{v}_\mathrm{D} = \frac{\mathbf{E}\times\mathbf{B}}{\mathrm{B}^2} \sim v\,t$

change frame of reference

$\mathbf{v} \to \mathbf{v} - \mathbf{v}_\mathrm{D}$

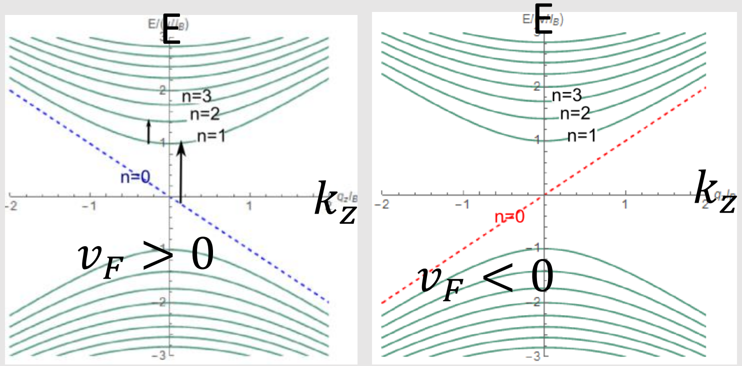
$(\boldsymbol{B}, \boldsymbol{E}) \to (\boldsymbol{B}', \boldsymbol{0})$

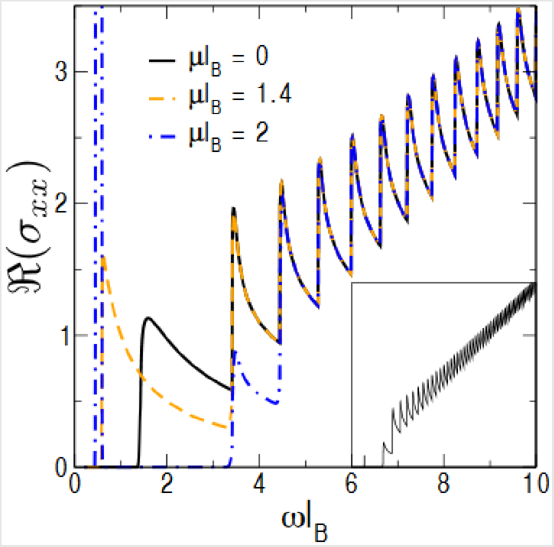
$\mathrm{B}^2 - \mathrm{E}^2 \sim 1 - \mathrm{t}^2 > 0$ is conserved



$\mathbf{V}'_\mathrm{D} = \mathbf{0}$

Landau bands





?

Selection rule:

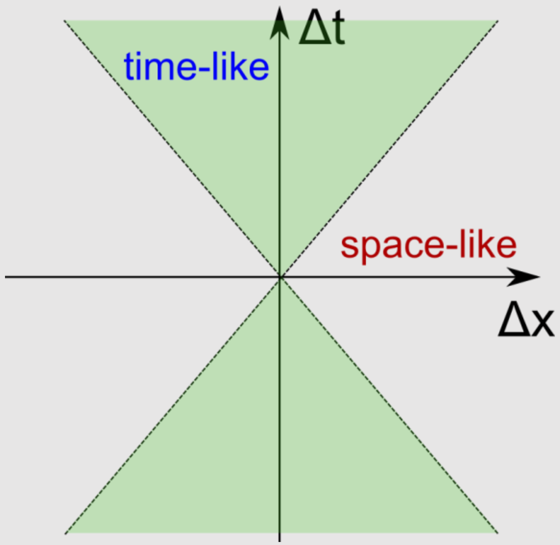
$\boldsymbol{n} \to \boldsymbol{n} \pm \boldsymbol{1}$

