Perspectives in Graphene Research and Beyond

Mark Oliver Goerbig

Disclaimer !

What I will not be talking about...

Applications of graphene

2013 : Graphene Flagship (10 Mrd Euros, European Union)

Potential applications: electronics, materials, optics,
captors, energetics, medicine, environment,…

(very long list !)

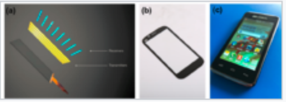
→ https://en.wikipedia.org/wiki/Potential_applications_of_graphene

Real applications: tennis racquets

Applications [edit]

Main article: Potential applications of graphene

Graphene is a transparent and flexible conductor that holds great promise for various material/device applications, including solar cells,[276] light-emitting diodes (LED), touch panels, and smart windows or phones.[277] According to information from Changzhou, China-based 2D Carbon Graphene Material Co.,Ltd, graphene-based touch panel modules have been sold in volume to cell phone, wearable device, and home appliance manufacturers. For instance, smartphone products with graphene touch screens are already on the market.



(a) The typical structure of a touch sensor in a touch panel. (Image courtesy of Synaptics, Incorporated.) (b) An actual example of 2D Carbon Graphene Material Co.,Ltd's graphene transparent conductor-based touchscreen that is employed in (c) a commercial smartphone.

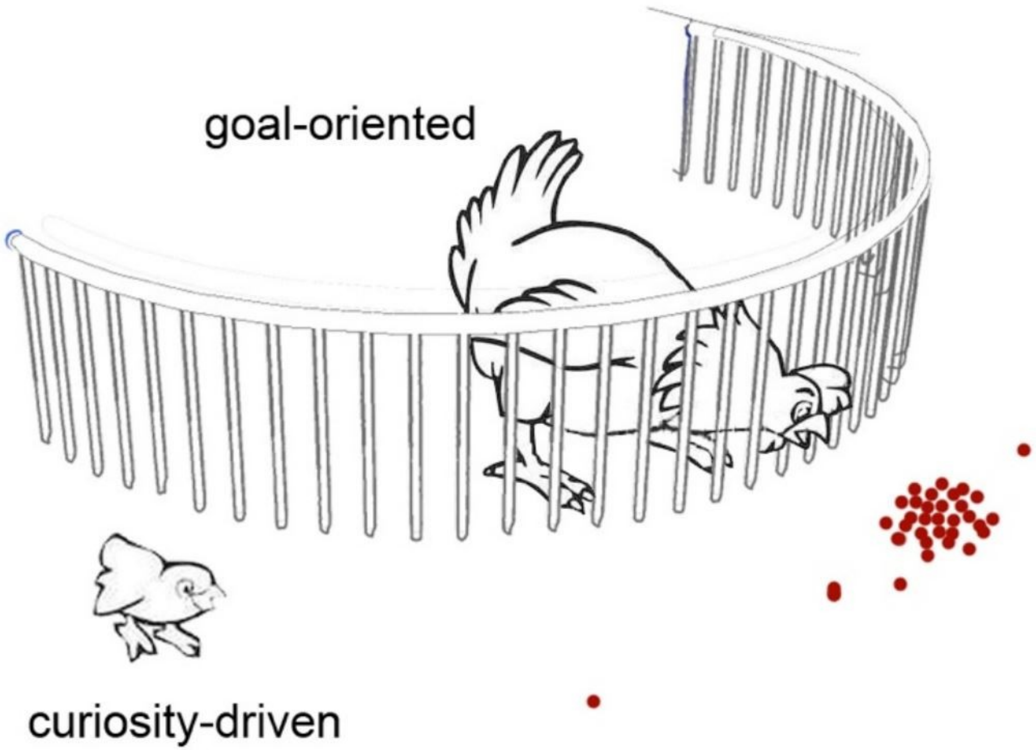
In 2013, Head announced their new range of graphene tennis racquets.[278]

As of 2015, there is one product available for commercial use: a graphene-infused printer powder.[279] Many other uses for graphene have been proposed or are under development, in areas including electronics, biological engineering, filtration, lightweight/strong composite materials, photovoltaics and energy storage.[211][280] Graphene is often produced as a powder and as a dispersion in a polymer matrix. This dispersion is supposedly suitable for advanced composites,[281][282] paints and coatings, lubricants, oils and functional fluids, capacitors and batteries, thermal management applications, display materials and packaging, solar cells, inks and 3D-printers' materials, and barriers and films.[283]

In 2016, researchers have been able to make a graphene film that can absorb 95% of light incident on it.[284] It is also getting cheaper; recently scientists at the University of Glasgow have produced graphene at a cost that is 100 times less than the previous methods.[285]

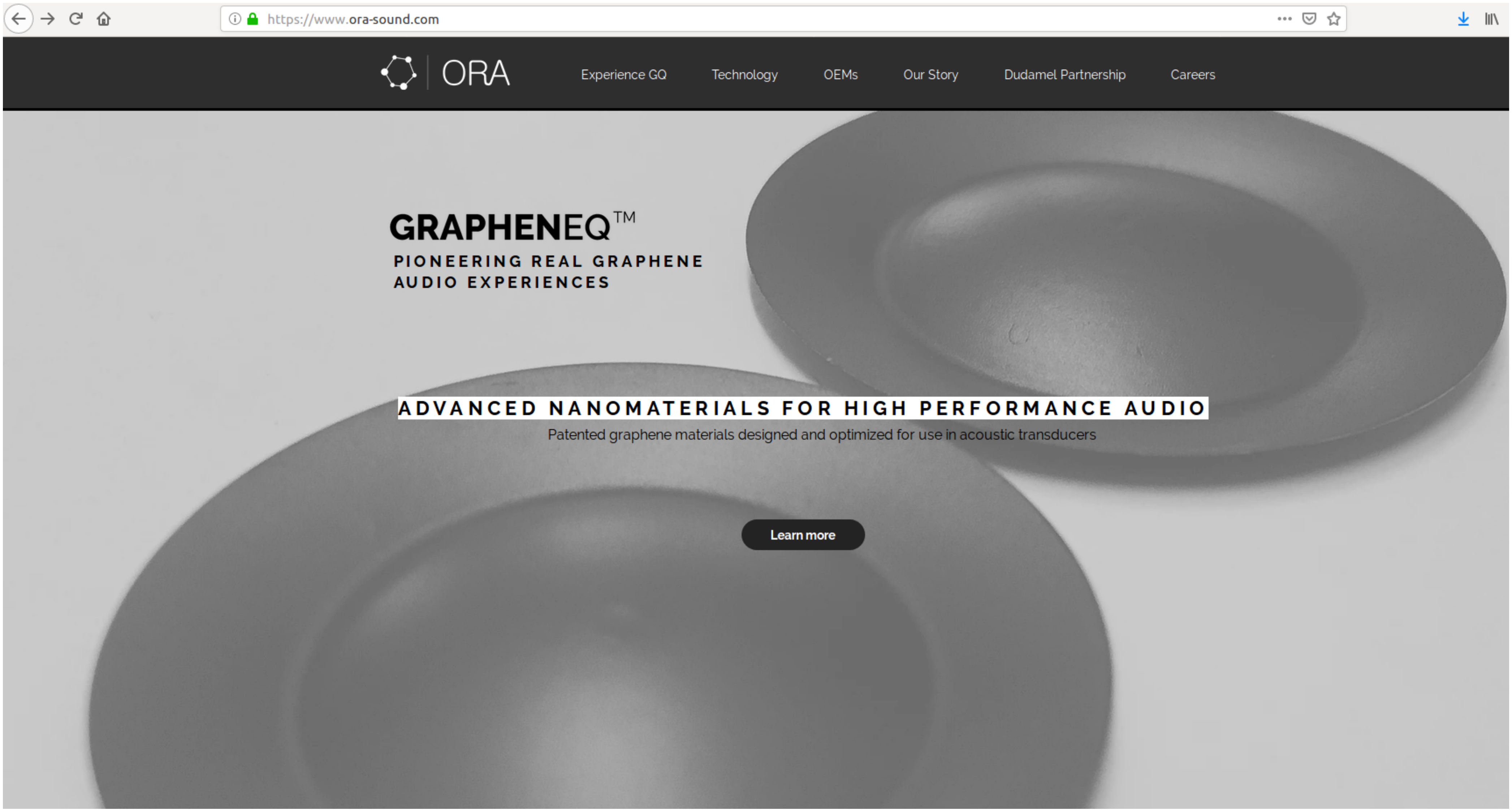
In August 2, 2016, BAC's new Mono model is said to be made out of graphene as a first of both a street-legal track car and a production car.[286]

Project-funding based research



https://www.nobelprize.org/nobel_prizes/physics/laureates/2005/hansch-slides.pdf

Graphene-based headphones



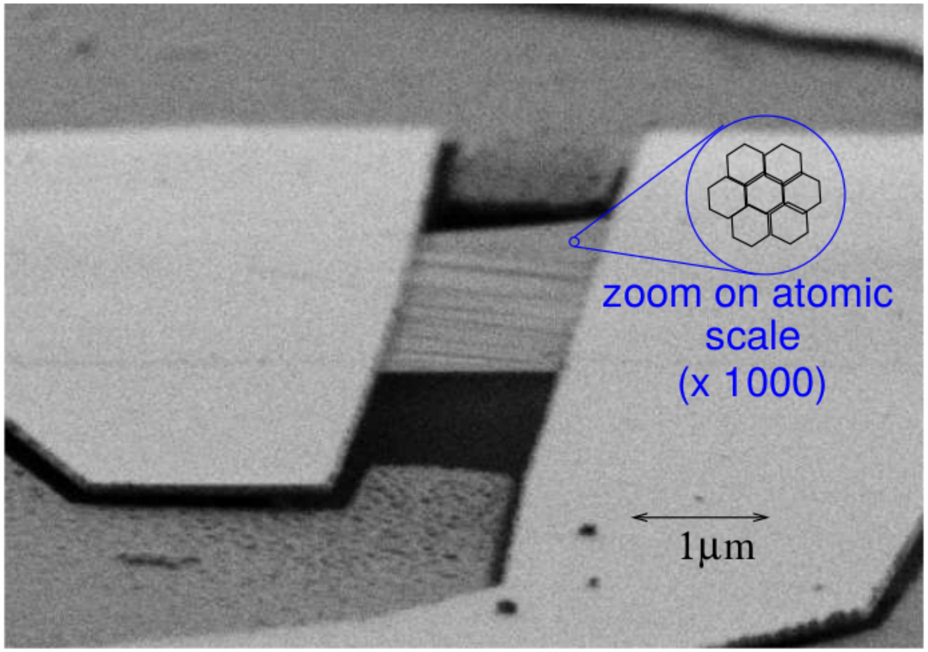
→ *Project emerged from fundamental research at McGill University, Montréal*

Fundamental condensed-matter research

Why do we care about graphene?

Prehistory: Graphene in a nutshell

- 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

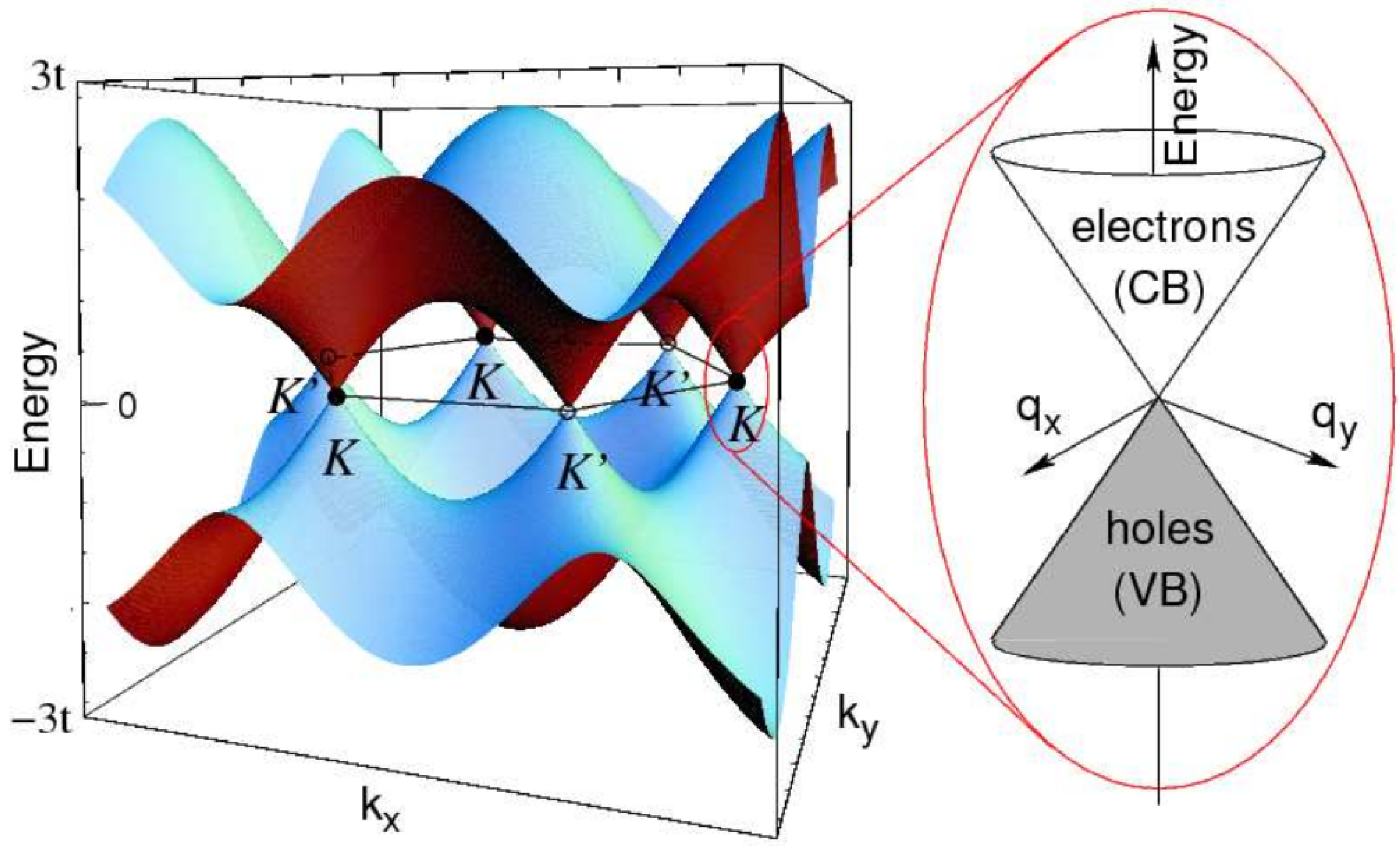
<u>Interest for fundamental research:</u>

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

Band structure of graphene

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

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



Wave functions and winding numbers

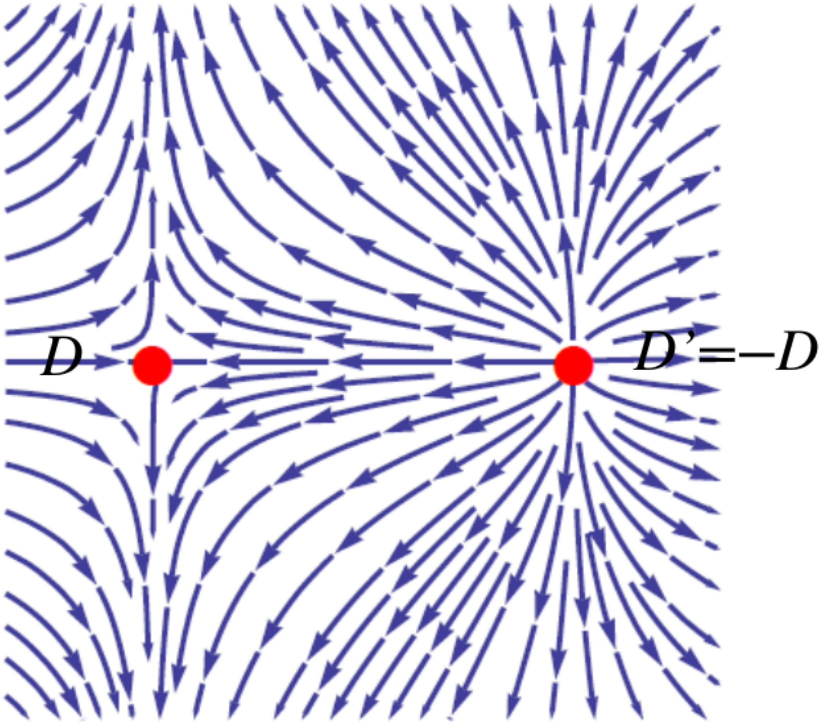
wave function

$$\psi_{\xi,\lambda;\mathbf{q}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \xi\lambda e^{-i\xi\phi_{\mathbf{q}}} \end{pmatrix} \qquad \tan\phi_{\mathbf{q}} = \frac{q_y}{q_x}$$

winding number ($\sim$ topol. charge)

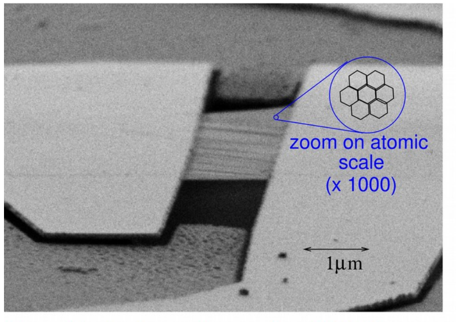
$$W_{\xi,\lambda} = \frac{\xi\lambda}{2\pi} \oint_{C_i} \nabla_{\mathbf{q}}\phi_{\mathbf{q}} \cdot d\mathbf{q} = \xi\lambda$$

Phase of wave function
(TRS−related Dirac points)



Time-reversal symmetry
$\rightarrow$ *Dirac points have opposite winding number*

Position of graphene in modern condensed-matter physics

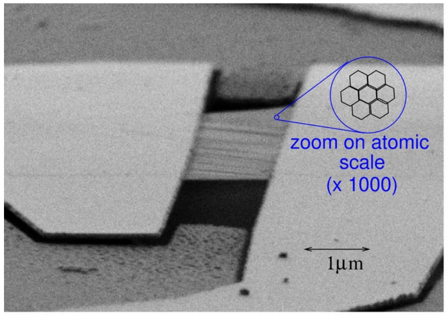


Chuan Li, physique mésoscopique, LPS, Orsay

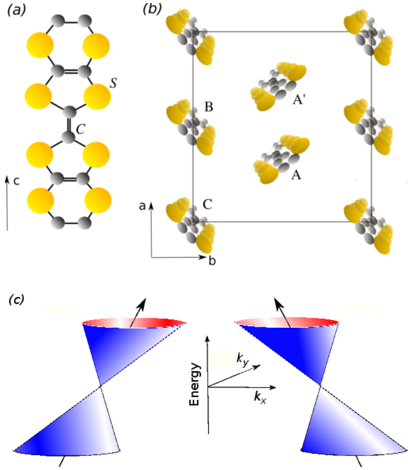
Since 2005: rewriting of the ***theory of the electron liquid*** for the case of graphene

→ plasmonics
→ electron-phonon coupling
→ superconductivity
→ electronic viscosity
→ SU(4) FQHE/quantum-Hall ferromagnetism

Position of graphene in modern condensed-matter physics



Chuan Li, physique mésoscopique, LPS, Orsay



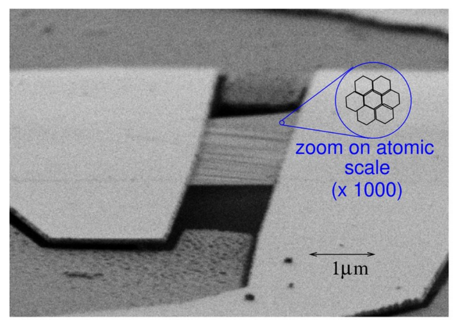
Since ~2006: ***other 2D materials hosting Dirac fermions***

→ organic materials

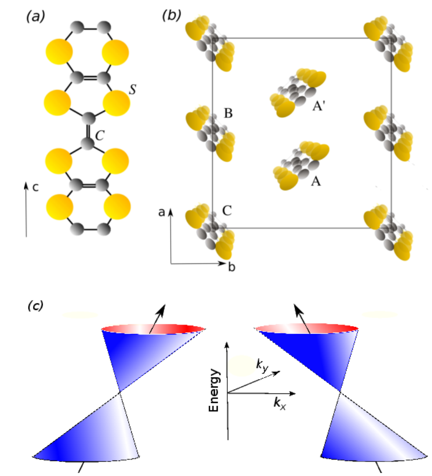
→ *tilted* Dirac cones

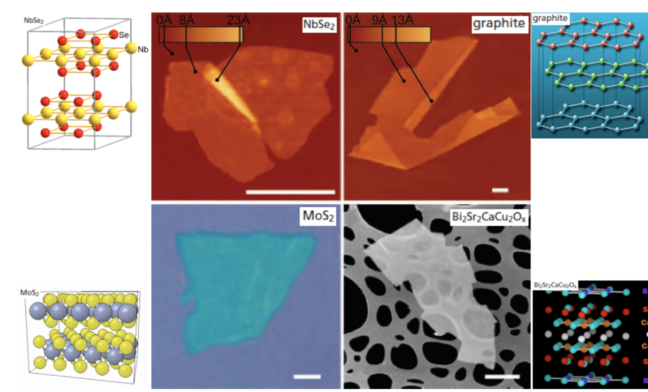
→ silicene...