Magnetooptical response

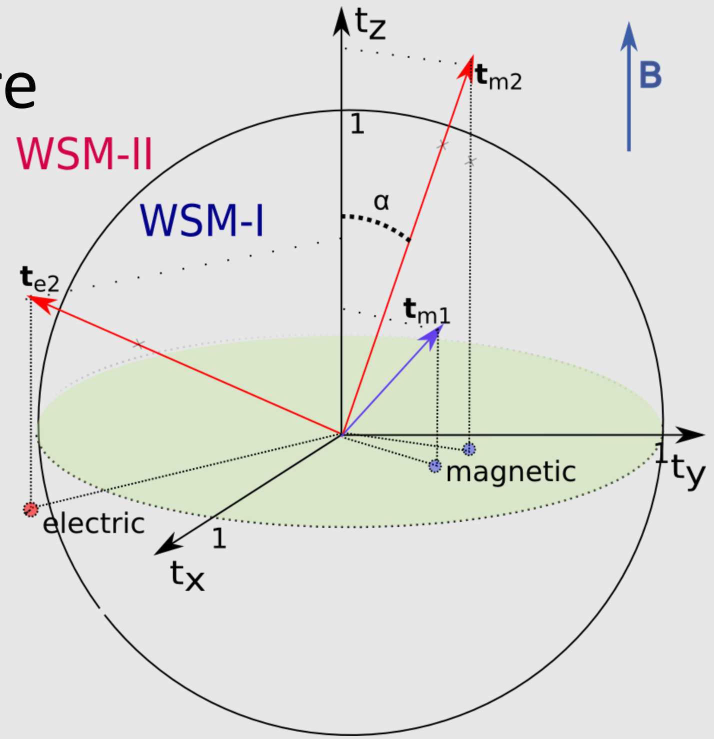
- Ashby et al., *Eur. Phys. J. B (2014) 87: 92*

Type-I and type-II Weyl semimetals

- Two different types of Weyl semimetals, based on the tilt **t**
  - $t^2 < 1$: type-I WSM,
  - $t^2 > 1$: type-II WSM.
- Similar to Minkowsky space of special relativity where



- vector $(\Delta\tau, \Delta x)$ has $s^2 = \Delta\tau^2 - \Delta x^2$ constant,
- $\Delta\tau^2 > \Delta x^2$: time − like coordinates,
- $\Delta\tau^2 < \Delta x^2$: space − like coordinates.



Special relativity : the Lorentz boost

- Lorentz boost in x-direction gives ${x'}_\mu = \Lambda_\mu^\nu x_\nu$ and

$$(V', \boldsymbol{A}')_\mu = \Lambda_\mu^\nu (V, \boldsymbol{A})_\nu$$

…and wave function also changes

$$\Psi'(\boldsymbol{x}', t') = S(\Lambda)\Psi(\boldsymbol{x}, t) \qquad \text{with} \qquad S(\Lambda) = e^{\eta \sigma_x / 2}$$

- **here** :
  - non-relativistic Bloch electrons ($v_F \sim c/300$),
  - tilt is not Lorentz covariant.

…but it works!

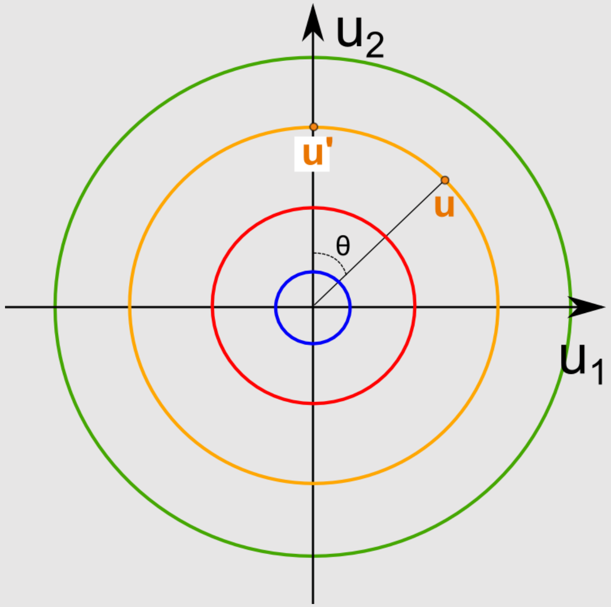
Lorentz boost from quantum mechanics

- Rotation of arbitrary $\boldsymbol{u}$ in $\widehat{H} = \boldsymbol{u} \cdot \widehat{\boldsymbol{\gamma}}$

$$|\psi\rangle \mapsto |\psi'\rangle = e^{i\theta\hat{\Gamma}/2}\,|\psi >$$

$$H \mapsto H' = e^{i\theta\hat{\Gamma}/2} H e^{-i\theta\hat{\Gamma}/2} = \boldsymbol{u} \cdot (\boldsymbol{R}_\theta^{-1}\boldsymbol{\gamma}) = (\boldsymbol{R}_\theta \boldsymbol{u}) \cdot \boldsymbol{\gamma}$$

with $[\hat{\Gamma}, \hat{\gamma}_1] = -i\hat{\gamma}_2, [\hat{\Gamma}, \hat{\gamma}_2] = i\hat{\gamma}_1$



$$\boldsymbol{R}_\theta = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

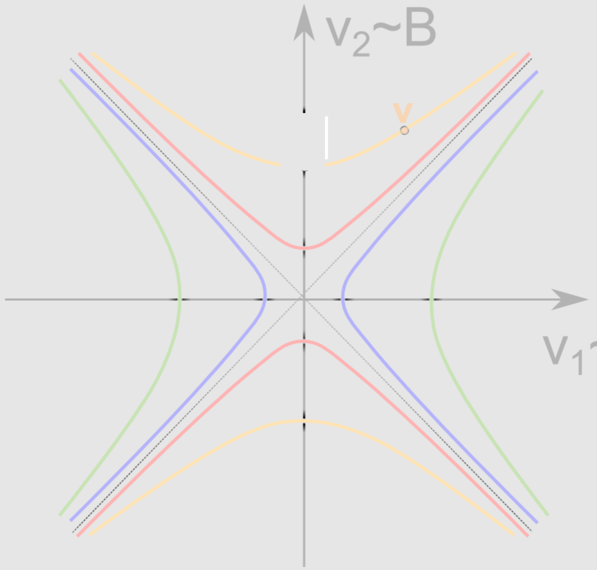
$$\tan\theta = u_2/u_1$$

- Lorentz boost of $\boldsymbol{v}$ in $\widehat{H} = \boldsymbol{v} \cdot \widehat{\boldsymbol{\gamma}}$

$$|\psi\rangle \mapsto |\psi'\rangle = \mathcal{N} e^{\eta\hat{\Gamma}/2}\,|\psi >$$

$$H - \mathcal{E}.I \mapsto (H - \mathcal{E}.I)' = \boldsymbol{v} \cdot (\boldsymbol{L}_\eta^{-1}\boldsymbol{\gamma}) - \mathcal{E}\, e^{-\eta\hat{\Gamma}} = (\boldsymbol{L}_\eta \boldsymbol{v}) \cdot \boldsymbol{\gamma} - \mathcal{E}\, e^{-\eta\hat{\Gamma}}$$

with $\{\hat{\Gamma}, \hat{\gamma}_1\} = \hat{\gamma}_2,\ \{\hat{\Gamma}, \hat{\gamma}_2\} = \hat{\gamma}_1$



$$\boldsymbol{L}_\eta = \begin{pmatrix} \cosh\eta & \sinh\eta \\ \sinh\eta & \cosh\eta \end{pmatrix}$$

$$\tanh\eta = v_2/v_1 = \beta$$

Lorentz boost from quantum mechanics

- Rotation of arbitrary $\boldsymbol{u}$ in $\widehat{H} = \boldsymbol{u} \cdot \widehat{\boldsymbol{\gamma}}$

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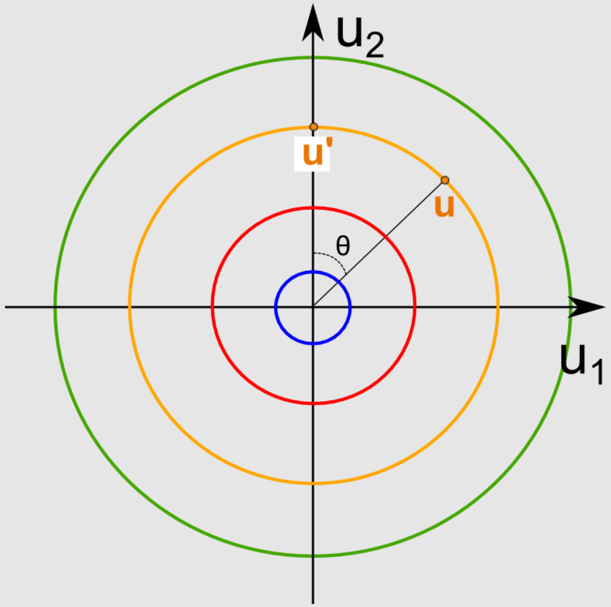