Position of graphene in modern condensed-matter physics



Chuan Li, physique mésoscopique, LPS, Orsay



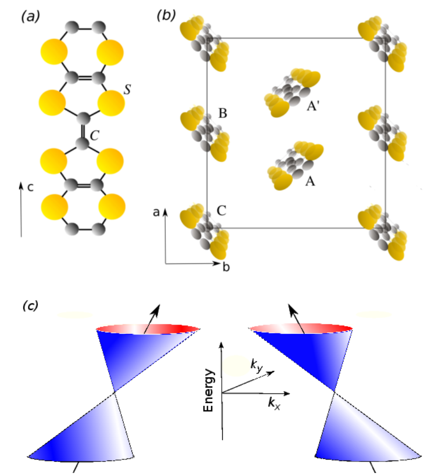


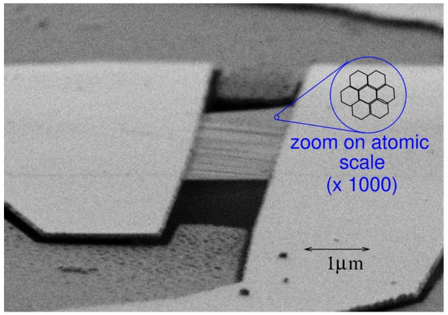
Since ~2006: ***other 2D crystals***

→ semiconductors (transition-metal dichalcogenides)

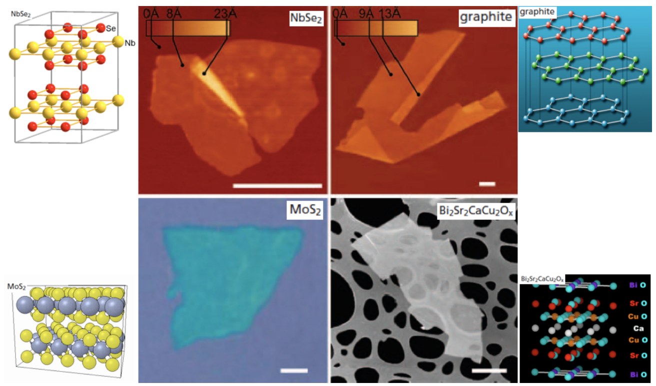
→ ***massive Dirac fermions (?)***

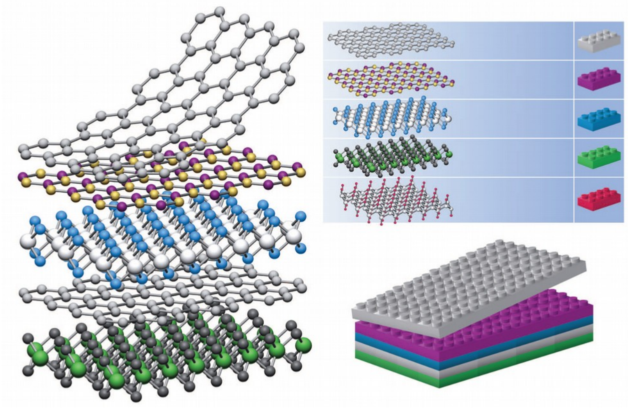
Position of graphene in modern condensed-matter physics





Chuan Li, physique mésoscopique, LPS, Orsay





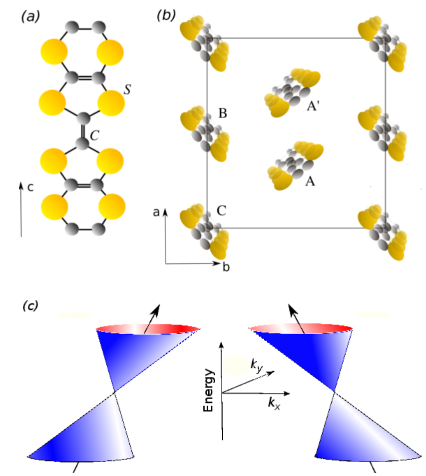
Since ~2010: ***heterostructures***

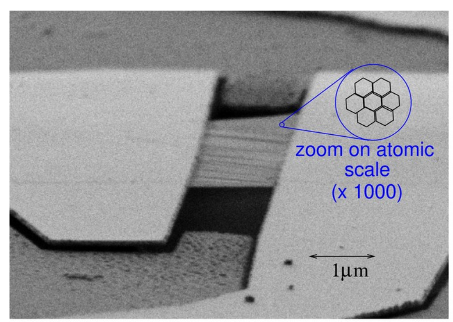
→ bilayer graphene

→ BN encapsulation

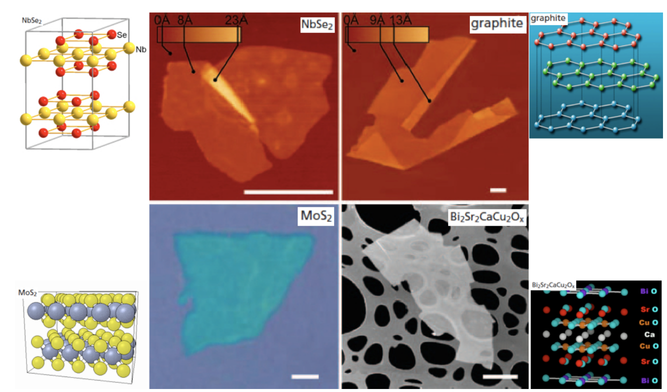
→ ***band-structure engineering (?)***

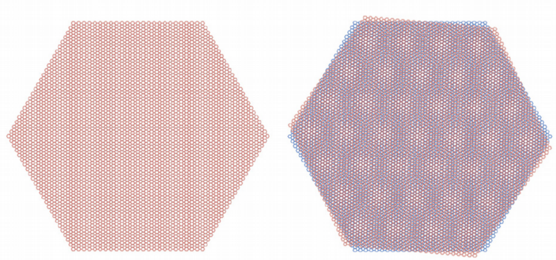
Position of graphene in modern condensed-matter physics

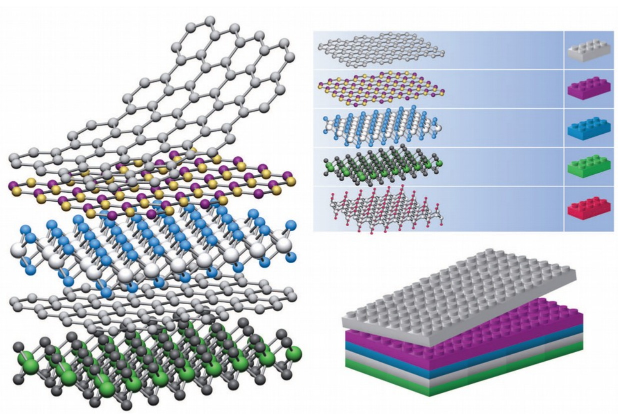




Chuan Li, physique mésoscopique, LPS, Orsay







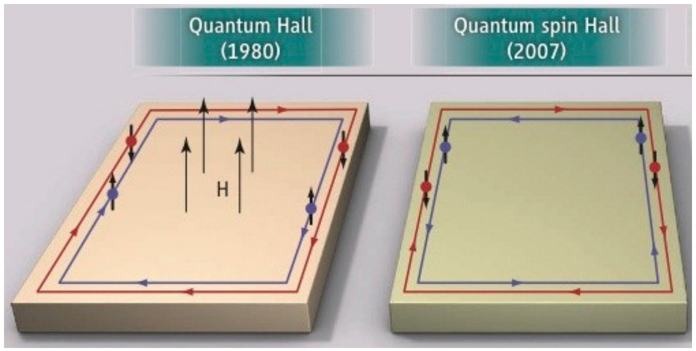
Since ~2009 (2018):

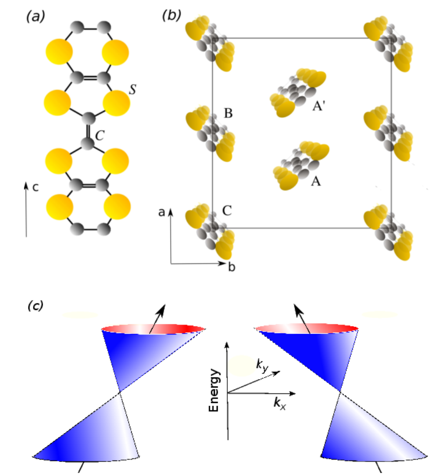
twisted bilayer graph.

→ Moiré patterns

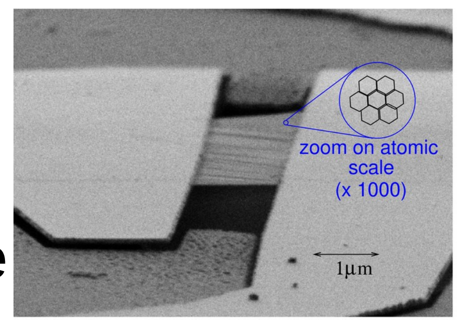
→ correlations and unconventional superconductivity

Position of graphene in modern condensed-matter physics

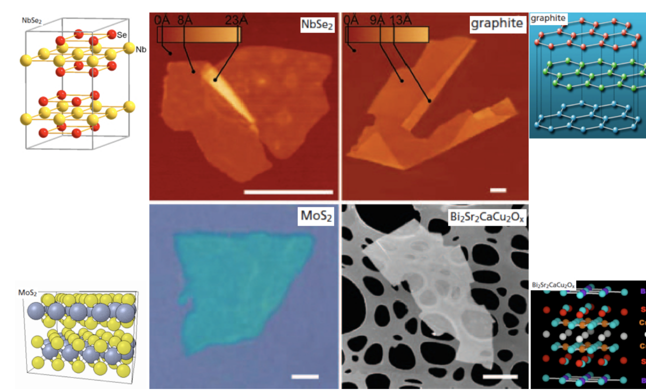


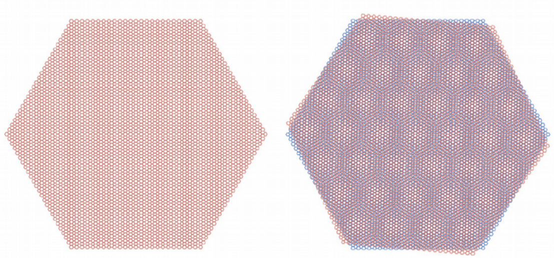


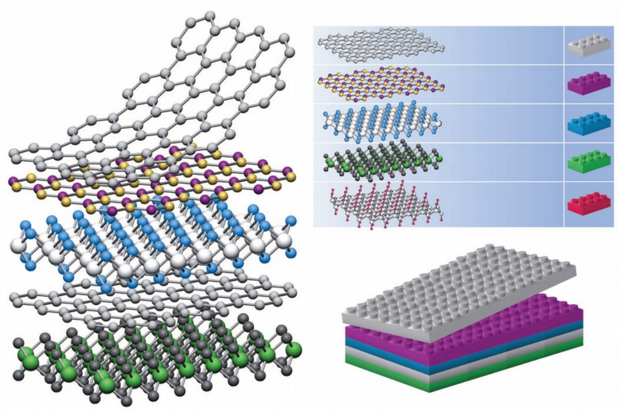
Since 2005: ***topological insulators and supercond.***
→ QAHE and QSHE
→ bulk-edge correspondence



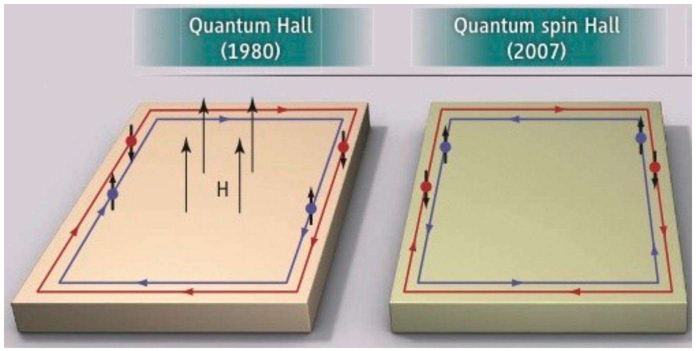
Chuan Li, physique mésoscopique, LPS, Orsay

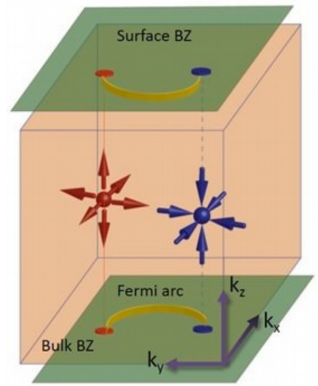




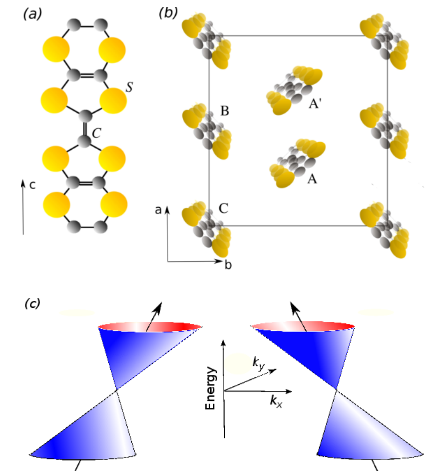


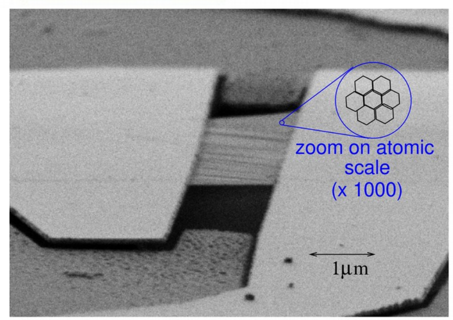
Position of graphene in modern condensed-matter physics



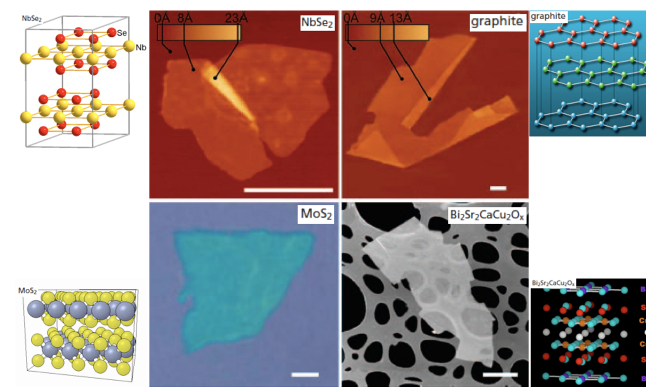


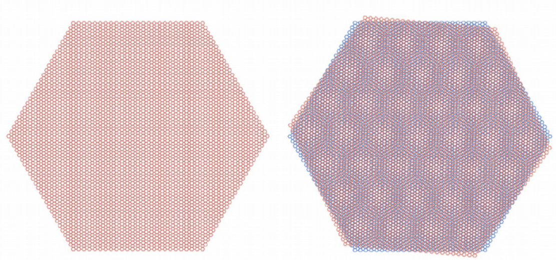
Since ~2014:
 Weyl semimetals
→ 3D graphene
→ Fermi arcs
→ chiral anomaly

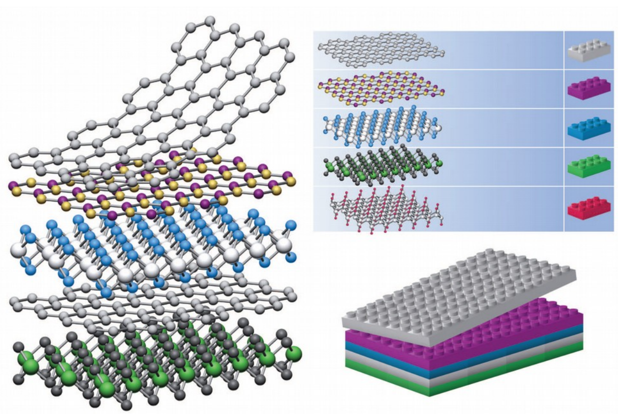




Chuan Li, physique mésoscopique, LPS, Orsay







Outline

- *Relativistic features* of graphene electrons

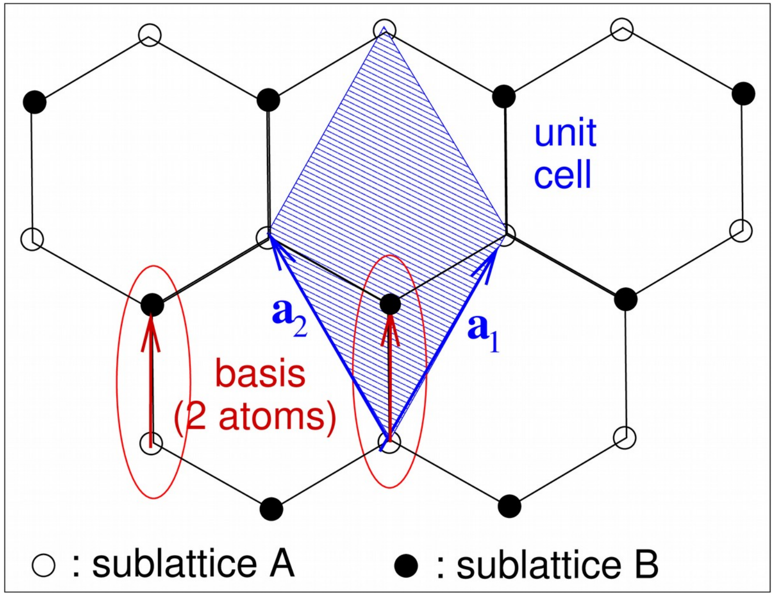
  (beyond the spectrum)
- *Massive Dirac fermions* in 2D transition-metal dichalcogenides (TMDC)
- How to unveil *geometry/topology in 2D materials*

  (the role of Berry curvature)
- Future research: interplay between *topology and correlations*

Band structure of graphene

Tight-binding model
(nearest-neighbour hopping) :

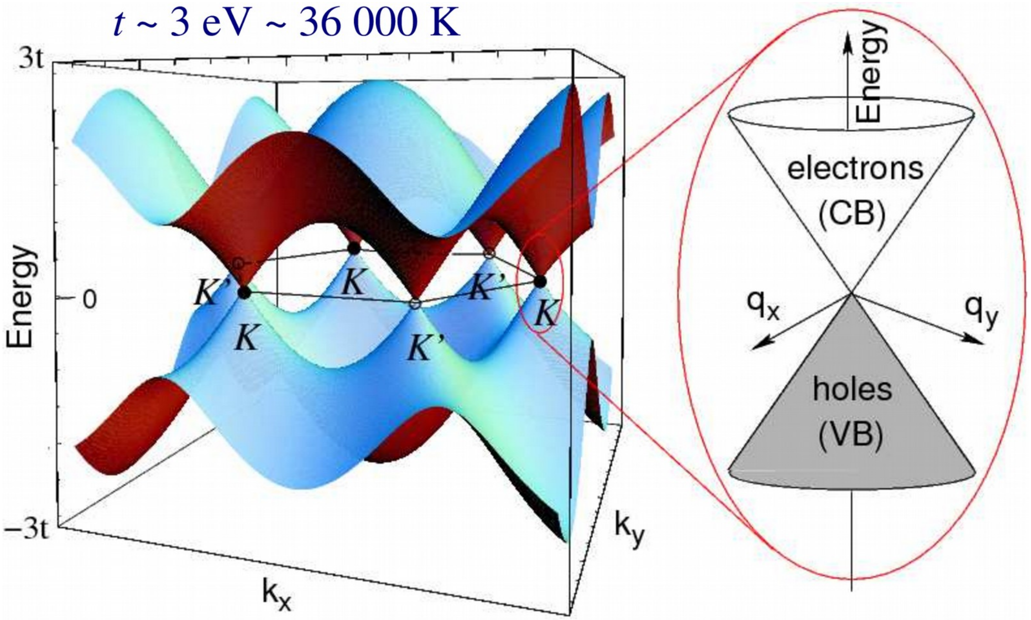
$$H_{\mathbf{k}} = \begin{pmatrix} \epsilon_0 & -t\gamma_{\mathbf{k}}^* \\ -t\gamma_{\mathbf{k}} & \epsilon_0 \end{pmatrix}$$



with (hopping from B to A) :

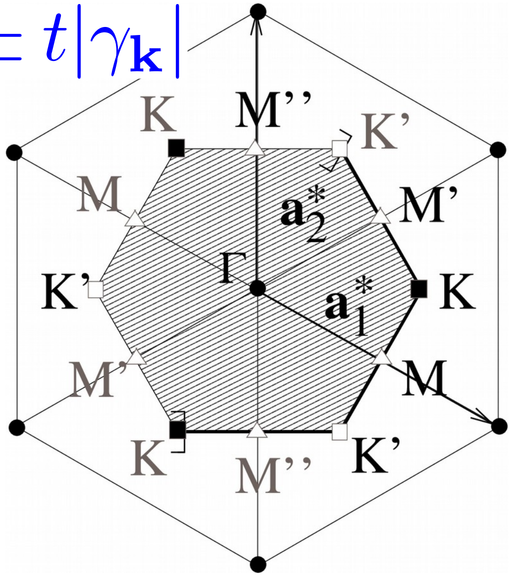
$$\gamma_{\mathbf{k}} = 1 + e^{i\mathbf{k}\cdot\mathbf{a}_1} + e^{i\mathbf{k}\cdot\mathbf{a}_2}$$

t ~ 3 eV ~ 36 000 K



energy bands :

$$E_{\pm}(\mathbf{k}) = \epsilon_0 \pm t|\gamma_{\mathbf{k}}|$$



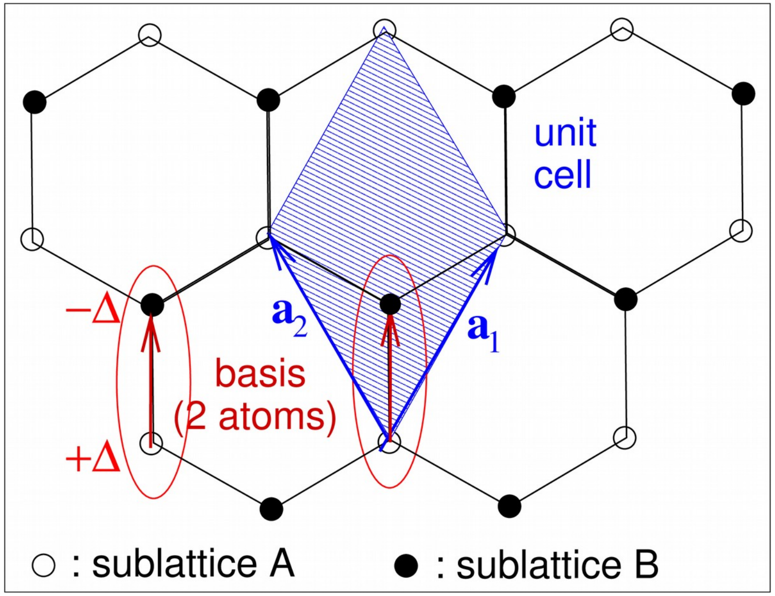
Band structure of *gapped* graphene

Tight-binding model
(nearest-neighbour hopping) :

$$H_{\mathbf{k}} = \begin{pmatrix} \epsilon_0 + \Delta & -t\gamma^*_{\mathbf{k}} \\ -t\gamma_{\mathbf{k}} & \epsilon_0 - \Delta \end{pmatrix}$$