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- Lorentz boost of $\boldsymbol{v}$ in $\widehat{H} = \boldsymbol{v} \cdot \widehat{\boldsymbol{\gamma}}$

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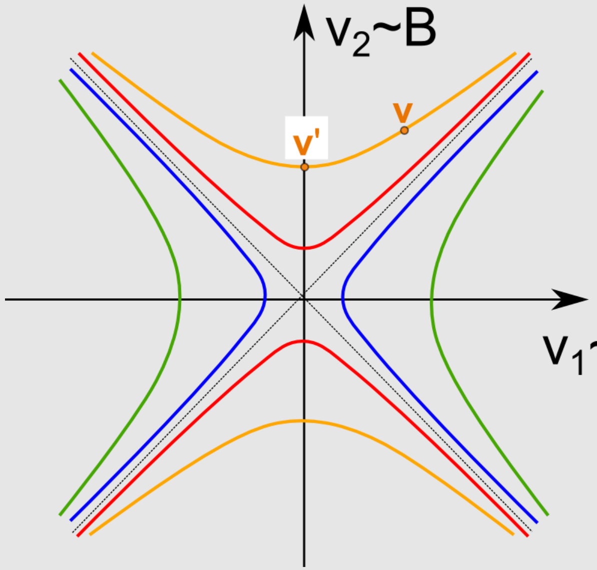
$$H - \mathcal{E}.I \longmapsto (H - \mathcal{E}.I)' = \boldsymbol{v} \cdot (\boldsymbol{L}_\eta^{-1}\boldsymbol{\gamma}) - \mathcal{E}\, e^{-\eta\widehat{\Gamma}} = (\boldsymbol{L}_\eta \boldsymbol{v}) \cdot \boldsymbol{\gamma} - \mathcal{E}\, e^{-\eta\widehat{\Gamma}}$$

with $\{\widehat{\Gamma}, \hat{\gamma}_1\} = \hat{\gamma}_2,\ \{\widehat{\Gamma}, \hat{\gamma}_2\} = \hat{\gamma}_1$



$$\boldsymbol{L}_\eta = \begin{pmatrix} \cosh\eta & \sinh\eta \\ \sinh\eta & \cosh\eta \end{pmatrix}$$

$$\tanh\eta = v_2/v_1 = \beta$$

Tilted Weyl cones Lorentz boost

- Z.-M. Yu et al., *Phys. Rev. Lett.* **117**, 077202 (2016)
- M. Udagawa et al, *Phys. Rev. Lett.* **117**, 086401 (2016)
- S. Tchoumakov et al., *Phys. Rev. Lett.* **117**, 086402 (2016)

- In a uniform magnetic field, Lorentz boost of tilted Weyl cone

$$H(k) = v_F(\boldsymbol{k} + e\boldsymbol{A})\sigma_i + v_F\boldsymbol{t}\cdot(\boldsymbol{k} + e\boldsymbol{A})I \;\rightarrow H'^{(k)} = v'_F(\boldsymbol{k} + e\boldsymbol{A}')\sigma_i + t v_F k_z I$$