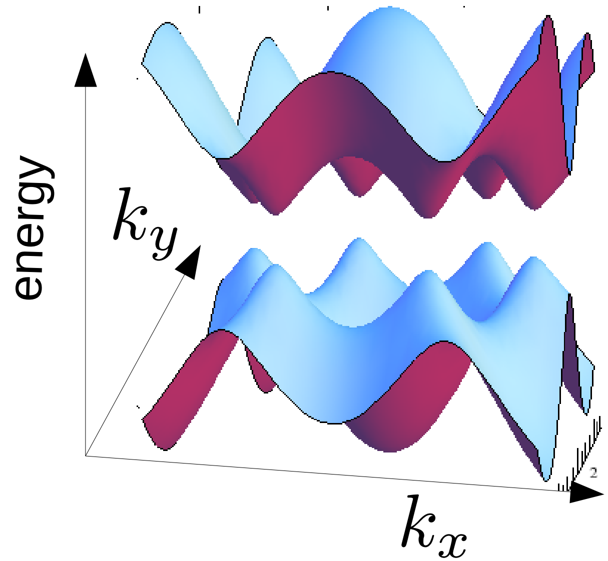
with (hopping from B to A) :

$$\gamma_{\mathbf{k}} = 1 + e^{i\mathbf{k}\cdot\mathbf{a}_1} + e^{i\mathbf{k}\cdot\mathbf{a}_2}$$



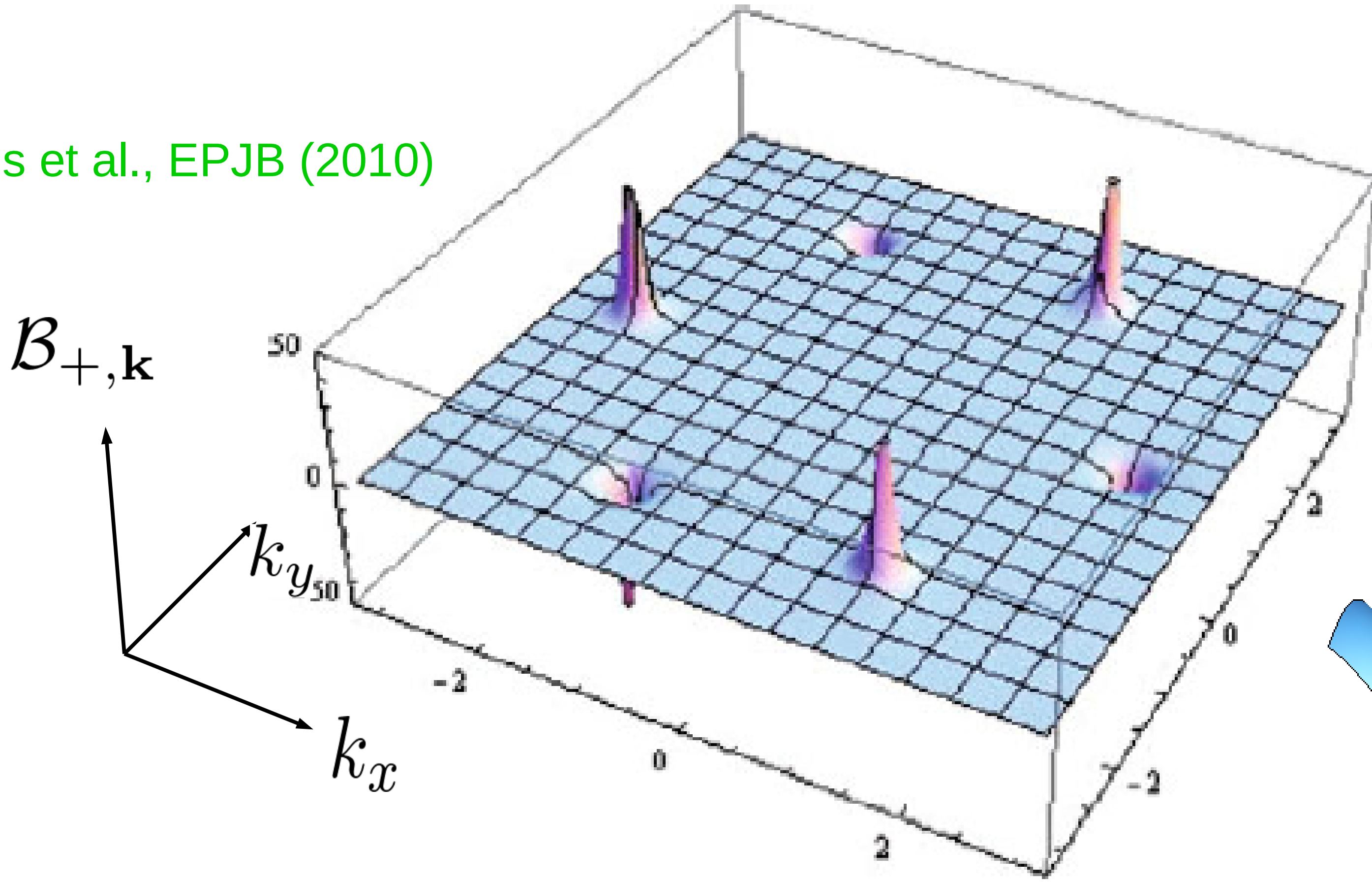
energy bands :

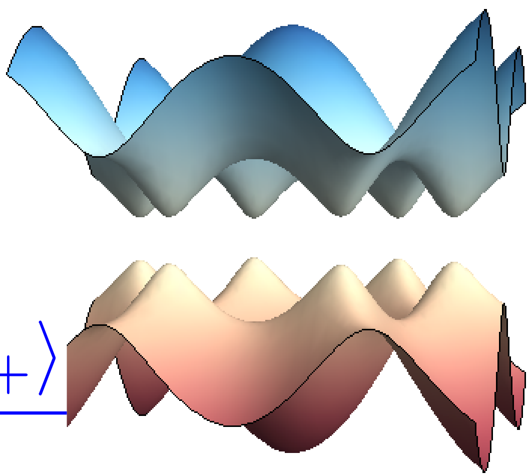
$$E_\lambda(\mathbf{k}) = \epsilon_0 + \sqrt{t^2|\gamma_{\mathbf{k}}|^2 + \Delta^2}$$



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

Band structure of *(gapped)* graphene (continuum limit)

Continuum limit = series expansion in qa :

$$(E - E_{\mathrm{Fermi}}) \ll t \qquad \text{i.e.} \qquad qa = |\mathbf{k} - \mathbf{K}|a \ll 1$$

$$\rightarrow \quad \gamma_{\mathbf{K}+\mathbf{q}} \simeq \gamma_{\mathbf{K}} + i\mathbf{q}\cdot\mathbf{a}_1 e^{2\pi/3} + i\mathbf{q}\cdot\mathbf{a}_2 e^{-2\pi/3}$$

$$\simeq \frac{3a}{2}(-q_x - iq_y)$$

$$\gamma_{-\mathbf{K}+\mathbf{q}} \simeq \gamma_{-\mathbf{K}} + i\mathbf{q}\cdot\mathbf{a}_1 e^{-2\pi/3} + i\mathbf{q}\cdot\mathbf{a}_2 e^{2\pi/3}$$

$$\simeq \frac{3a}{2}(q_x - iq_y)$$

$$\Delta = m v_F^2$$

Dirac Hamiltonian (*massive fermions*) :

ξ : valley index (K or K')

$$\boxed{H_\xi(\mathbf{q}) = \begin{pmatrix} \Delta & \hbar v_F(\xi q_x - iq_y) \\ \hbar v_F(\xi q_x + iq_y) & -\Delta \end{pmatrix}} \qquad v_F = \frac{3at}{2\hbar}$$

Landau levels (→ magnetic field)

$$H_\xi = \begin{pmatrix} \Delta & \xi v(\Pi_x - \xi i \Pi_y) \\ \xi v(\Pi_x + i\xi\Pi_y) & -\Delta \end{pmatrix}$$

with (Peierls substitution):

$$\Pi_{x/y} = p_{x/y} + eA_{x/y}(\mathbf{r})$$

$$H_K = \begin{pmatrix} \Delta & \sqrt{2}\frac{\hbar v}{l_B} a \\ \sqrt{2}\frac{\hbar v}{l_B} a^\dagger & -\Delta \end{pmatrix} \qquad H_{K'} = \begin{pmatrix} \Delta & -\sqrt{2}\frac{\hbar v}{l_B} a^\dagger \\ -\sqrt{2}\frac{\hbar v}{l_B} a & -\Delta \end{pmatrix}$$

fermions de Dirac massifs

Landau-level spectrum:

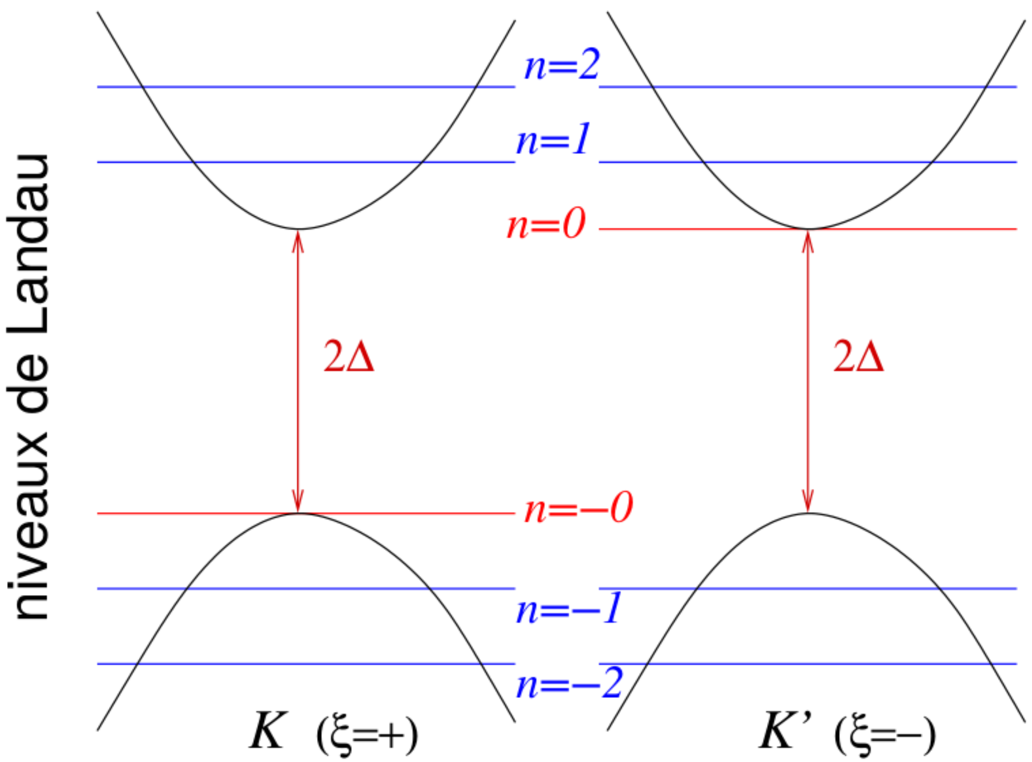
$$\epsilon^\xi_{\lambda, n\neq 0} = \lambda\sqrt{\Delta^2 + 2\hbar^2\frac{v^2}{l_B^2}n}$$

$$\simeq \lambda\left[\Delta + \hbar\frac{eB}{\Delta/v^2}n\right]$$

$$\epsilon^\xi_{n=0} = -\xi\Delta$$

→ *parity anomaly*

[Semenoff, PRL (1984)]



Dirac fermions in condensed matter

Are there relativistic signatures beyond the spectrum ?

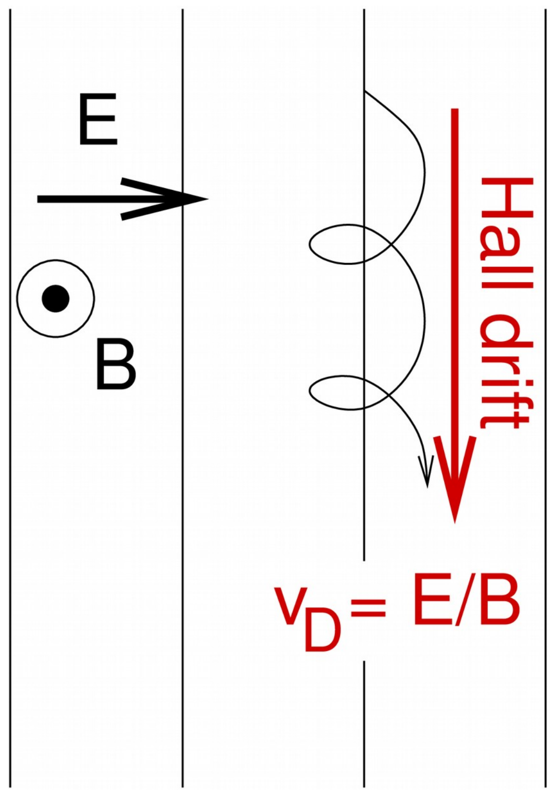
→ *Covariance*
→ *Coupling to electromagnetic field*

2D electrons in crossed magnetic and electric fields

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

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

→ 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

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

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

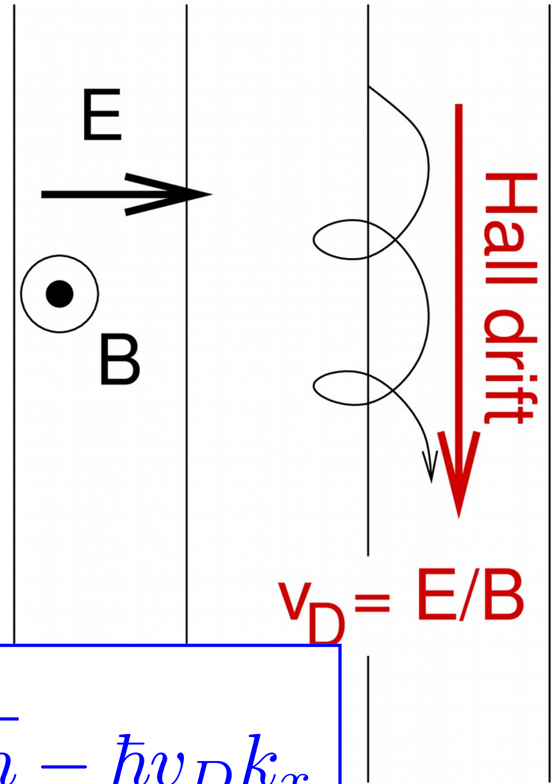
→ Relativistic (Dirac) fermions:
Lorentz transformation to comoving frame of reference with velocity $v_D = E/B$

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

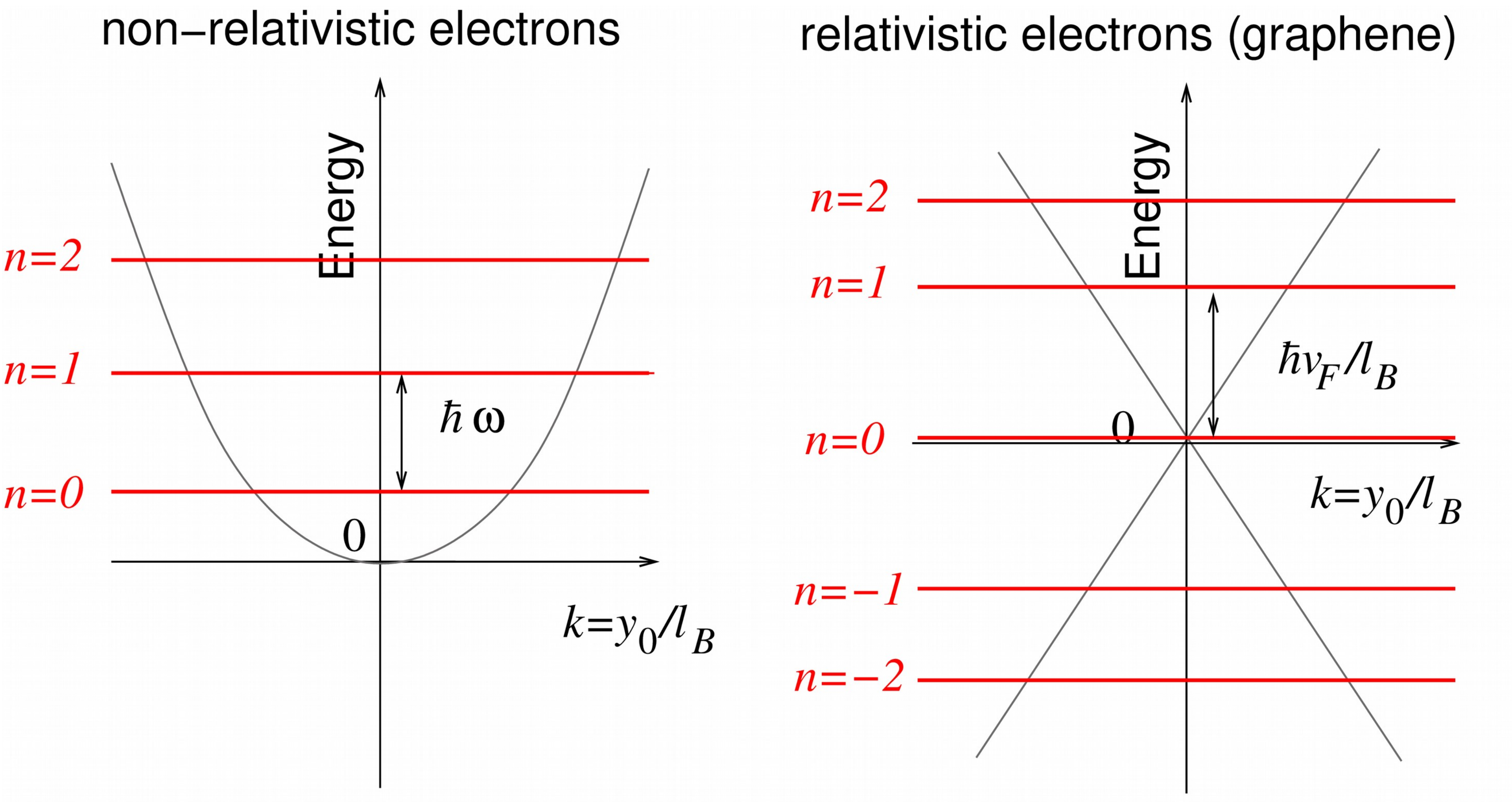
$$\epsilon \to \epsilon' = \epsilon/\sqrt{1 - (v_D/v)^2} \propto 1/l_{B'} \propto \sqrt{B'}$$

→ Landau levels (in lab frame):

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

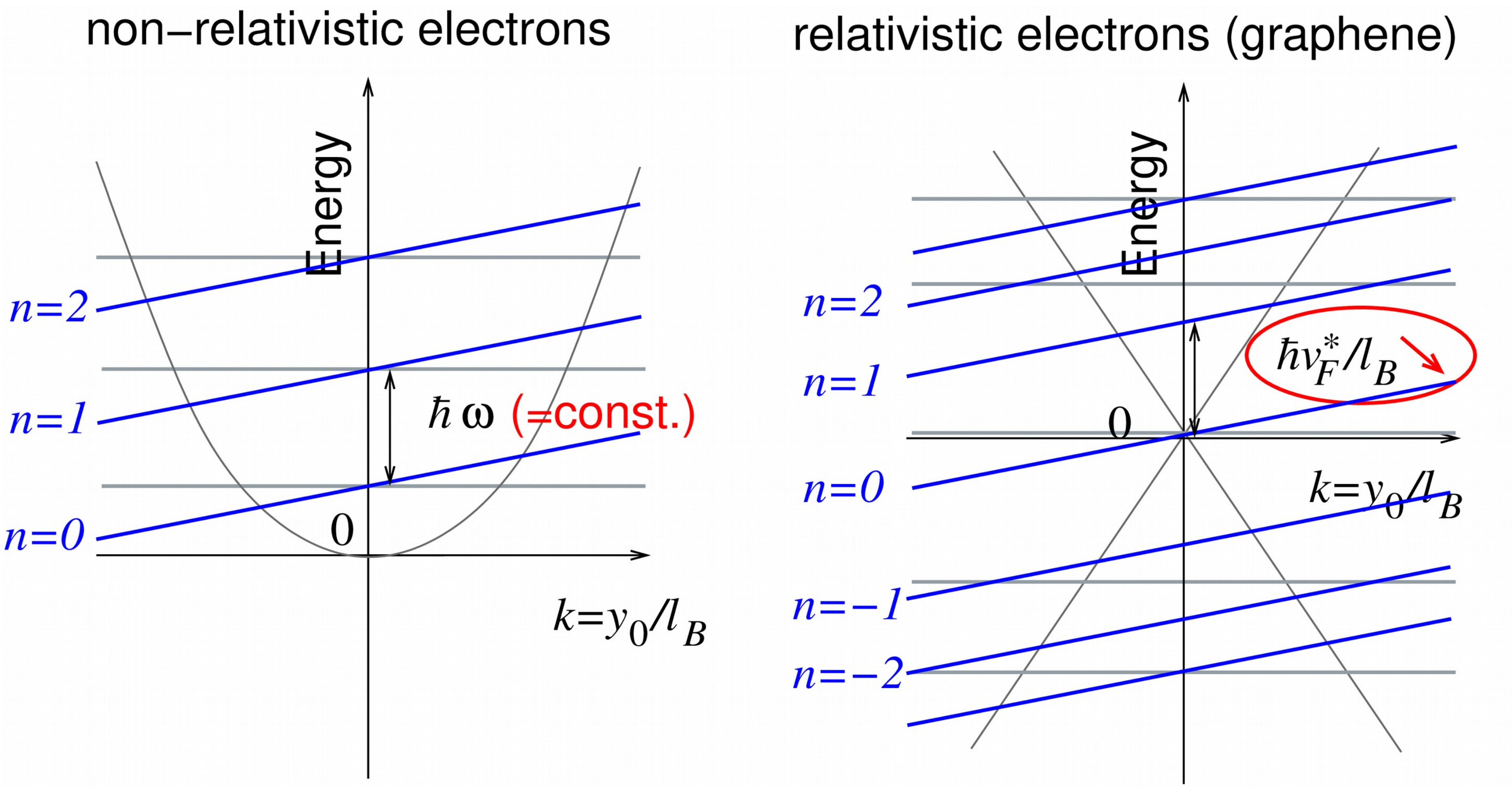


2D electrons in crossed magnetic and electric fields



no electric field

2D electrons in crossed magnetic and electric fields



in the presence of an electric field

[Lukose et al., PRL (2007)]

Relativistic breakdown of Landau levels

Relativistic Landau levels:

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

Condition for drift velocity (upper critical electric field):

$$v_D = E/B < v \qquad \leftrightarrow \qquad E < E_c = vB$$

→ *"magnetic regime" ~ existence of frame of reference with closed orbits*

→ *"electric regime" ~ open orbits in any frame of reference for*

$$v_D > v \qquad \leftrightarrow \qquad E > vB$$

Pseudo-covariance in tilted Dirac and Weyl cones

Generalised Dirac/Weyl Hamiltonian:

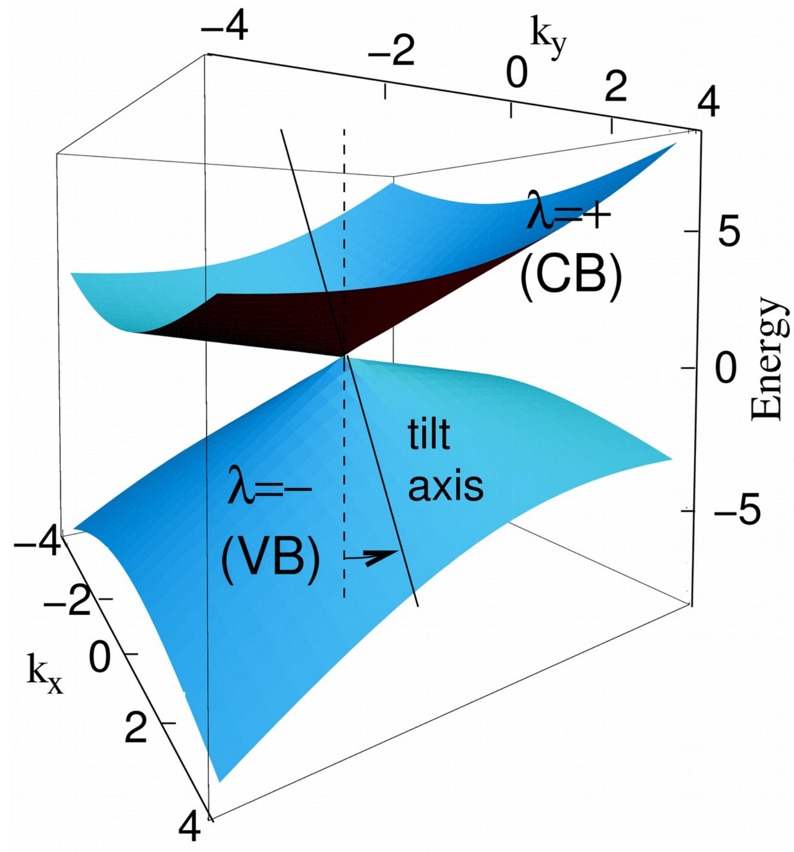
$$H_\xi = \xi\hbar v\left(q_x\sigma_x + \xi q_y\sigma_y + q_z\sigma_z\right) + \xi\hbar\mathbf{w}_0\cdot\mathbf{q}\sigma_0$$

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

σ_0 : *2x2 one matrix*

Energy dispersion:

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



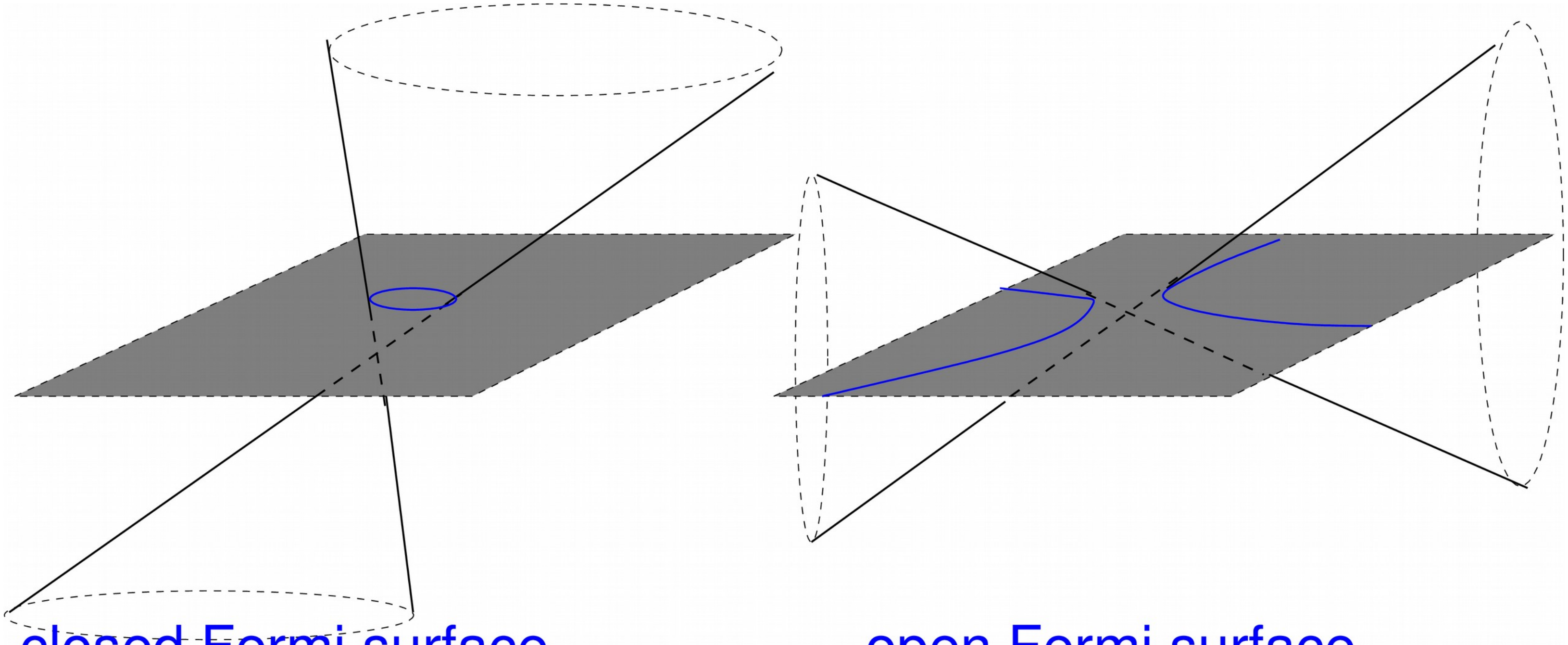
Criterion for maximal tilt

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

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)

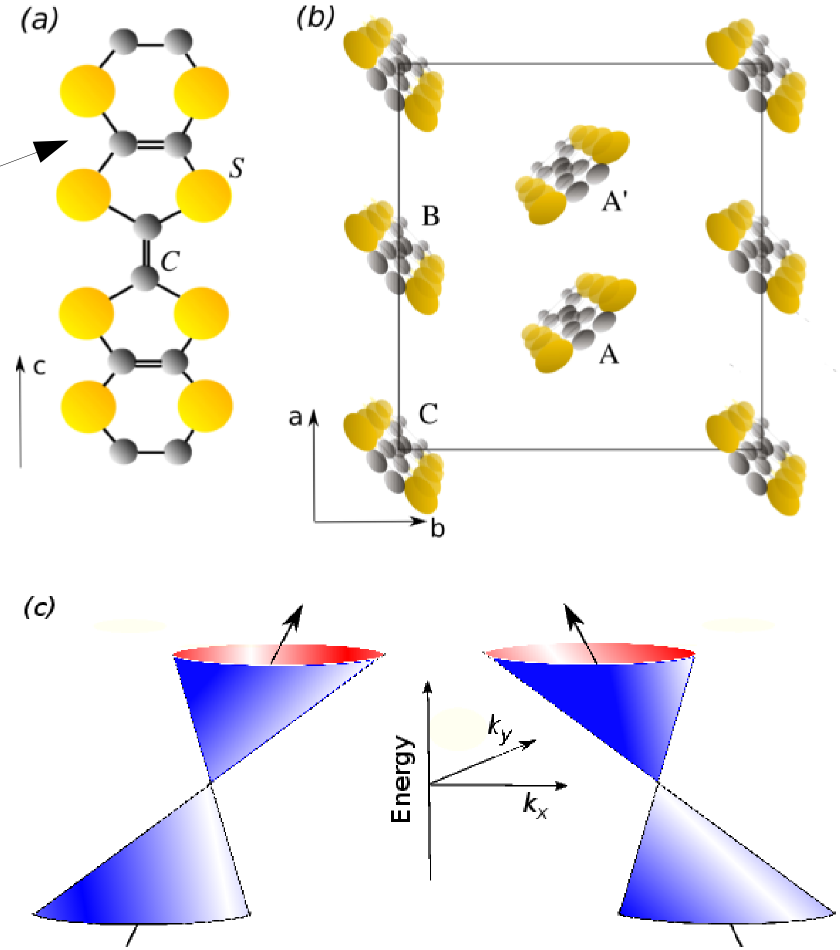
open Fermi surface
(hyperbolas)

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

Materials with tilted Dirac cones

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 $t_i \sim 20...140\ \mathrm{meV}$

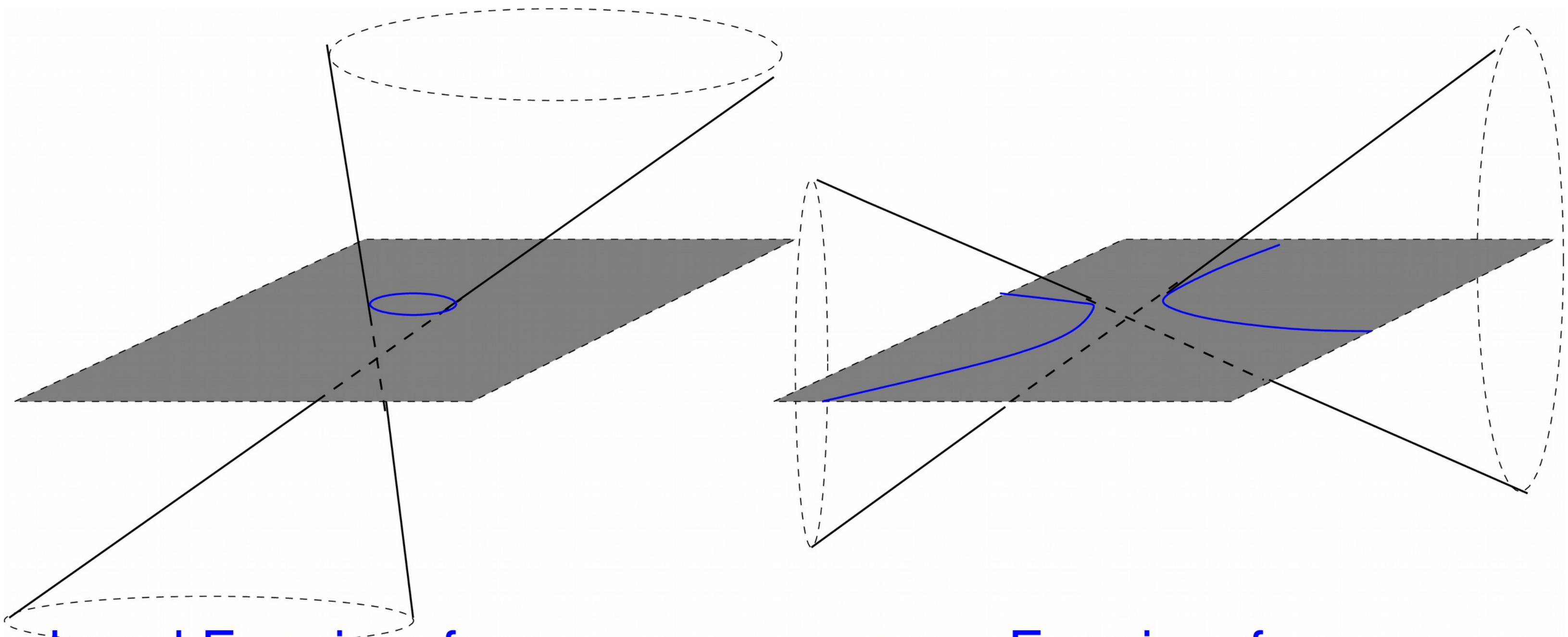
→ Dirac semimetal under pressure

Katayama et al., JPSJ (2006)

Criterion for maximal tilt/relation with relativistic electrons in crossed fields

$\tilde{w}_0 = (w_{0x}^2 + w_{0y}^2 + w_{0z}^2)/v^2 < 1$ $\qquad$ $\tilde{w}_0 > 1$

type-I Dirac/Weyl semimetal $\qquad$ type-II Dirac/Weyl semimetal



closed Fermi surface (ellipse) $\qquad$ 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

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

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

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

trivial part

covariant part

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

$E_{\text{eff}} = w_0 B \qquad \rightarrow \qquad w_0 = v_D$: ***tilt = drift velocity !***

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

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

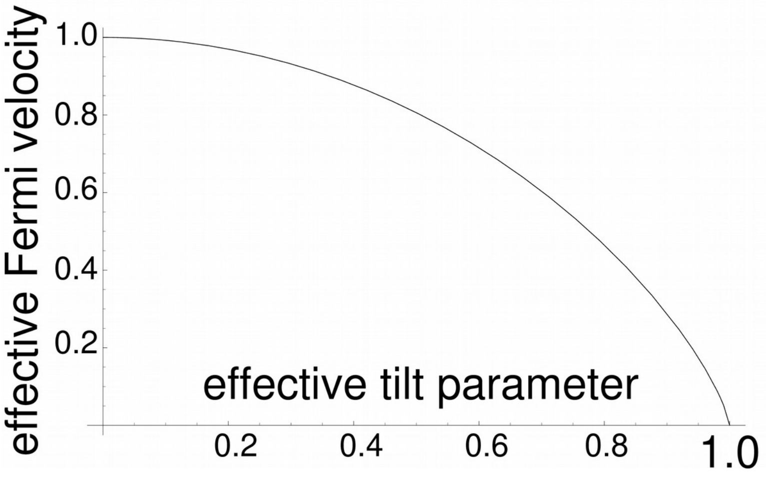
Diagonalisation yields Landau-level spectrum:

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

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

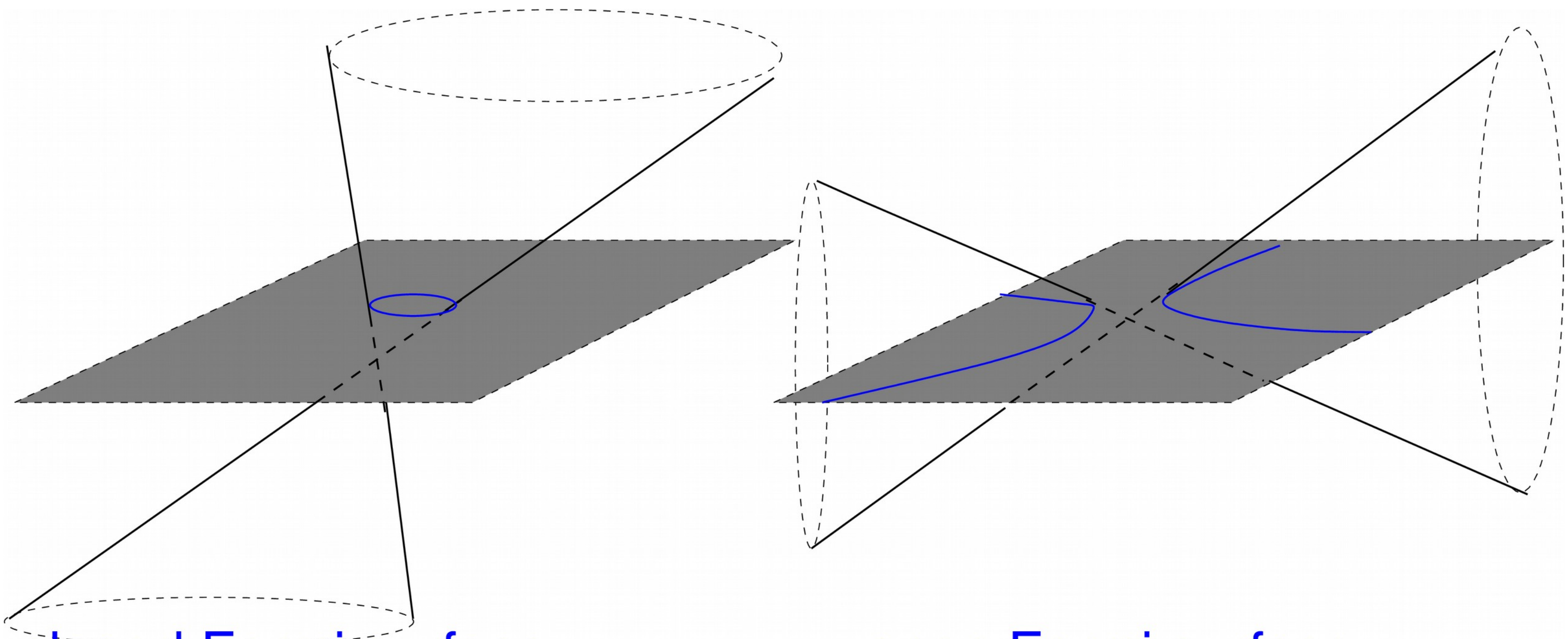
with renormalised velocity:

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



Pseudo-covariance in tilted Dirac and Weyl cones

$\tilde{w}_0 < 1$ $\tilde{w}_0 > 1$



closed Fermi surface (ellipse)

open Fermi surface (hyperbolas)

~ "magnetic" regime

~ "electric" regime

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

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

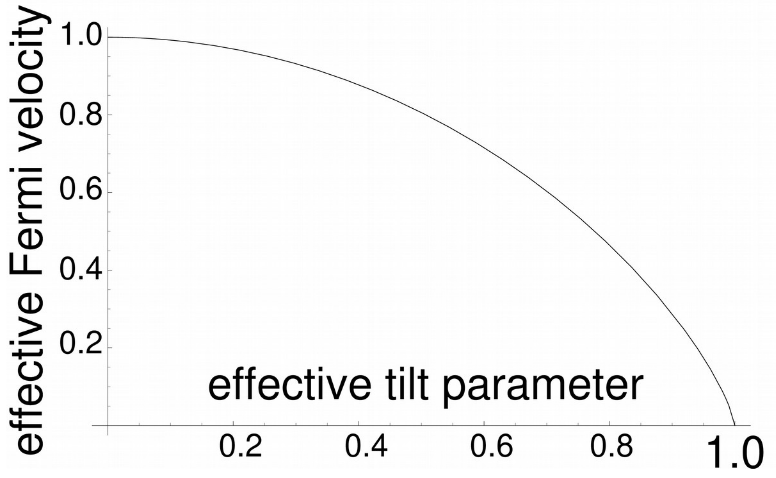
Diagonalisation yields Landau-level spectrum:

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:

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



Light-matter coupling

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

→ 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

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

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

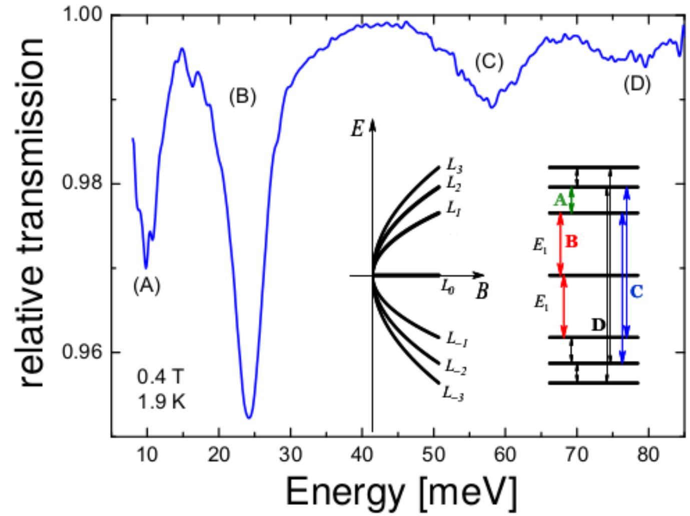
→ graphene (no tilt, no electric field): $m = (n \pm 1)$

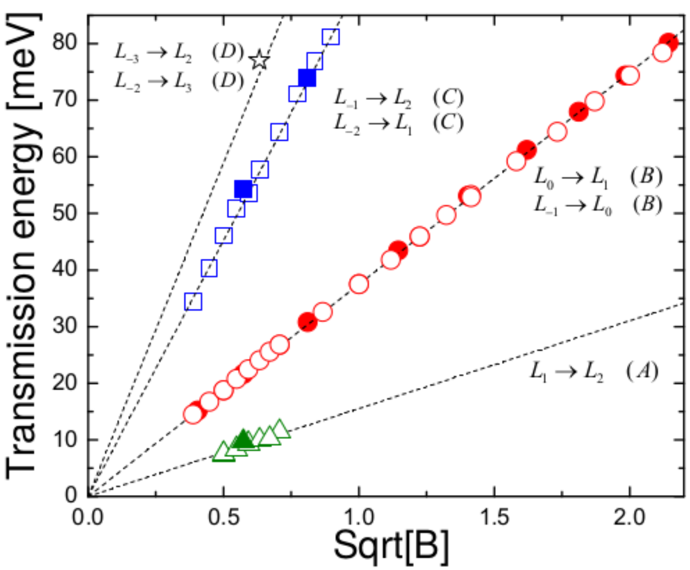
<u>dipolar selection rules (in comoving frame):</u>