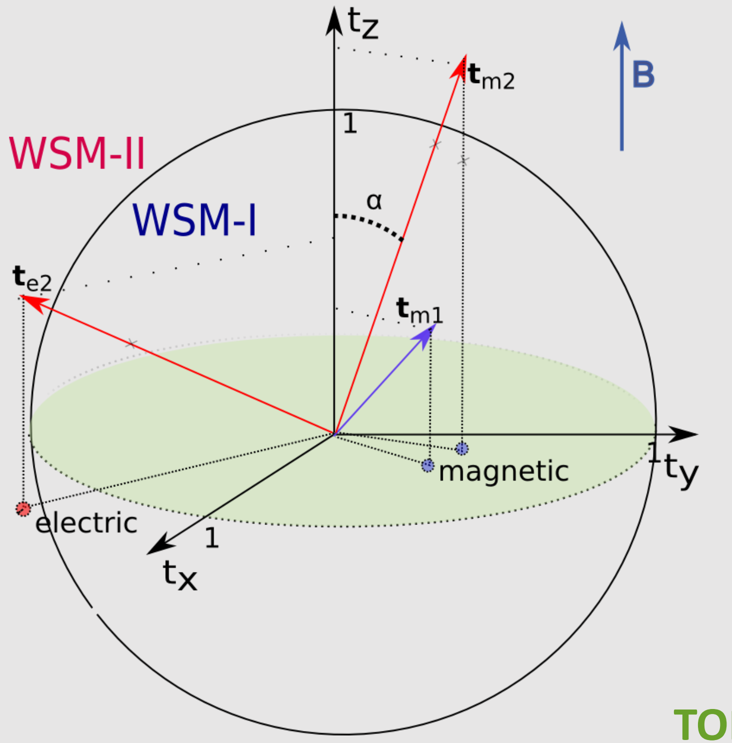
- **In-plane tilt**

$$\boldsymbol{t}_\perp = \frac{\boldsymbol{t}\times\boldsymbol{B}}{B} = (t_y, -t_x)$$

⇒ Landau quantization only for **B** close to tilt axis

$$\beta = |\boldsymbol{t}_\perp| < 1 \Rightarrow |\sin\alpha| < 1/t$$

Speed ratio, characterizing Lorentz boost



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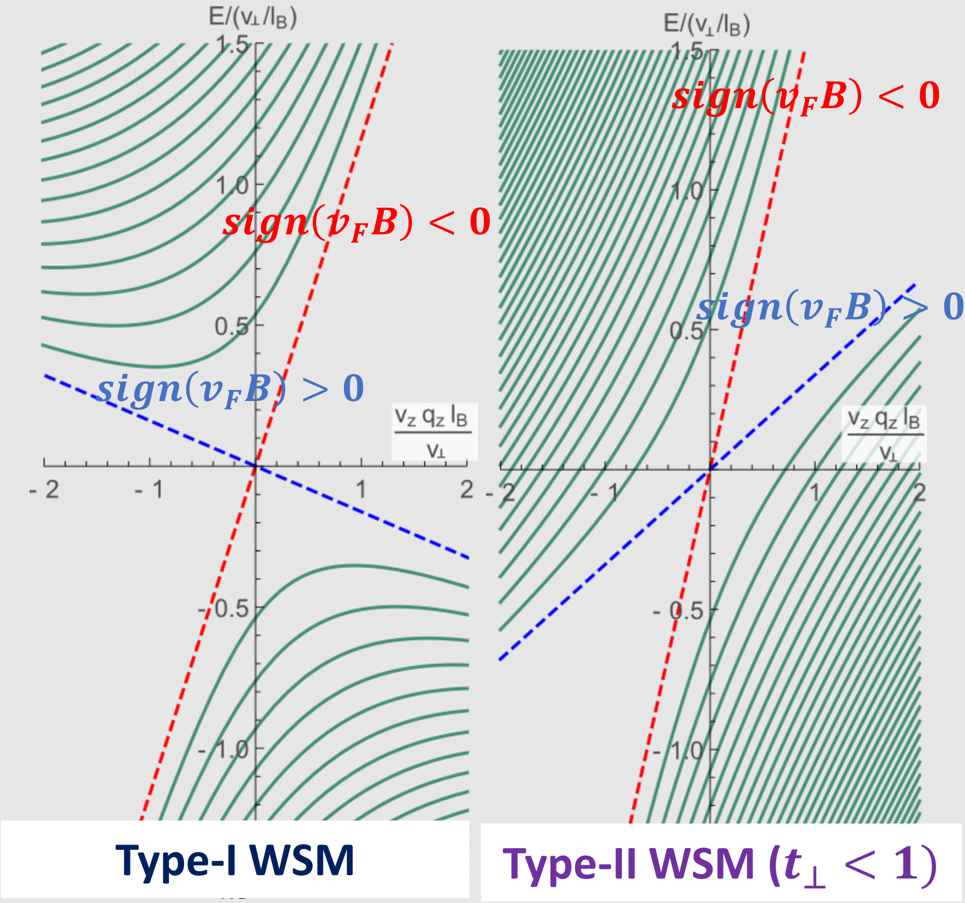
Tilted Weyl cones Landau levels spectrum