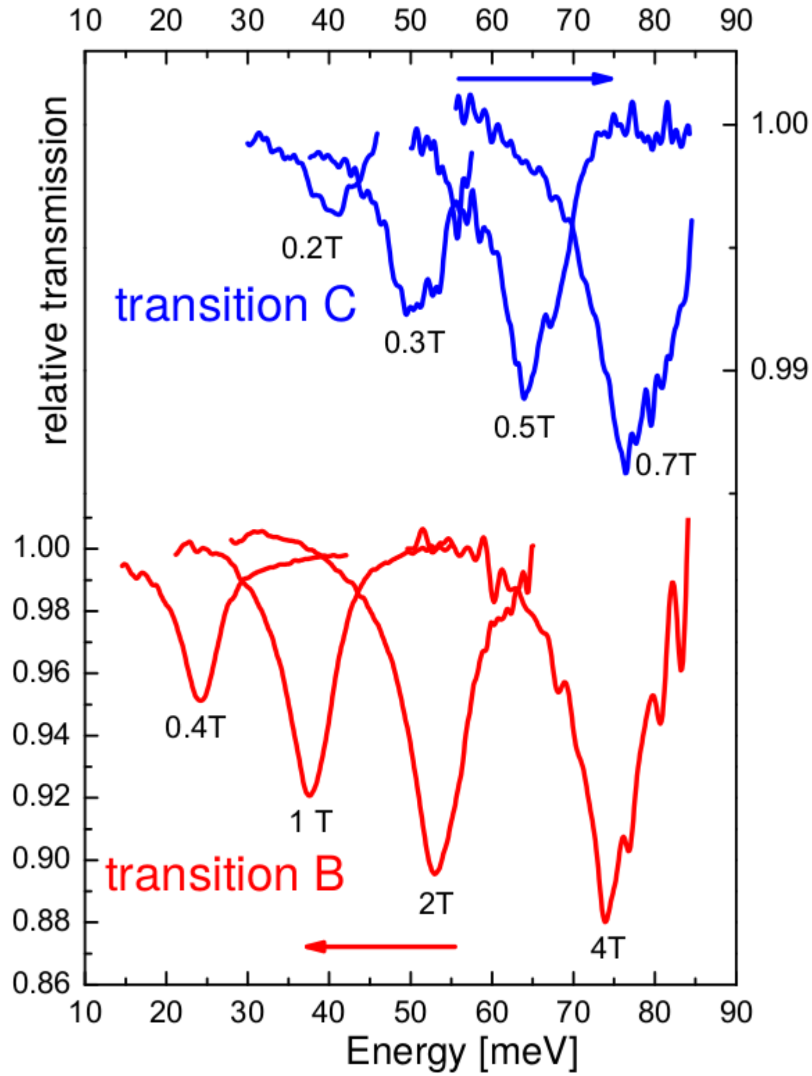
$$\lambda n \to \lambda'(n+1) \qquad \text{for} \quad \text{right}-\text{handed light} \quad \circlearrowleft$$

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

Infrared transmission spectroscopy in graphene







selection rules :

$$\lambda, n \to \lambda', n\pm1$$

Grenoble high–field group: Sadowski et al., PRL 97, 266405 (2007)

Light-matter coupling for tilted Dirac cones

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

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

(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 $\psi'^{\dagger}_{\lambda n}\mathbf{v}\psi'_{\lambda'(n\pm1)}$

WANTED: selection rules in lab frame !

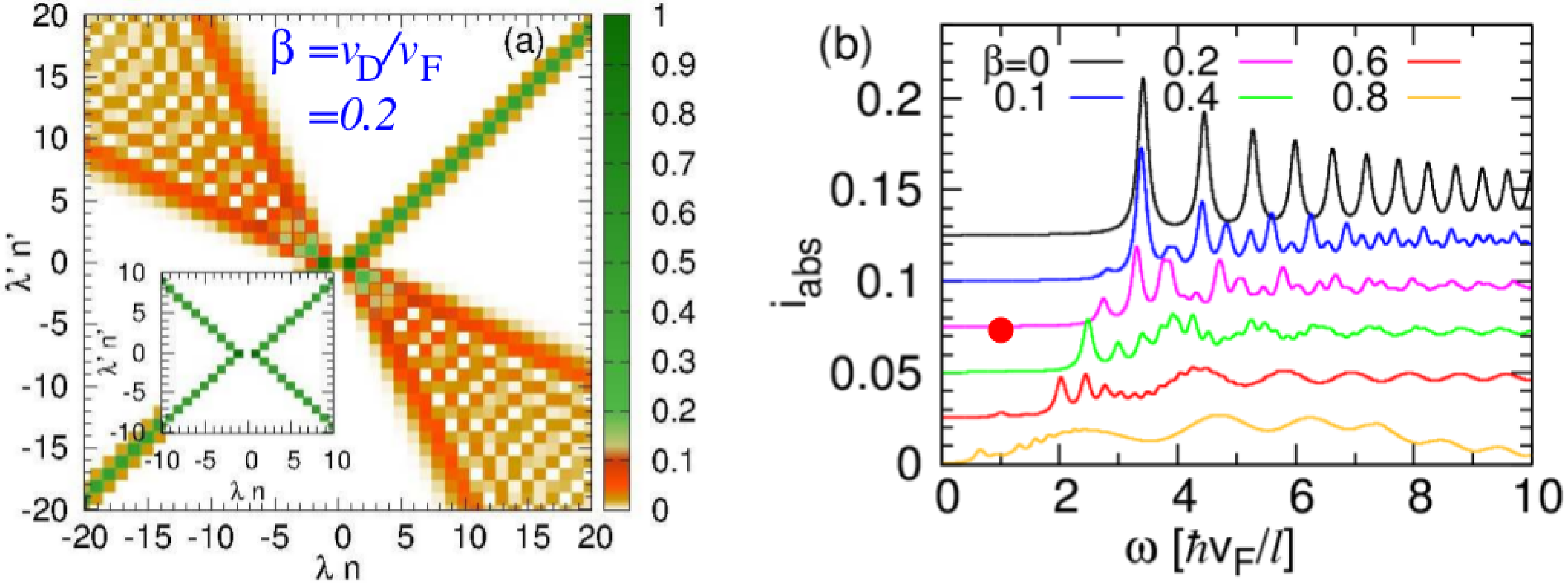
Light-matter coupling for tilted Dirac cones

- 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



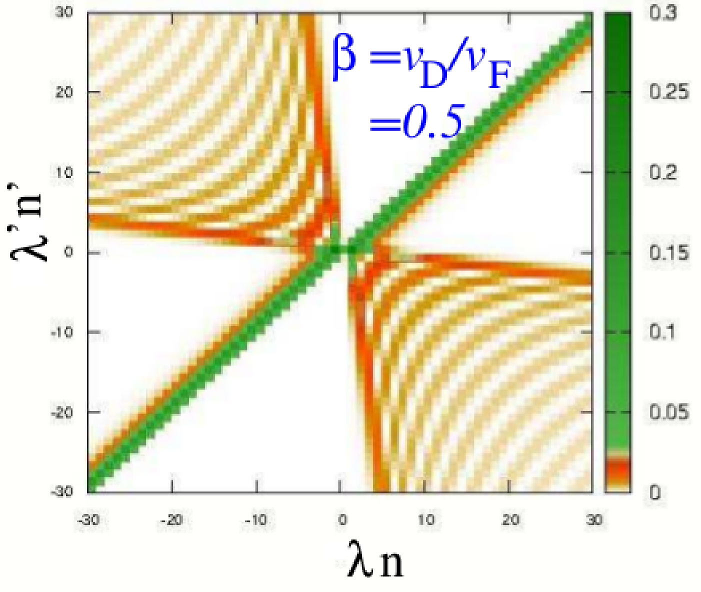
Light-matter coupling for tilted Dirac cones

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

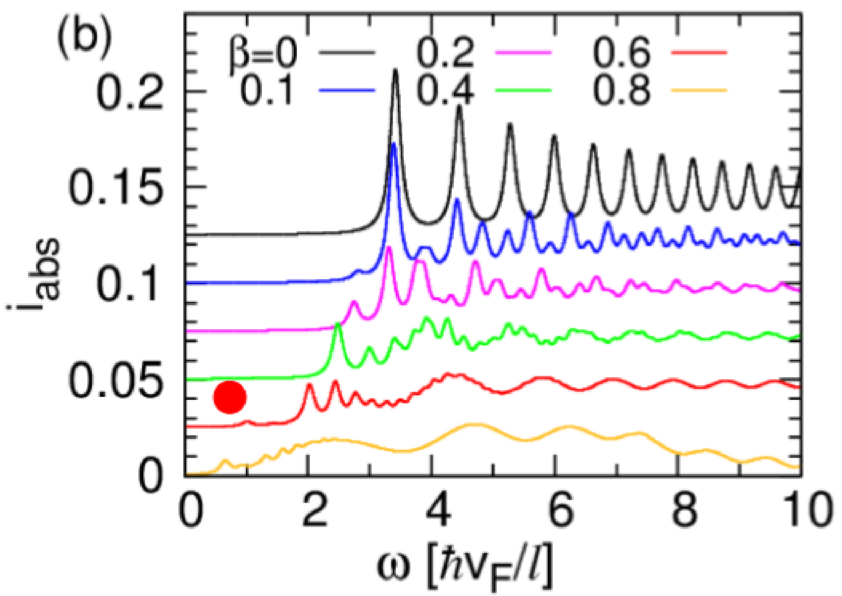
$$\lambda n \to \lambda'(n \pm 1)$$

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

matrix elements



absorption coefficient



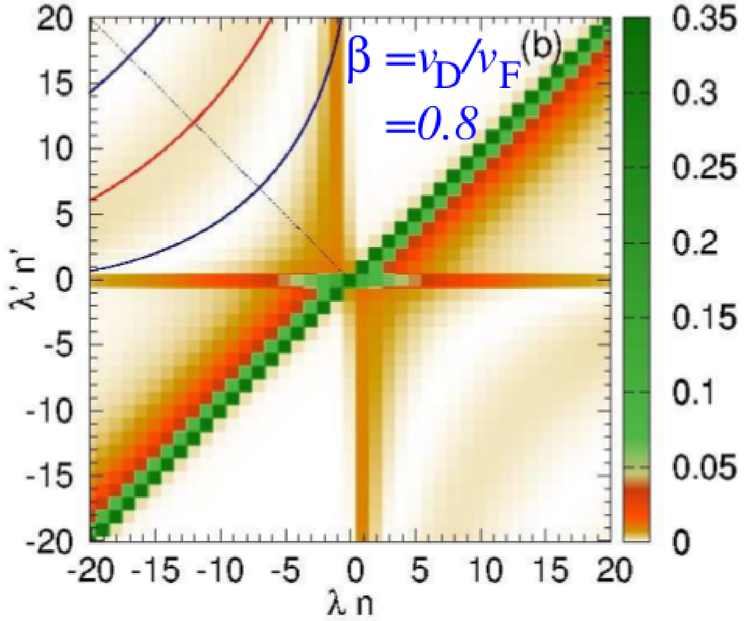
Light-matter coupling for tilted Dirac cones

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

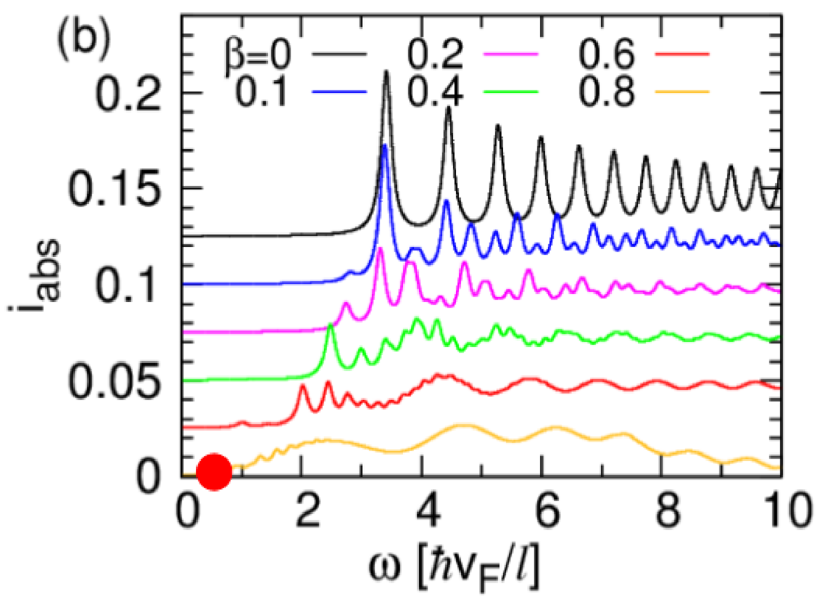
$$\lambda n \to \lambda'(n \pm 1)$$

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

matrix elements



absorption coefficient



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

Pseudo-covariance in 3D Weyl semimetals

Novelty with respect to 2D:

Tilt direction no longer necessarily perpendicular to the magnetic field

→ *magnetic and electric regimes no longer directly related to type-I and type-II Weyl semimetals*

Pseudo-covariance in 3D Weyl semimetals

tilt parameter (vector)

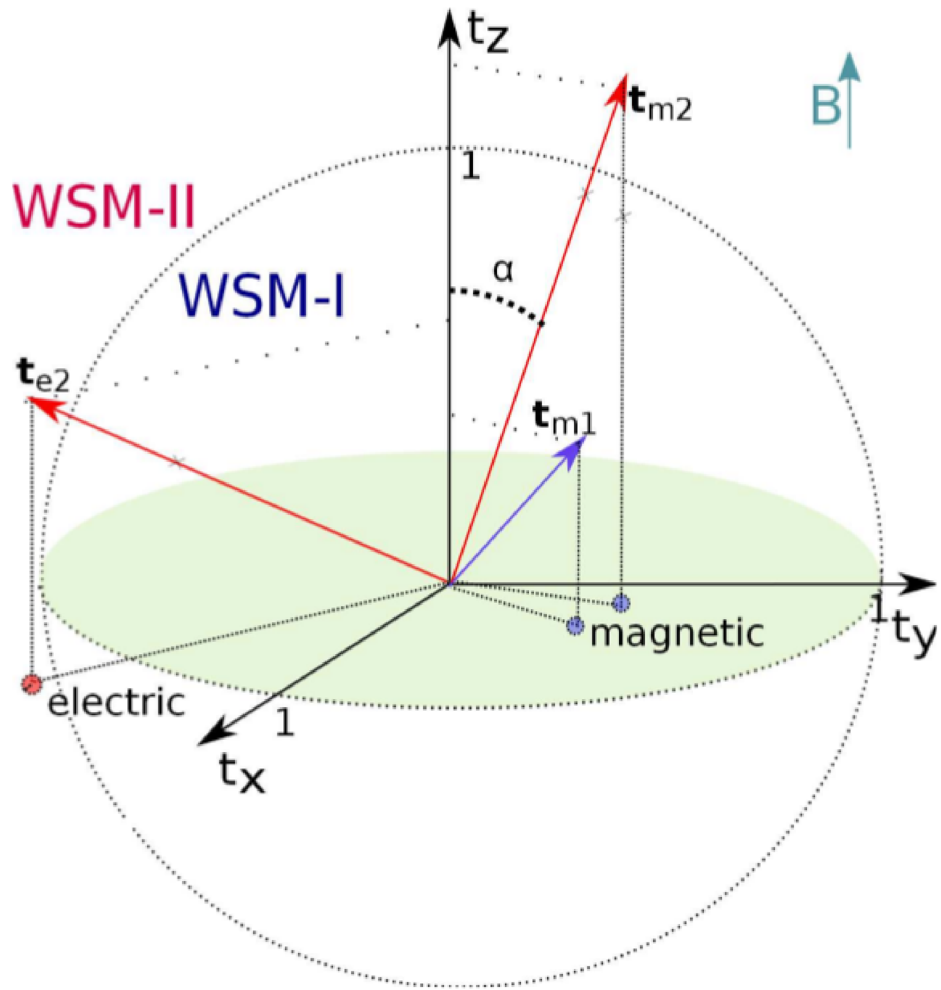
$$\mathbf{t} = \left(\frac{w_{0x}}{w_x}, \frac{w_{0y}}{w_y}, \frac{w_{0z}}{w_z} \right)$$

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

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



Pseudo-covariance in 3D Weyl semimetals – Landau levels

same recipe as for 2D:

Lorentz boost to a frame of reference, where $\mathbf{t}_\perp$ vanishes

1D Landau bands

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

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

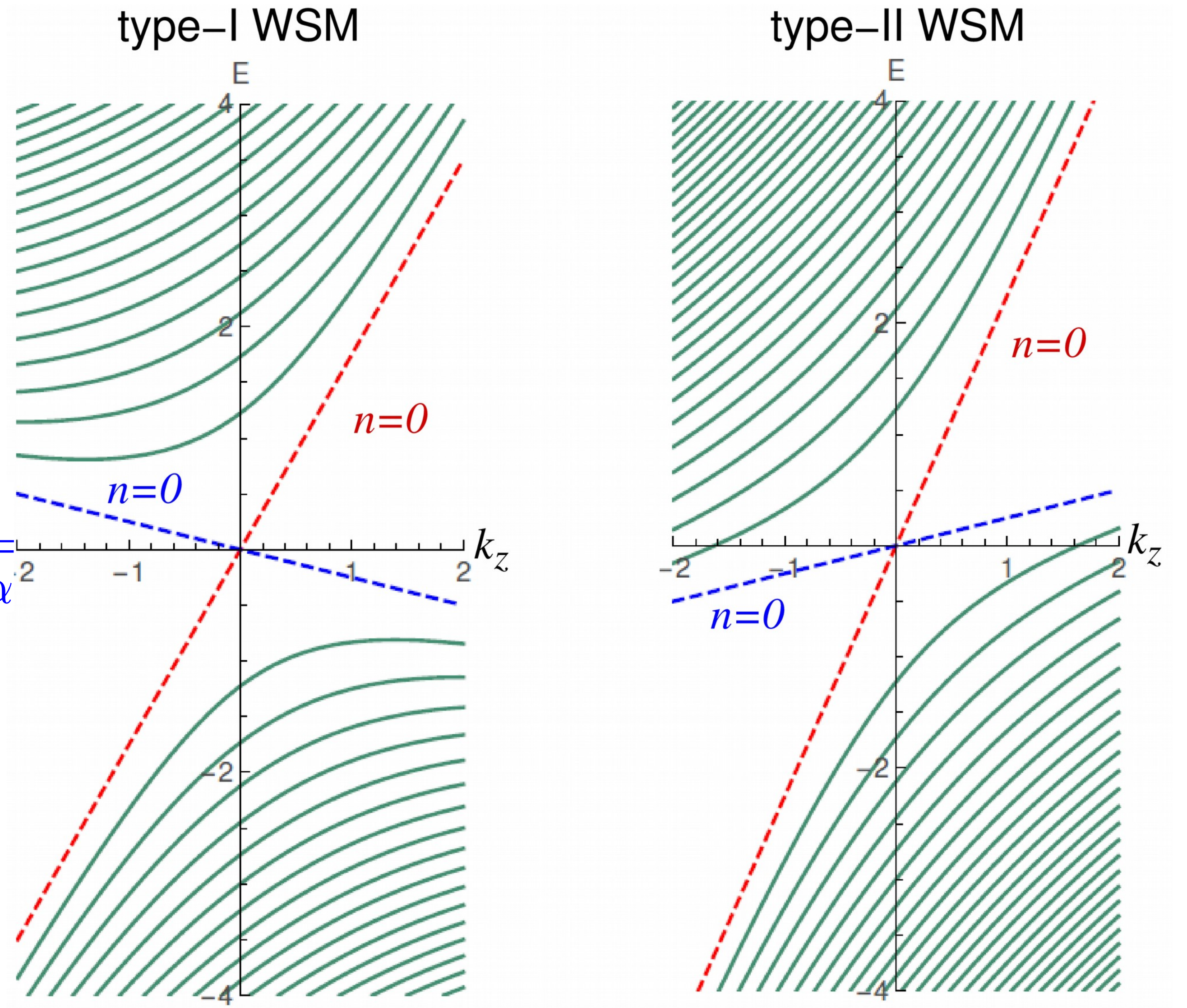
3-dimensional Weyl semimetals	$\lvert\mathbf{t}_\perp\rvert = \beta < 1$	$\lvert\mathbf{t}_\perp\rvert = \beta > 1$
$\lvert\mathbf{t}\rvert < 1$	type-I WSM *magnetic* regime	type-I WSM *electric* regime ?
$\lvert\mathbf{t}\rvert > 1$	type-II WSM *magnetic* regime	type-II WSM *electric* regime

Pseudo-covariance in 3D Weyl semimetals – Landau levels

WSM type conferred to 1D bands

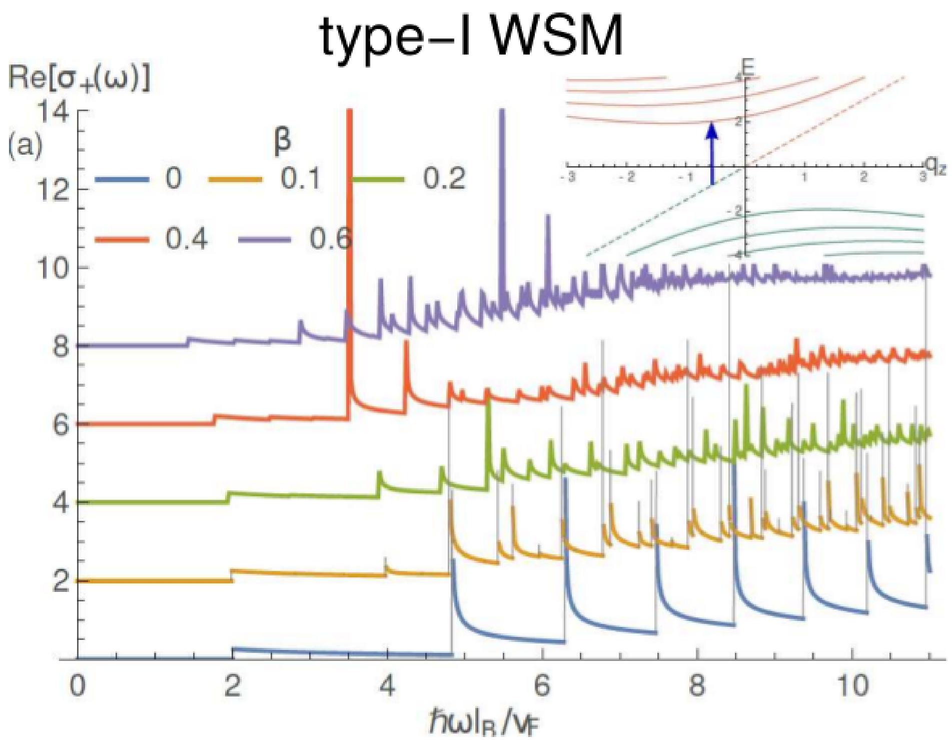
$$t_z = \frac{w_{0z}}{w'_z} = \frac{|\mathbf{t}\cos\alpha|}{\sqrt{1-t^2\sin^2\alpha}}$$

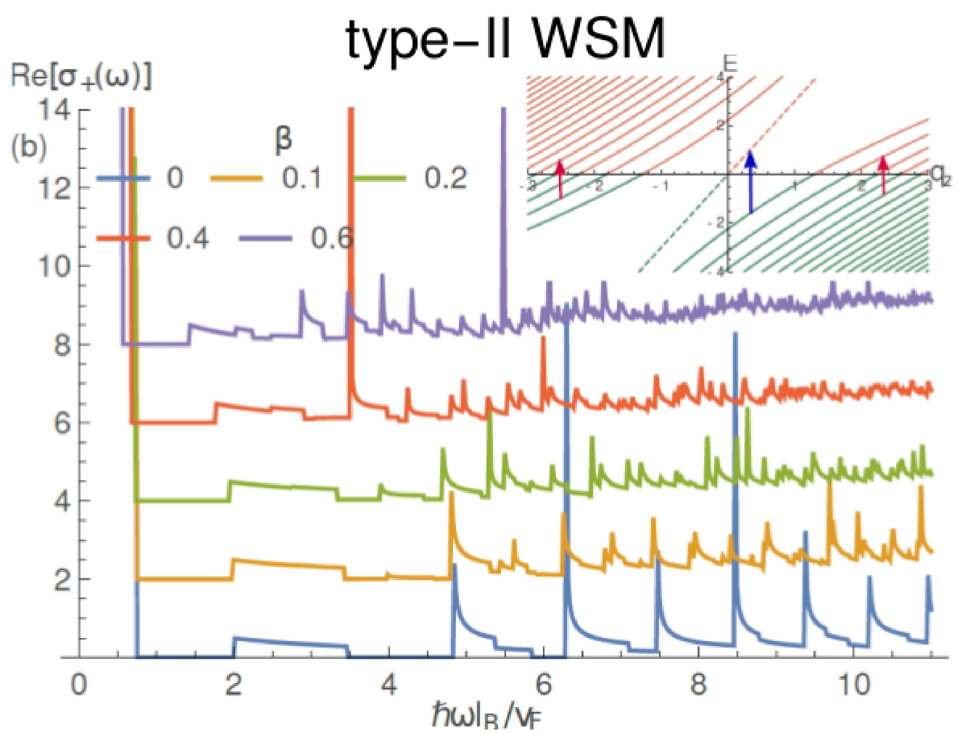
(1D tilt parameter)



Optical conductivity

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





again: *violation of dipolar selection rules*

Outline

- *Relativistic features* of graphene electrons

  (beyond the spectrum)

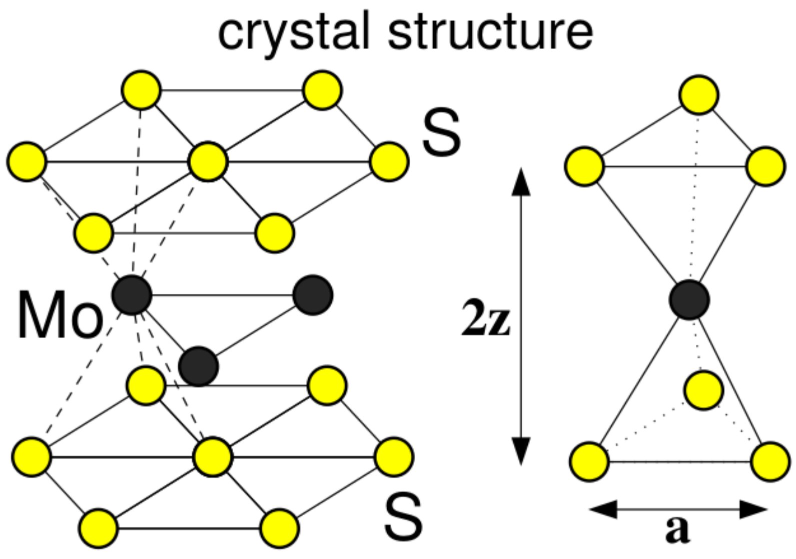
- *Massive Dirac fermions* in 2D transition-metal dichalcogenides (TMDC)

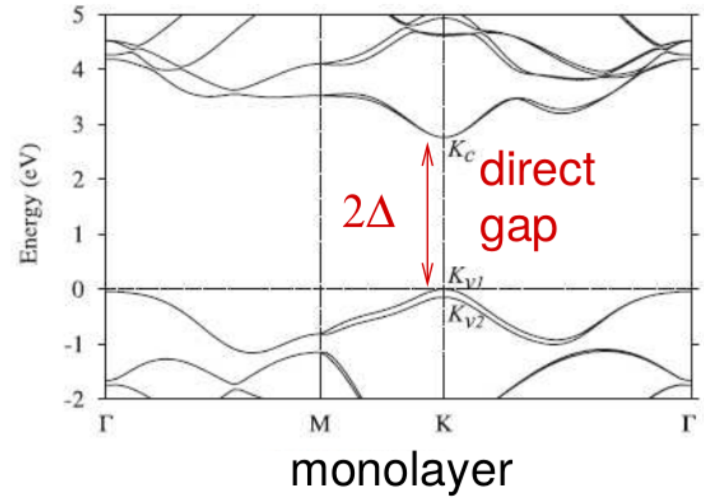
- How to unveil *geometry/topology in 2D materials*

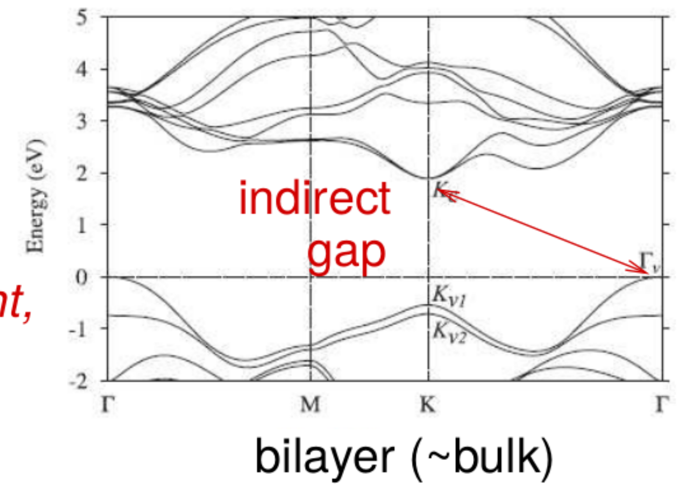
  (the role of Berry curvature)

- Future research: interplay between *topology and correlations*

Example of TMDC: Molybdenum Disulfide (MoS_2)



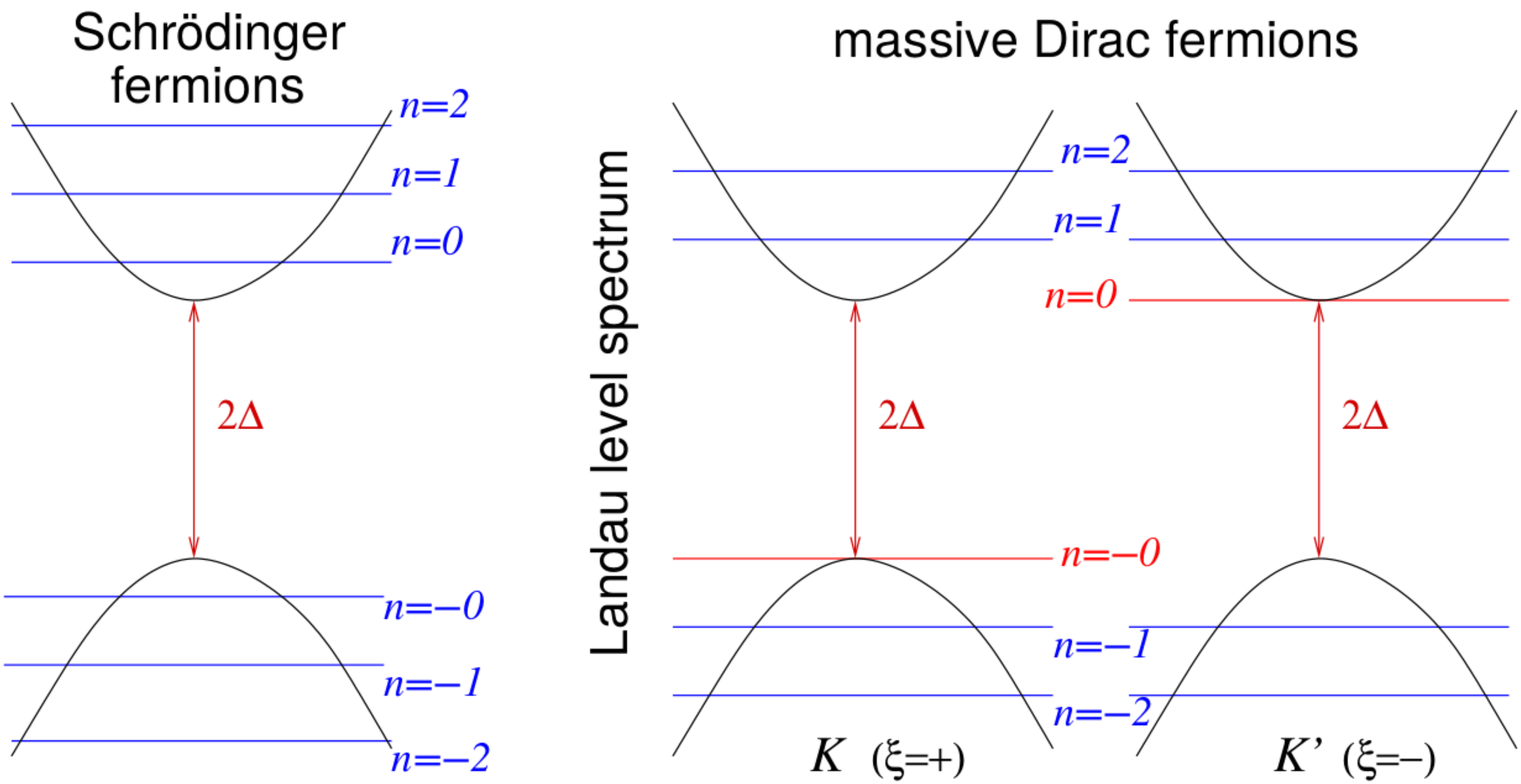




many ab initio calculations, here: *Cheiwchanchamnangij & Lambrecht, PRB (2012)*

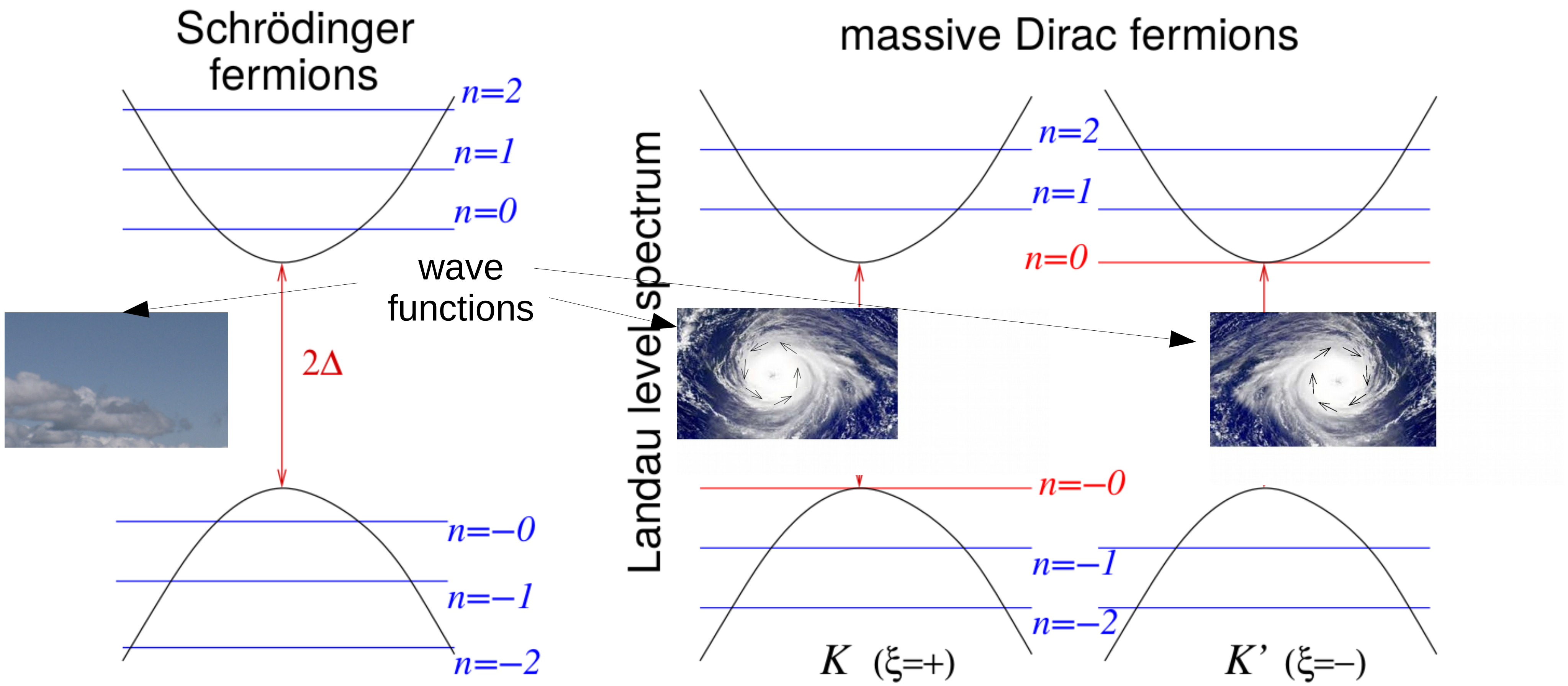
- 3 p orbitals per S, 5 d orbitals per Mo = 11 orbitals
- at K points: $|d_{3\mathrm{r}^2-\mathrm{z}^2}\rangle$ and $(|d_{\mathrm{xy}}\rangle + i\xi|d_{\mathrm{x}^2-\mathrm{y}^2}\rangle)/\sqrt{2}$

Schrödinger or massive Dirac fermions ?



$$\mathcal{H}(\mathbf{q}) = \begin{pmatrix} \Delta + \frac{\hbar^2}{2m} q^2 & 0 \\ 0 & -\Delta - \frac{\hbar^2}{2m} q^2 \end{pmatrix} \qquad \mathcal{H}(\mathbf{q}) = \begin{pmatrix} \Delta & \hbar v_D (q_x - i q_y) \\ \hbar v_D (q_x + i q_y) & -\Delta \end{pmatrix}$$

Schrödinger or massive Dirac fermions ?



$$\mathcal{H}(\mathbf{q}) = \begin{pmatrix} \Delta + \frac{\hbar^2}{2m}q^2 & 0 \\ 0 & -\Delta - \frac{\hbar^2}{2m}q^2 \end{pmatrix}$$

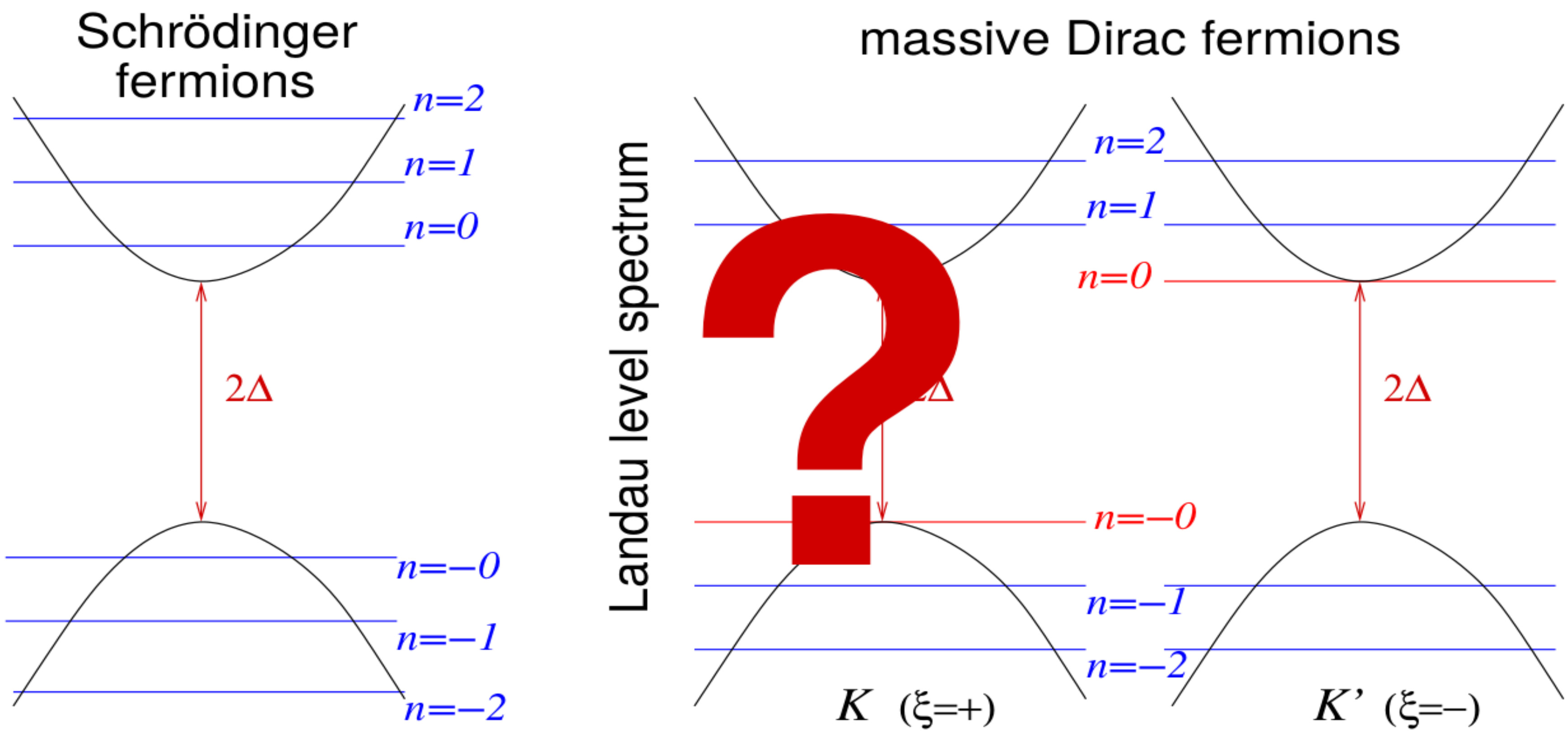
$$\boxed{\Omega_\lambda = 0}$$

no Berry curvature

$$\boxed{\Omega_{\lambda,\xi}(\mathbf{q}) = -\frac{\lambda\xi}{2}\frac{\hbar^2 v^2 \Delta}{(\Delta^2 + \hbar^2 v^2 q^2)^{3/2}}}$$

Berry curvature

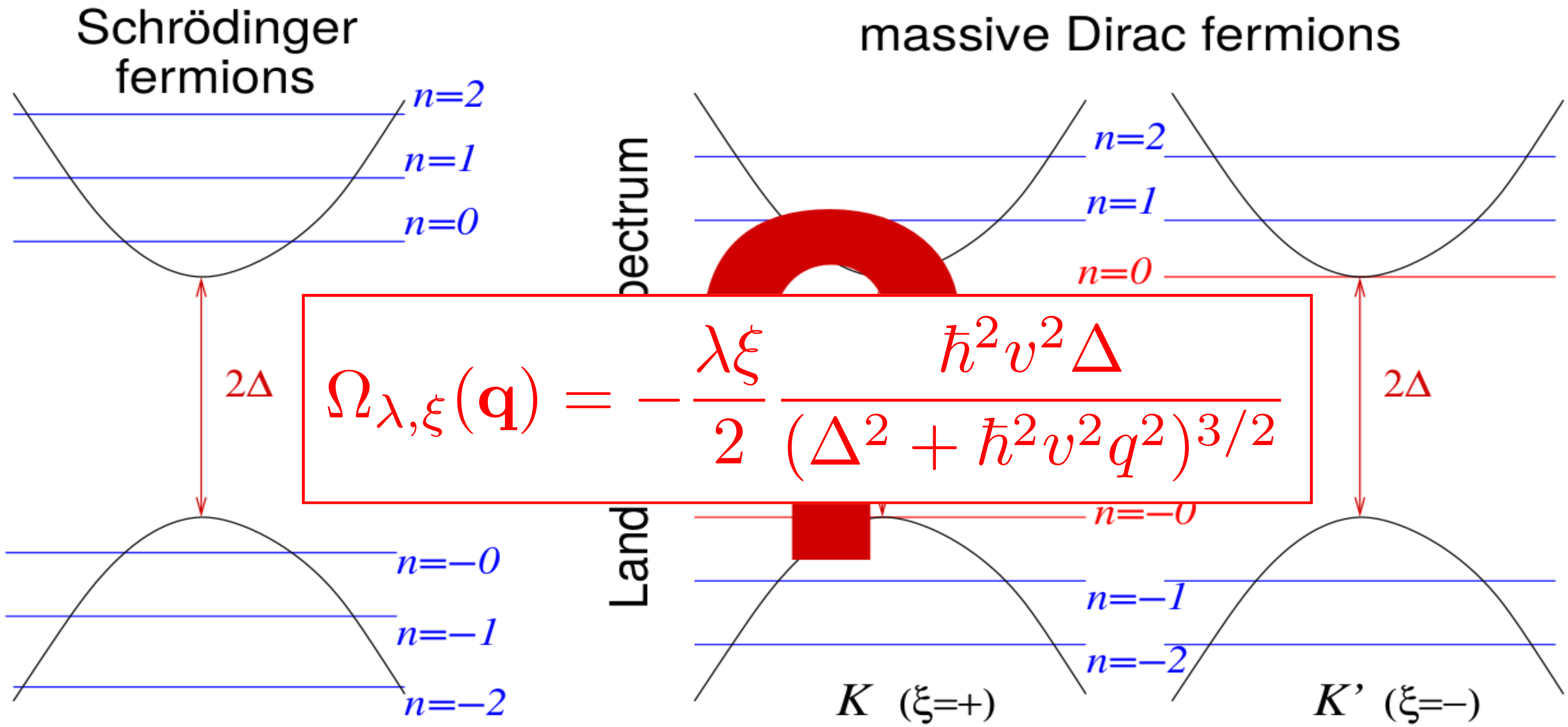
Schrödinger or massive Dirac fermions ?