- One dimensional Landau bands

$$E_n^{\pm}(k_z) = t_z v_z k_z \pm \sqrt{1 - {t_\perp}^2} \sqrt{v_z^2 k_z^2 + 2 v_x v_y \sqrt{1 - {t_\perp}^2} eB\, n}$$

3D Weyl semimetals	$\lvert \boldsymbol{t}_\perp \rvert < 1$	$\lvert \boldsymbol{t}_\perp \rvert > 1$
$\lvert \boldsymbol{t} \rvert < 1$	**Type-I WSM** magnetic regime	**Type-I WSM** electric regime
$\lvert \boldsymbol{t} \rvert > 1$	**Type-II WSM** magnetic regime	**Type-II WSM** electric regime

magnetic regime



Magnetooptical response of tilted WSM

- **2D** : J. Sári et al., *Phys. Rev. B* **92**, 035306 (2015)
- **3D :** S. Tchoumakov et al., *Phys. Rev. Lett.* **117**, 086402 (2016)

$$Re[\sigma_{ll}] = \frac{\sigma_0 eB}{2\pi\omega} \sum_{jj'} \left| u_l \cdot v_{jj'} \right| \left[f_D(E_j) - f_D(E_{j'}) \right] \delta(\omega - \Delta E_{jj'})$$