$$\mathcal{H}(\mathbf{q}) = \begin{pmatrix} \Delta + \frac{\hbar^2}{2m^0_{\mathrm{el}}} q^2 & \hbar v_D (q_x - i q_y) \\ \hbar v_D (q_x + i q_y) & -\Delta - \frac{\hbar^2}{2m^0_{\mathrm{h}}} q^2 \end{pmatrix}$$

band masses: $1/m_\lambda = 1/m^0_\lambda + 1/m_D$, Dirac mass: $m_D = \Delta / v_D^2$

Schrödinger or massive Dirac fermions ?



$$\boxed{\Omega_{\lambda,\xi}(\mathbf{q}) = -\frac{\lambda\xi}{2}\frac{\hbar^2 v^2 \Delta}{(\Delta^2 + \hbar^2 v^2 q^2)^{3/2}}}$$

$$\mathcal{H}(\mathbf{q}) = \begin{pmatrix} \Delta + \frac{\hbar^2}{2m^0_{\rm el}} q^2 & \hbar v_D (q_x - i q_y) \\ \hbar v_D (q_x + i q_y) & -\Delta - \frac{\hbar^2}{2m^0_{\rm h}} q^2 \end{pmatrix}$$

band masses: $1/m_\lambda = 1/m^0_\lambda + 1/m_D$, Dirac mass: $m_D = \Delta/v_D^2$

Landau levels

$$\epsilon_{\lambda,n} = \delta\omega n - \frac{\Omega}{2} + \lambda\sqrt{\left(\Delta + \Omega n - \frac{\delta\omega}{2}\right)^2 + \omega'^2 n}$$

three frequencies: $\Omega = eB/M$, $\delta\omega = eB/\mu$, $\omega' = \sqrt{2}v_D/l_B$

bare electron mass: $1/m_\mathrm{e}^0 = 1/M + 1/\mu$

bare hole mass: $1/m_\mathrm{h}^0 = 1/M - 1/\mu$

<u>spectrum in parabolic approximation:</u>

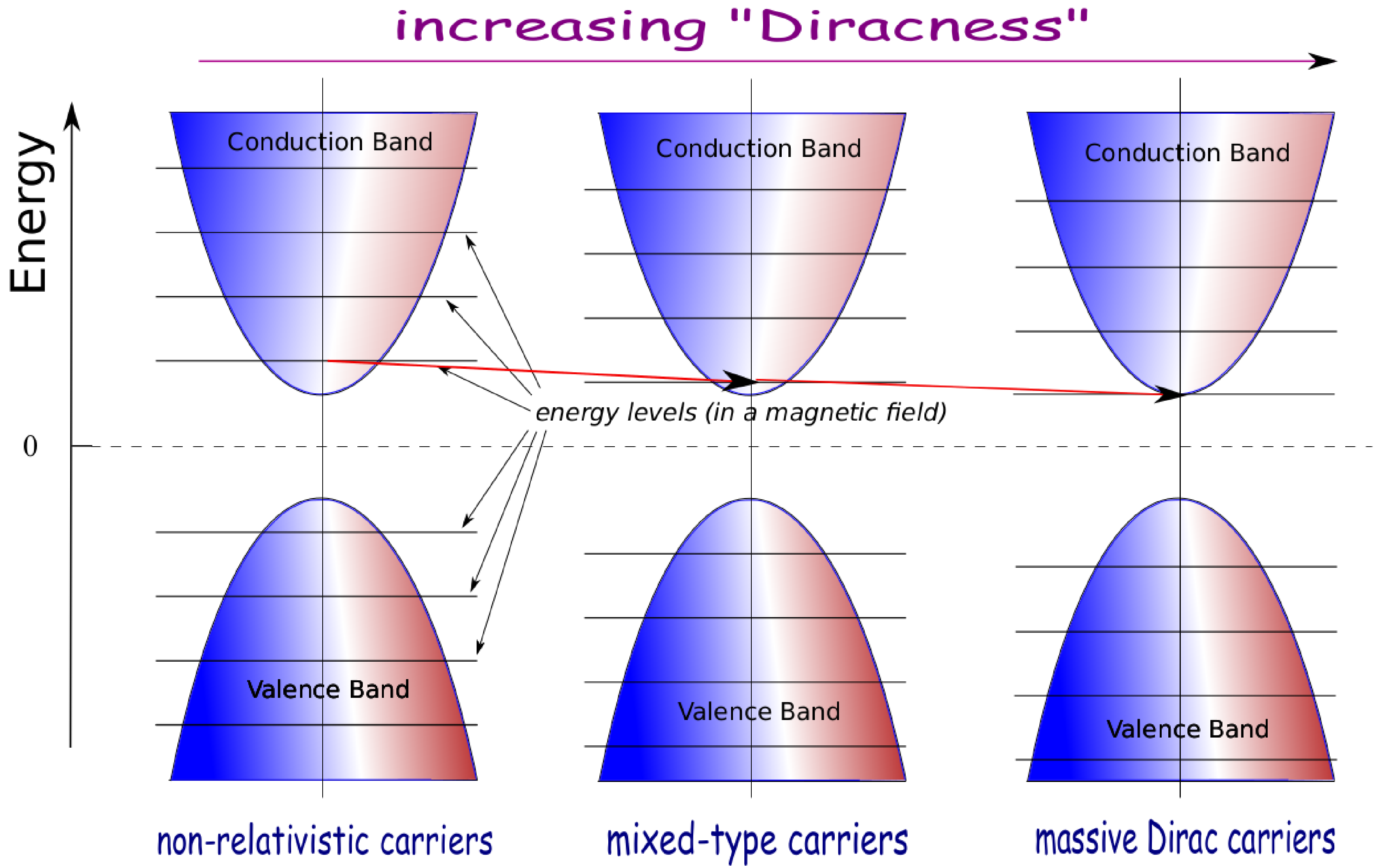
$$\epsilon_{\lambda,n} = \lambda\left[\Delta + \hbar\omega_\lambda(n + \gamma_\lambda)\right], \qquad \omega_\lambda = eB/m_\lambda$$

$\rightarrow$ Phase offset γ_λ no longer quantised !

[$\sim$ surface states of 3D TIs, Wright & MacKenzie, PRB (2013)]

(pure Schrödinger: $\gamma = 1/2$, pure Dirac: $\gamma = 0$)

Landau levels

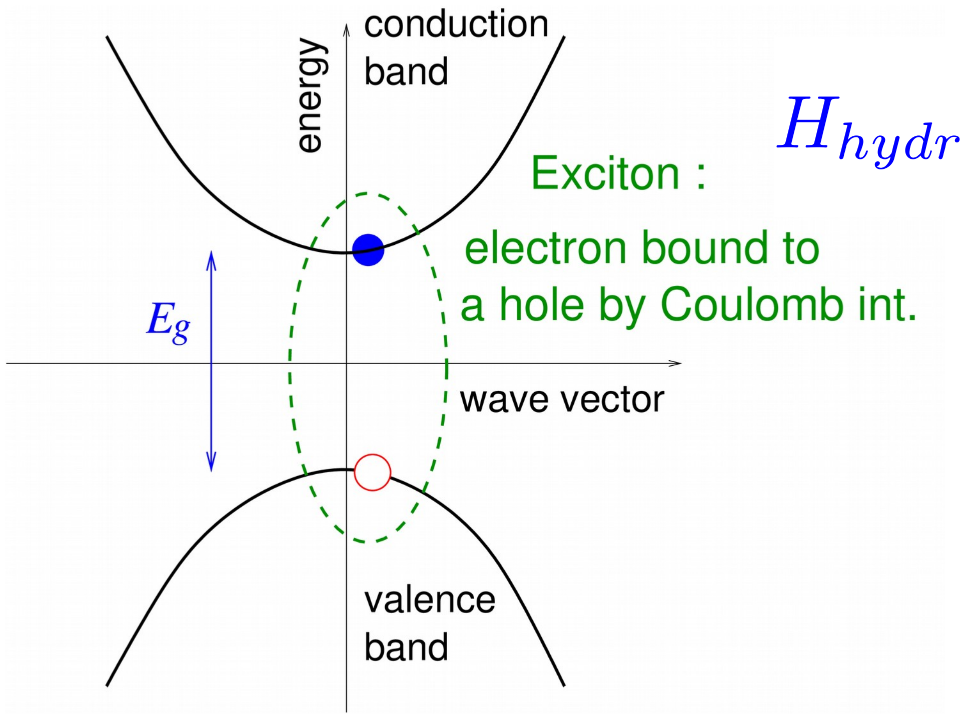


$\gamma = 1/2$ $\gamma = 1/4(3/4)$ $\gamma = 0$

Outline

- *Relativistic features* of graphene electrons (beyond the spectrum)
- *Massive Dirac fermions* in 2D transition-metal dichalcogenides (TMDC)
- How to unveil *geometry/topology in 2D materials* (the role of Berry curvature)
- Future research: interplay between *topology and correlations*

Exciton spectrum in 2D TMDC



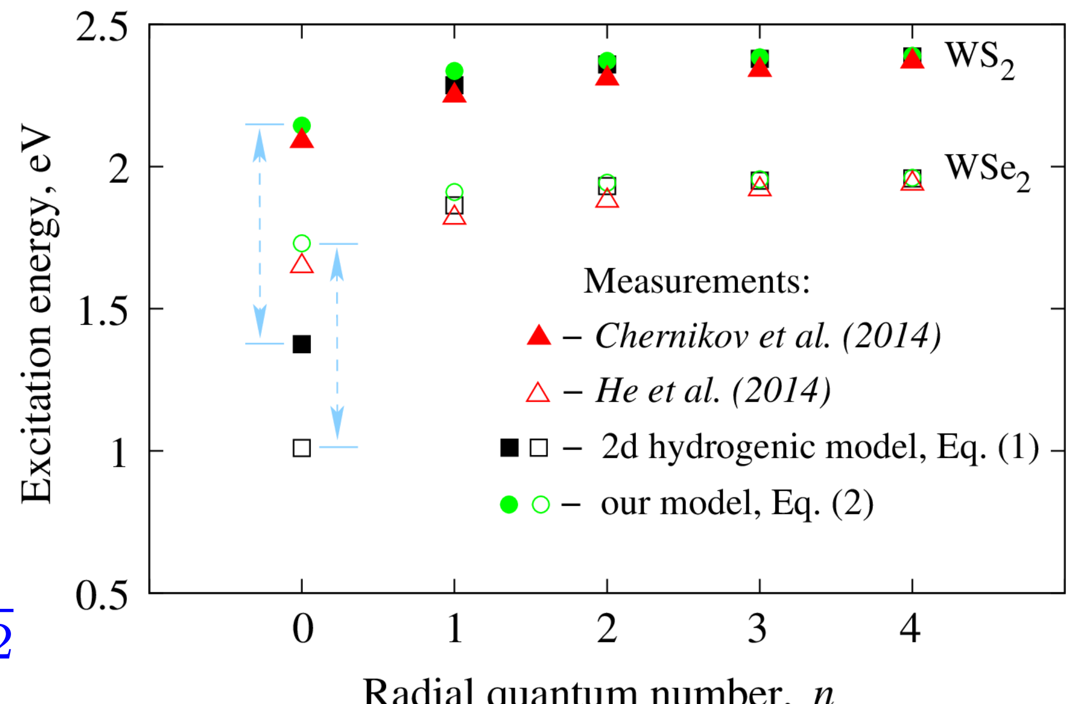
Hydrogen model of excitons:

$$H_{hydr.} = E_g + \frac{\mathbf{p}_e^2}{2m_e} + \frac{\mathbf{p}_h^2}{2m_h} - \frac{e^2}{\kappa|\mathbf{r}_e - \mathbf{r}_h|}$$

$$= E_g + \frac{\mathbf{p}^2}{2\mu} - \frac{e^2}{\kappa r}$$

Spectrum of hydrogen model (2D):

$$E_n = E_g - \frac{e^4\mu}{2\kappa^2\hbar^2}\frac{1}{(n+1/2)^2}$$



Possible reasons for failure of 2D hydrogen model at small n

- more realistic interaction potential to take into account screening effects (→ *Keldysh potential*)

- band-coupling effects (→ *Berry curvature* $\boldsymbol{\Omega}_\alpha(\mathbf{P})$)

→ semiclassical equations of motion :

$$\dot{\mathbf{P}}_j = -\frac{\partial V(\mathbf{R})}{\partial \mathbf{R}_j} - e\dot{\mathbf{R}}_j \times \mathbf{B}$$

$$\dot{\mathbf{R}}_j = \frac{\partial E_\alpha(\mathbf{P})}{\partial \mathbf{P}_j} - \frac{1}{\hbar}\dot{\mathbf{P}}_j \times \boldsymbol{\Omega}_\alpha(\mathbf{P}_j)$$

Modified "single-band" Hamiltonian (*toolbox*)

- Hamiltonian:

$$H = H_0(\mathbf{p}) + V(\mathbf{r})$$

- Generalised Peierls substitution:

$$\mathbf{p} \to \mathbf{p} + e\mathbf{A} \qquad \mathbf{r} \to \mathbf{r} + \frac{1}{2\hbar}\boldsymbol{\Omega}_\alpha \times \mathbf{p}$$

→ *justification: reproduction (at linear order) of semiclassical equations of motion (Heisenberg)*

- Linearised Hamiltonian:

Due to Coulomb interaction

$$H = H_0(\mathbf{p}) + V(\mathbf{r}) + \cancel{\frac{e}{2\hbar}\frac{\partial H_0}{\partial \mathbf{p}} \cdot (\mathbf{B} \times \mathbf{r})} + \frac{1}{2\hbar}\frac{\partial V}{\partial \mathbf{r}} \cdot (\boldsymbol{\Omega}_\alpha \times \mathbf{p})$$

Zero B field

Exciton Hamiltonian

- Hamiltonian in center-of-mass frame:

$$H_{exc} = E_g + \underbrace{\frac{\mathbf{p}^2}{2\mu} + V(r)}_{\text{Hydrogenic part}} + \underbrace{\frac{1}{2\hbar}\frac{\partial V}{\partial \mathbf{r}} \cdot [\boldsymbol{\Omega}(\mathbf{p}) \times \mathbf{p}] + \frac{1}{4}|\boldsymbol{\Omega}(\mathbf{p})|\nabla^2 V(\mathbf{r})}_{\text{Berry-curvature correction + Darwin term}}$$

- Exciton Berry curvature:

$$\boldsymbol{\Omega}(\mathbf{p}) = \boldsymbol{\Omega}_e(\mathbf{p}) - \boldsymbol{\Omega}_h(-\mathbf{p}) \simeq 2\Omega_e(\mathbf{p} = 0)$$

Zhou et al., PRL (2015)
Srivastava & Imamoglu, PRL (2015)
Trushin et al., PRL (2018)

Exciton Hamiltonian *(orders of magnitude)*

- Hamiltonian in center-of-mass frame:

$$H_{exc} = E_g + \frac{\mathbf{p}^2}{2\mu} + V(r) + \frac{1}{2\hbar}\frac{\partial V}{\partial \mathbf{r}} \cdot [\mathbf{\Omega}(\mathbf{p}) \times \mathbf{p}] + \frac{1}{4}|\mathbf{\Omega}(\mathbf{p})|\nabla^2 V(\mathbf{r})$$

Hydrogenic part

Berry-curvature correction + Darwin term

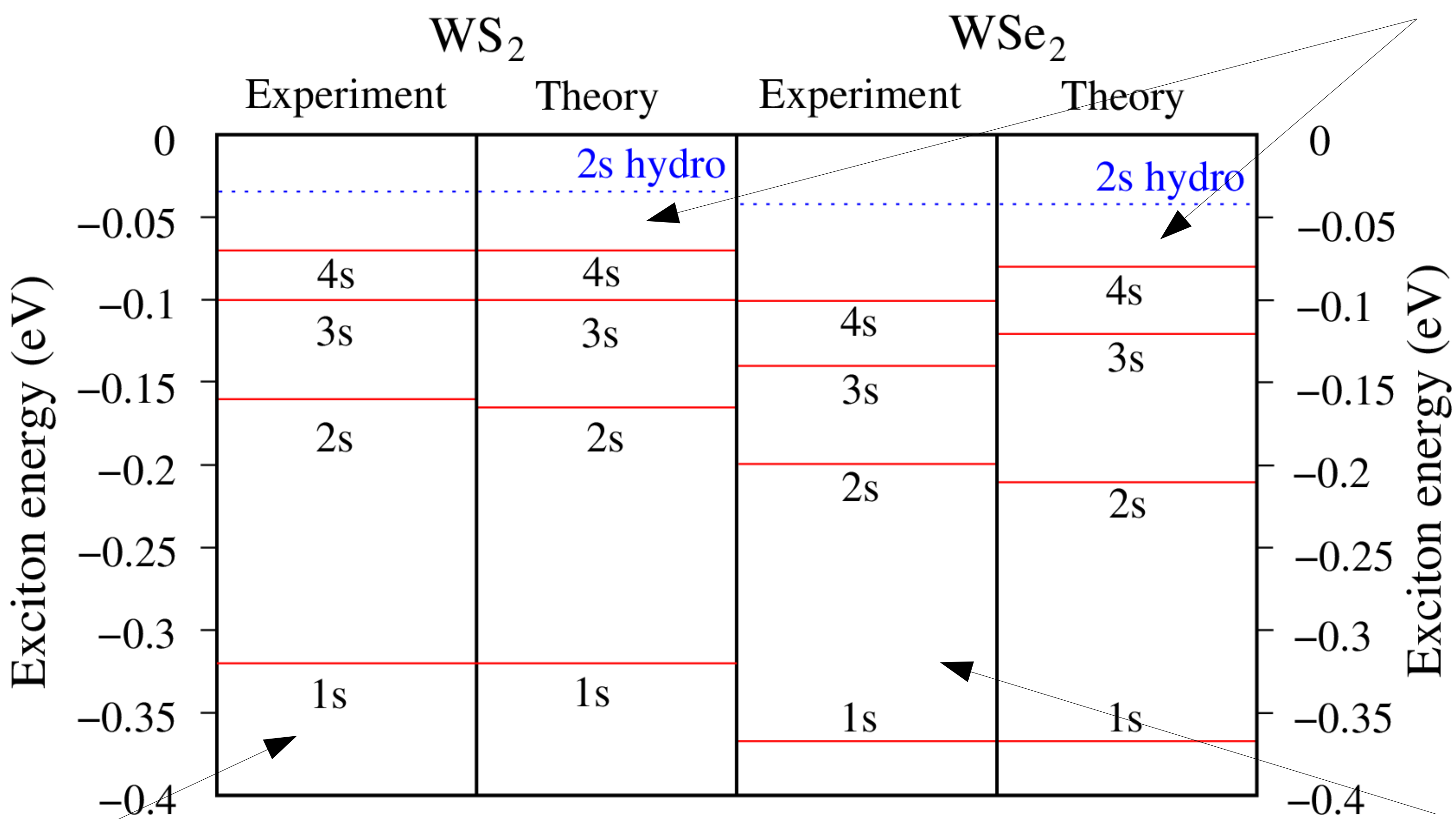
$$\sim \mathrm{Ry}^* = 13\mathrm{eV} \times \frac{\mu}{m_0}\frac{1}{\kappa^2} \qquad \sim \mathrm{Ry}^* \times \left(\frac{\lambda_C}{a_B}\right)^2 = \alpha^2 \mathrm{Ry}^*$$

$$a_B = \hbar^2\kappa/\mu e^2 \sim 5\text{Å}$$ (effective Bohr radius)

$$\lambda_C = \sqrt{\Omega} \leq \hbar/\sqrt{E_g \mu} = \alpha a_B$$ (effective Compton length)

$$\alpha = (e^2/\hbar\kappa)\sqrt{\mu/E_g} \simeq 1$$ ("fine-structure constant")

Exciton spectrum (Berry + Keldysh)



Trushin et al., PRL (2018)

Chernikov et al. PRL (2014)

He et al., PRL (2014)

$$\mu = 0.16 m_0 \qquad \mu = 0.17 m_0$$

$$r_0 = 4.65\text{nm} \qquad r_0 = 3.84\text{nm}$$

(Keldysh length)

ab initio calculations: $r_0 \simeq 4\text{nm}$ Berkelbach et al., PRB (2013)

Outline

- *Relativistic features* of graphene electrons

  (beyond the spectrum)
- *Massive Dirac fermions* in 2D transition-metal dichalcogenides (TMDC)
- How to unveil *geometry/topology in 2D materials*

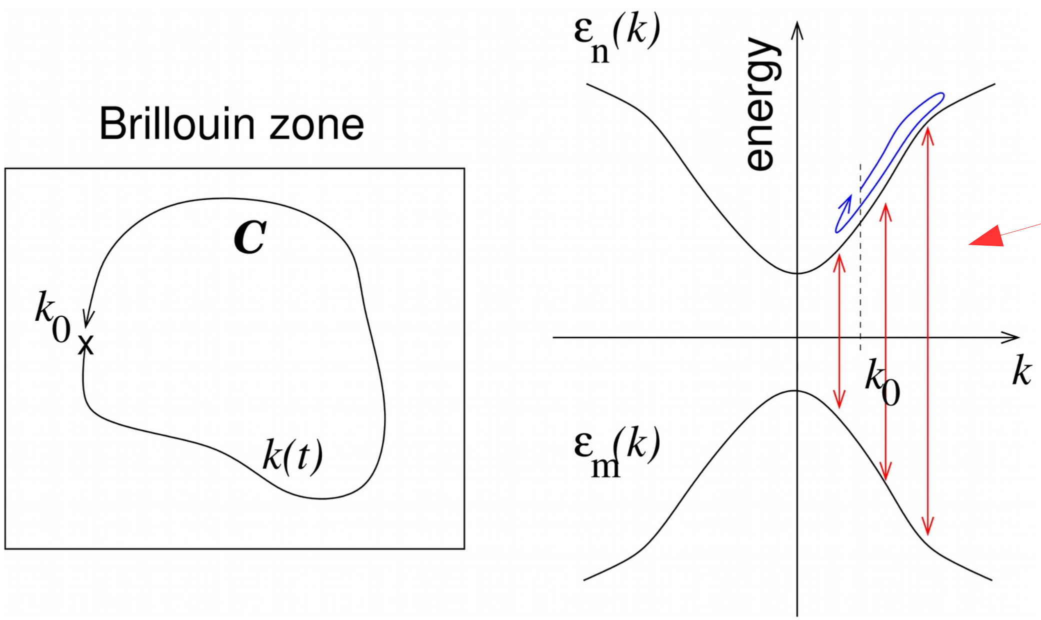
  (the role of Berry curvature)
- Future research: interplay between *topology and correlations*

Berry curvature – band projection

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

→ link to perturbation theory :

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



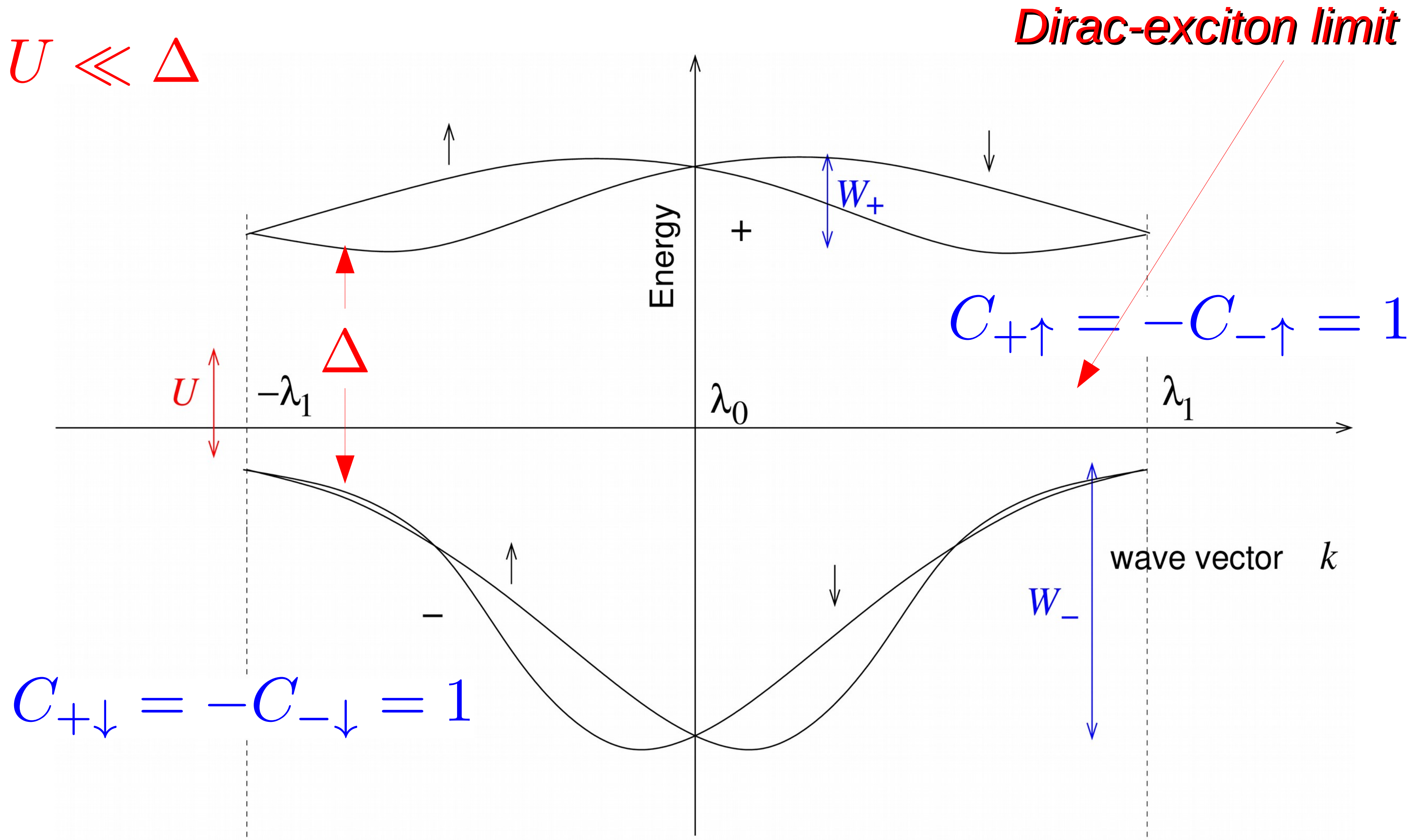
virtual transitions

sum rule:

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

The fate of topological bands in the presence of correlations

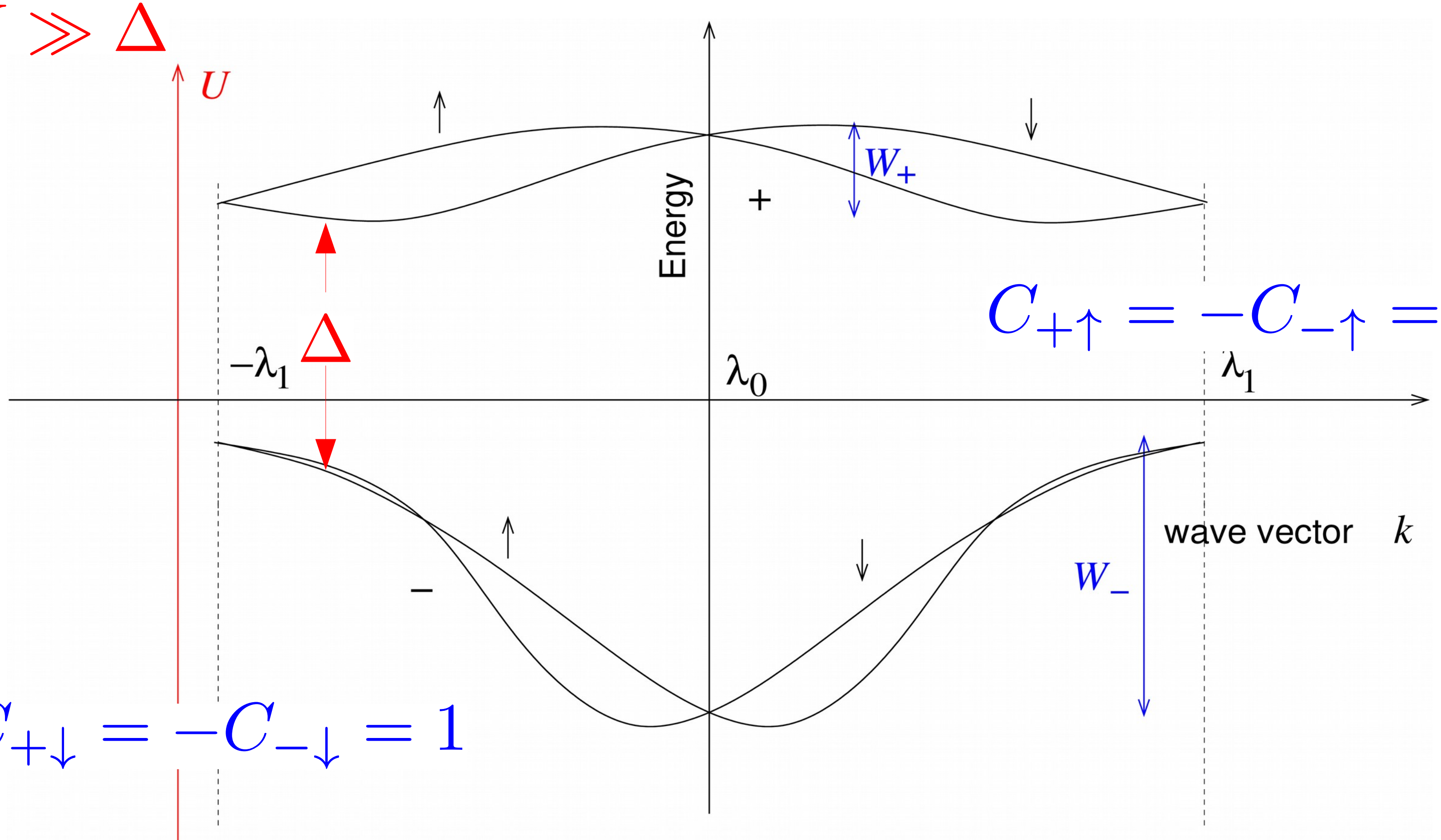
1) QSHE insulator (+weak correlations)



The fate of topological bands in the presence of correlations

1) QSHE insulator → Mott insulator (AF, topologically trivial) ?

$U \gg \Delta$



$C_{+\downarrow} = -C_{-\downarrow} = 1$

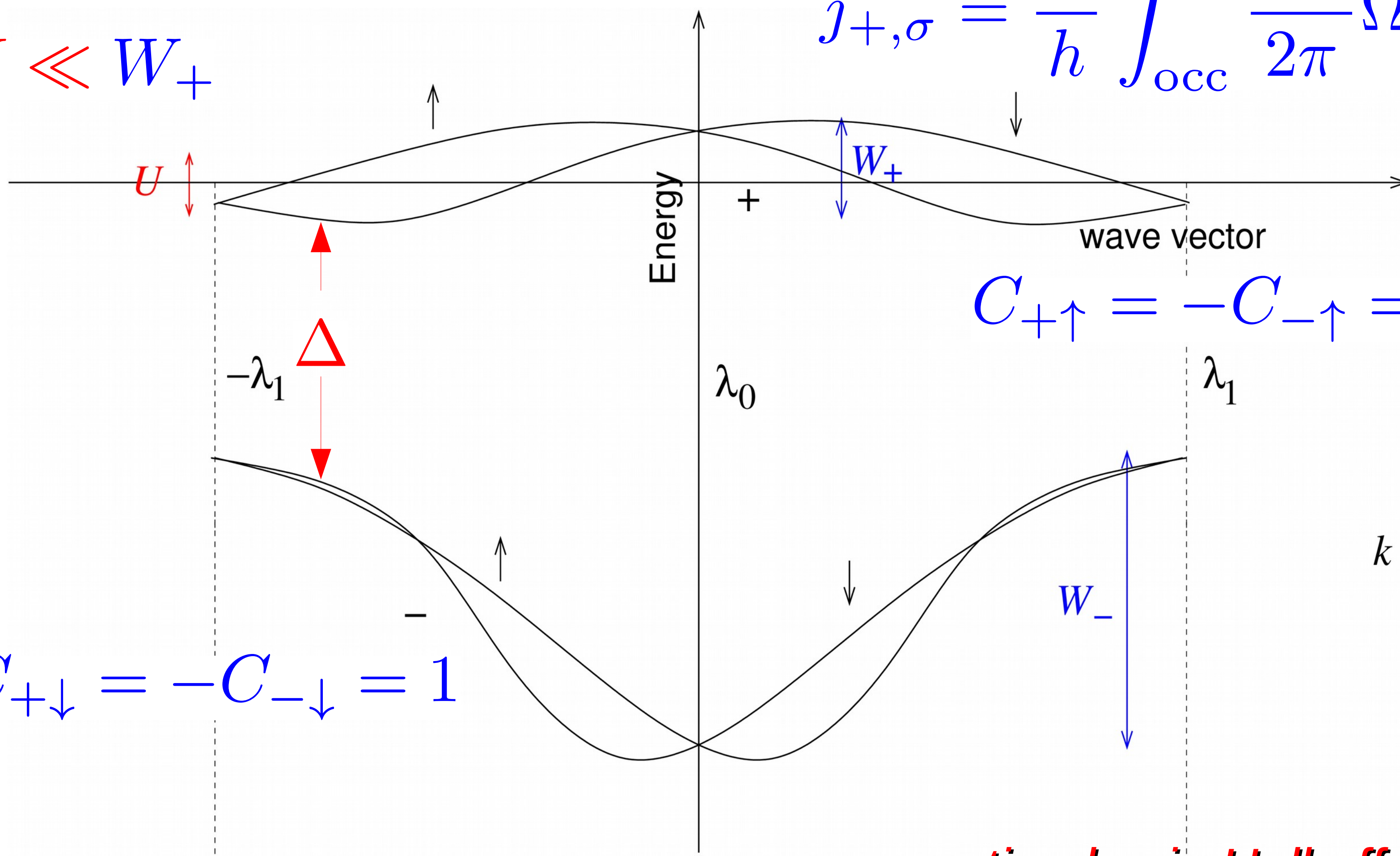
How does the (topo?) transition takes place from QSHE to MI?

The fate of topological bands in the presence of correlations

2) SH metal

$$U \ll W_+$$

$$j_{+,\sigma} = \frac{e^2}{h} \int_{\mathrm{occ}} \frac{d^2 k}{2\pi} \Omega_{+\sigma}(\mathbf{k})$$



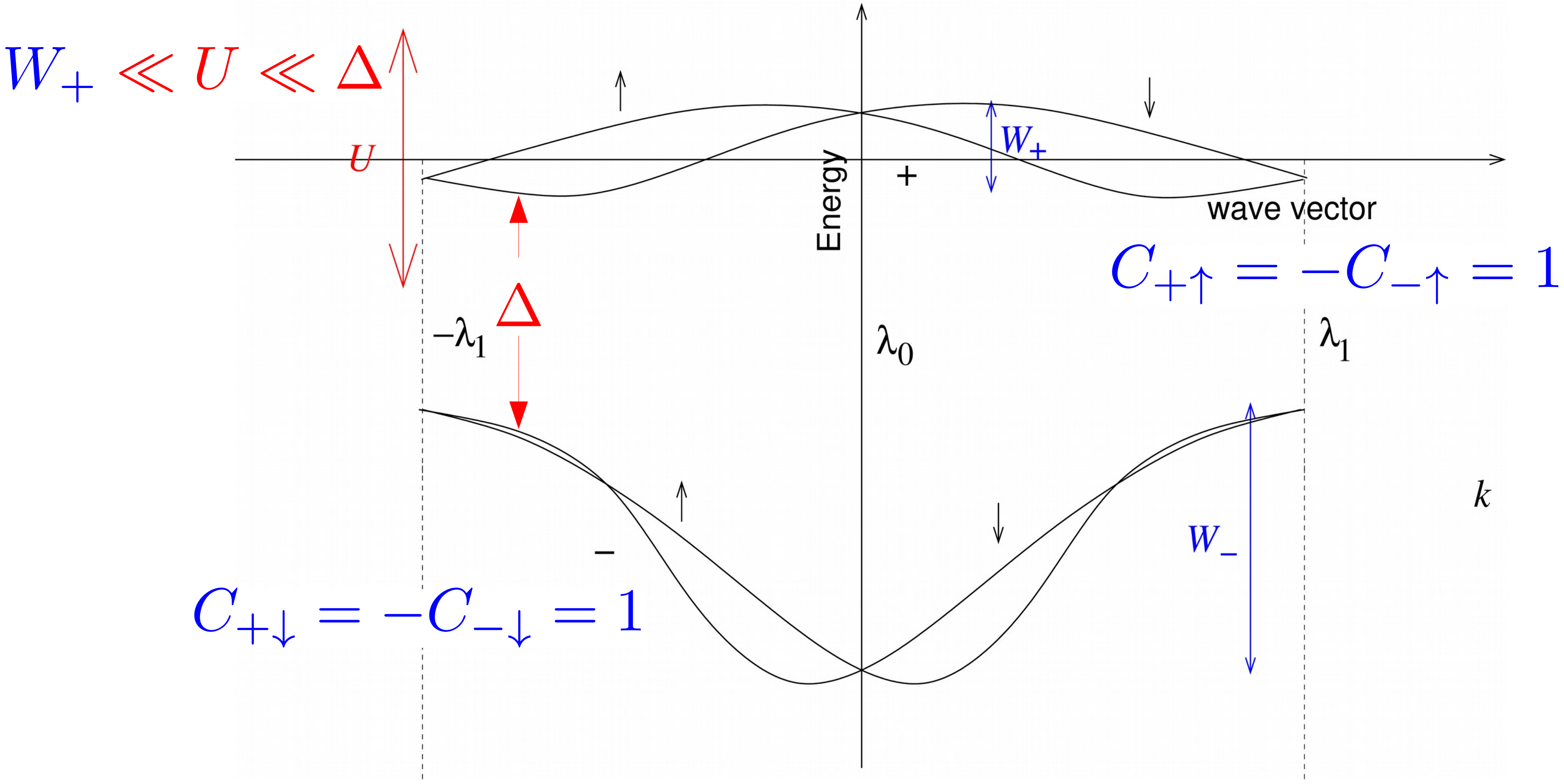
$$C_{+\uparrow} = -C_{-\uparrow} = 1$$

$$C_{+\downarrow} = -C_{-\downarrow} = 1$$

non-quantised spin Hall effect

The fate of topological bands in the presence of correlations

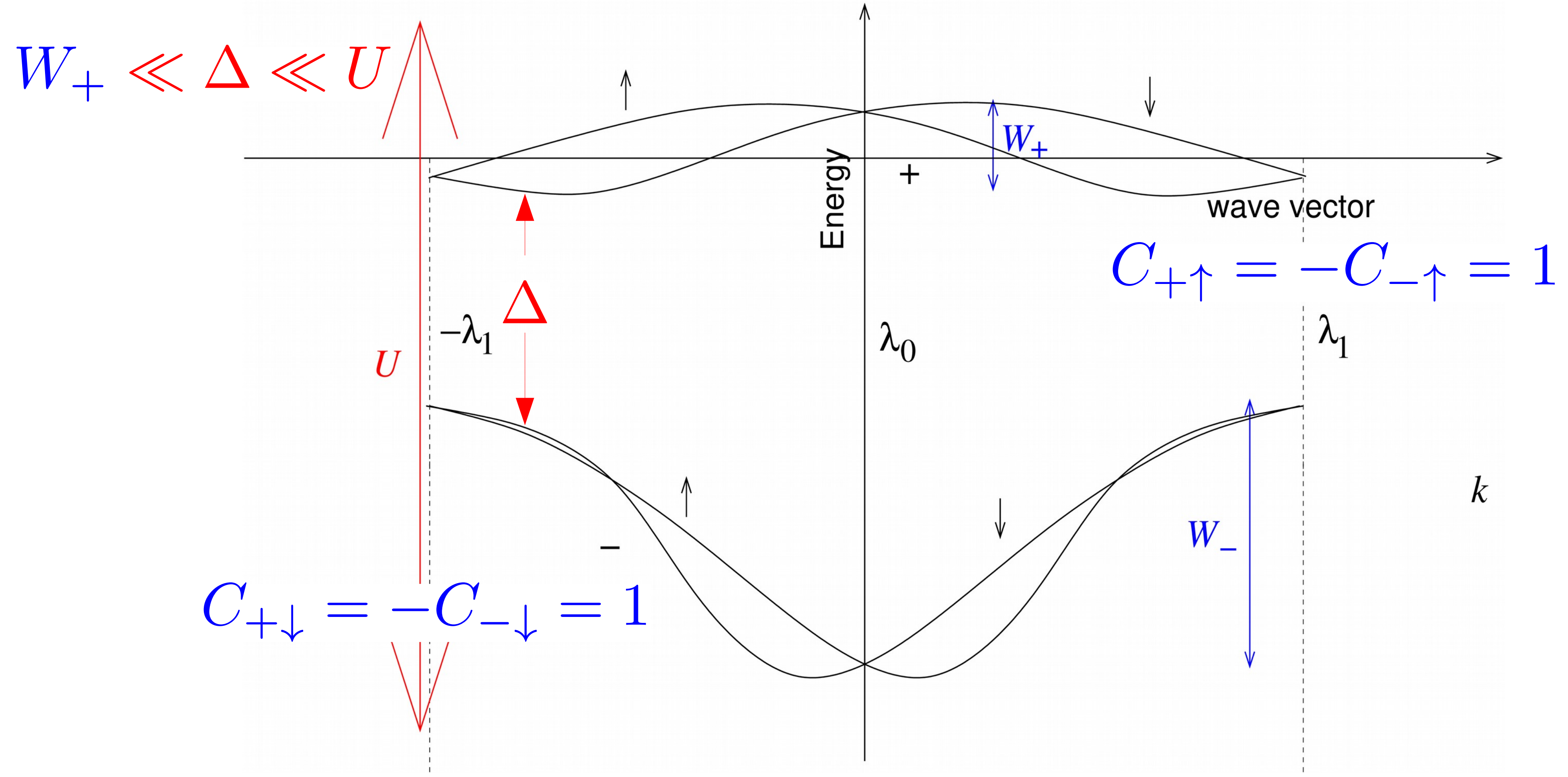
2) SH metal → FQHE



Fractional Chern insulator/quantum spin Hall effect

The fate of topological bands in the presence of correlations

2) SH metal → FQHE → Mott insulator (topologically trivial) ?



How does the (topo?) transition takes place from SHE to MI?

Outline → Summary

- *Relativistic features* of graphene electrons

  (beyond the spectrum)
- *Massive Dirac fermions* in 2D transition-metal dichalcogenides (TMDC)
- How to unveil *geometry/topology in 2D materials*

  (the role of Berry curvature)
- Future research: interplay between *topology and correlations*