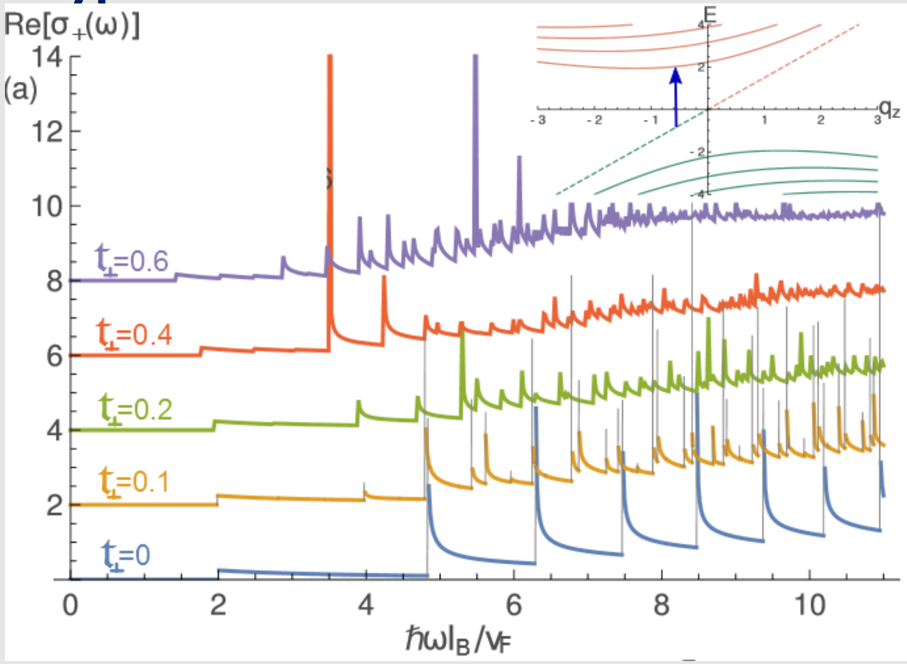
selection rules ~~$n \to n \pm 1$~~

Fermi distribution

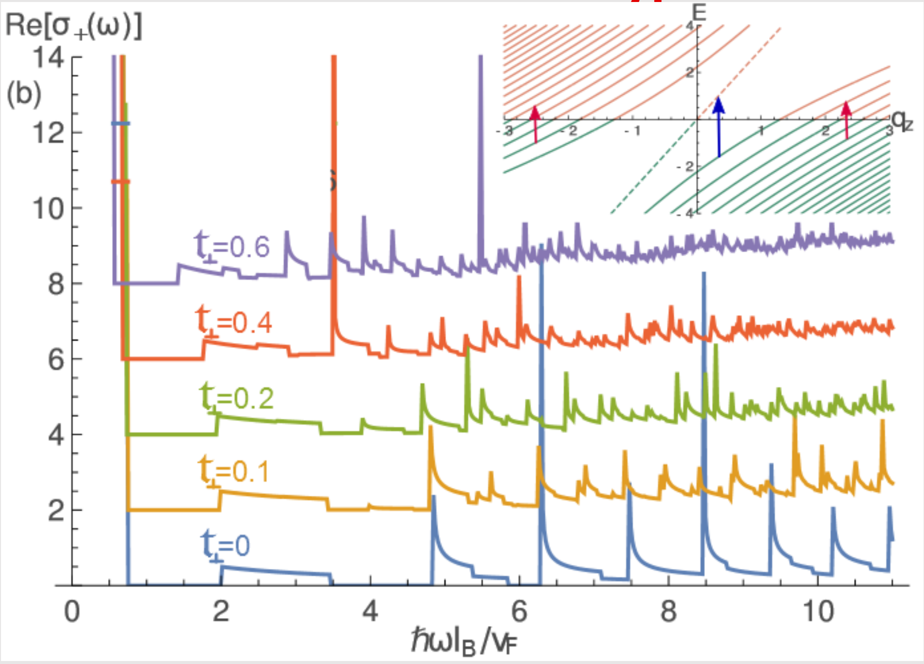
density of states

Breaking of dipolar selection rules

Type-I WSM



Type-II WSM



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Electric regime of a type-I WSM

- One can add a true electric field to the effective one

$$\boldsymbol{t}(\boldsymbol{E}) = \boldsymbol{t} - \frac{\boldsymbol{E} \times \boldsymbol{B}}{v_F B^2}$$

the spectrum is, for $\boldsymbol{t} = \boldsymbol{0}$,

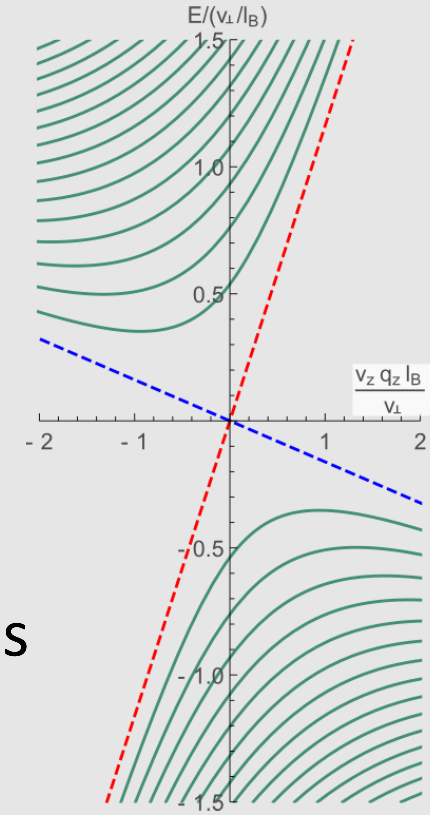
$$E_n^{\pm}(k_z) = \frac{E}{B} k_z \pm \sqrt{1 - w^2} \sqrt{v_z^2 k_z^2 + 2 v_x v_y \sqrt{1 - w^2} eB\, n}$$

with $\boldsymbol{w} = [\boldsymbol{E} \times \boldsymbol{B} / (v_F B^2)]$

Electric regime if $\frac{|\boldsymbol{E} \times \boldsymbol{B}|}{B^2} > v_F$

Conclusions

- Tilted Weyl cones in 2D and 3D
  - 2D : organic compound $\alpha - (BEDT - TTF)_2$,
  - 3D : Weyl semimetals ($MoTe_2, Cd_3As_2, \ldots$)
- Magnetic field effect simplified with Lorentz boosts, various regimes



3D Weyl semimetals	$\lvert t_\perp \rvert < 1$	$\lvert t_\perp \rvert > 1$
$\lvert t \rvert < 1$	**Type-I WSM** magnetic regime	**Type-I WSM** electric regime
$\lvert t \rvert > 1$	**Type-II WSM** magnetic regime	**Type-II WSM** electric regime

- Signature in magnetooptical selection rules (violation of dipolar $n \to n \pm 1$)

S. Tchoumakov et al., *Phys. Rev. Lett.* **117**, 086402 (2016)