Électrons dans des cristaux 2D

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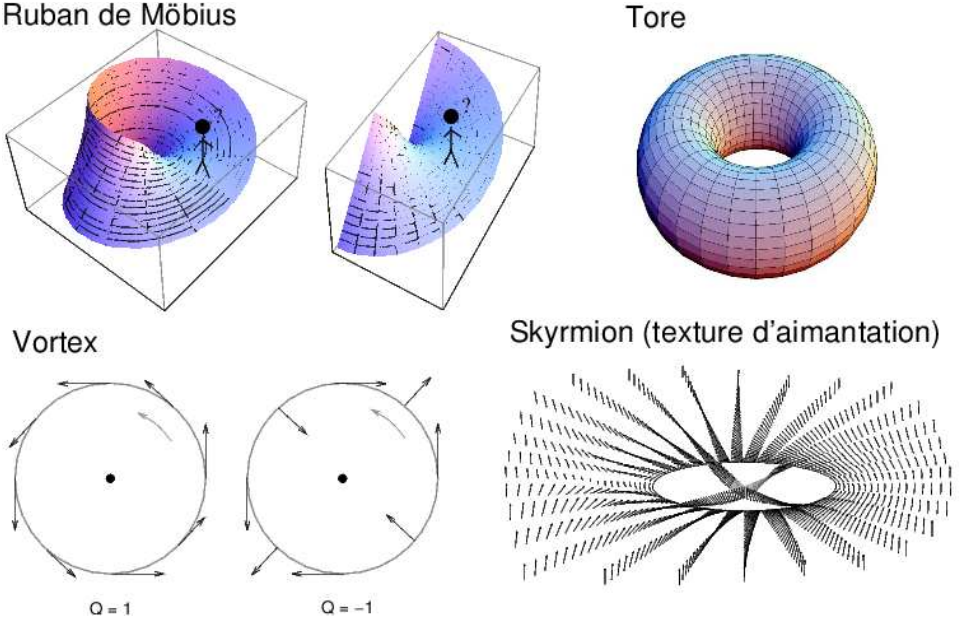
Séminaire Général du LAL, Orsay, 27/03/2015

Some modern topics of condensed-matter physics

- Graphene and other 2D crystals (since 2005)
- Topological aspects of condensed-matter systems

– Phases not described by local order parameters ($\rightarrow$ Landau theory of phase transitions, e.g. magnetism, superconductivity, superfluidity, ...)

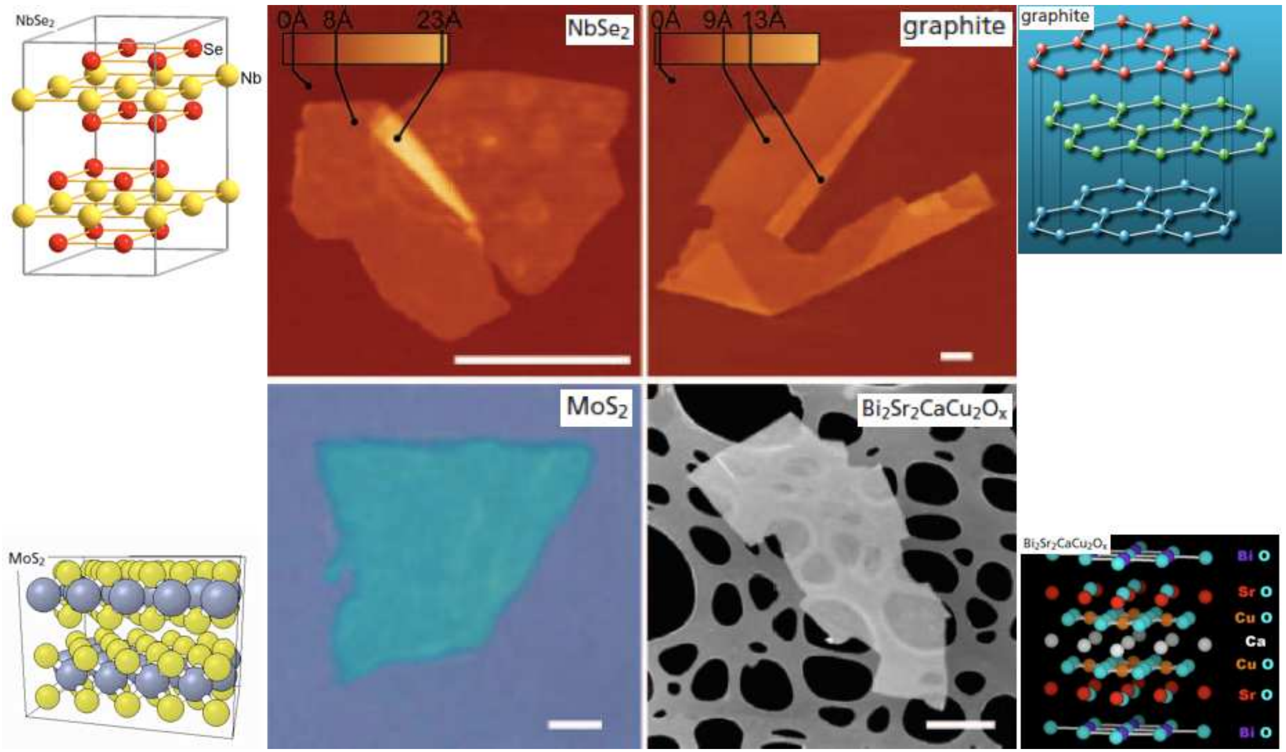
– Classification in terms of topological invariants ($=$ integrated quantities)



– (Fractional) quantum Hall effect

- Simulation of condensed-matter systems in cold atoms

Graphene and other 2D crystals

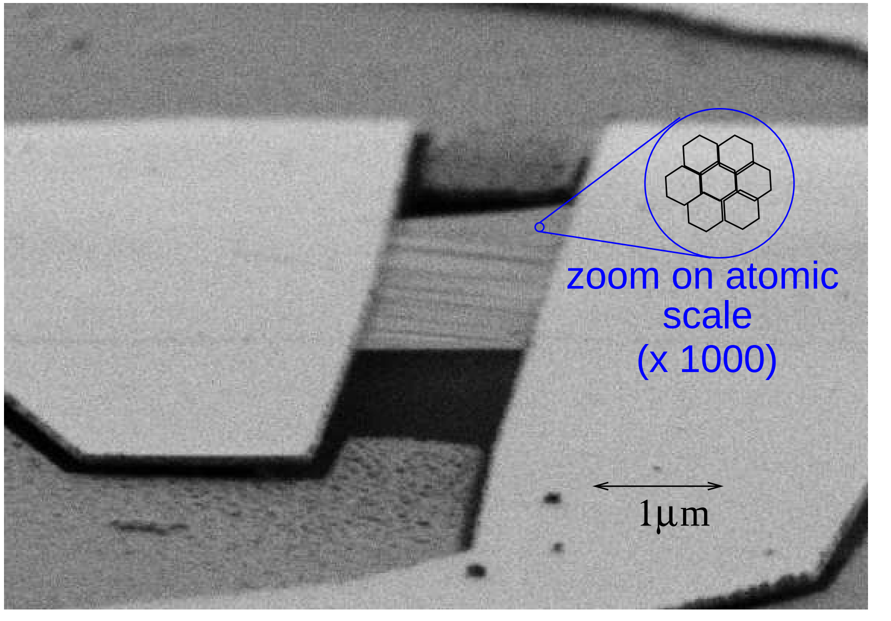


<u>Electronic properties:</u>

- similarity with graphene ?
- role of (massive) 2D Dirac fermions ?

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>

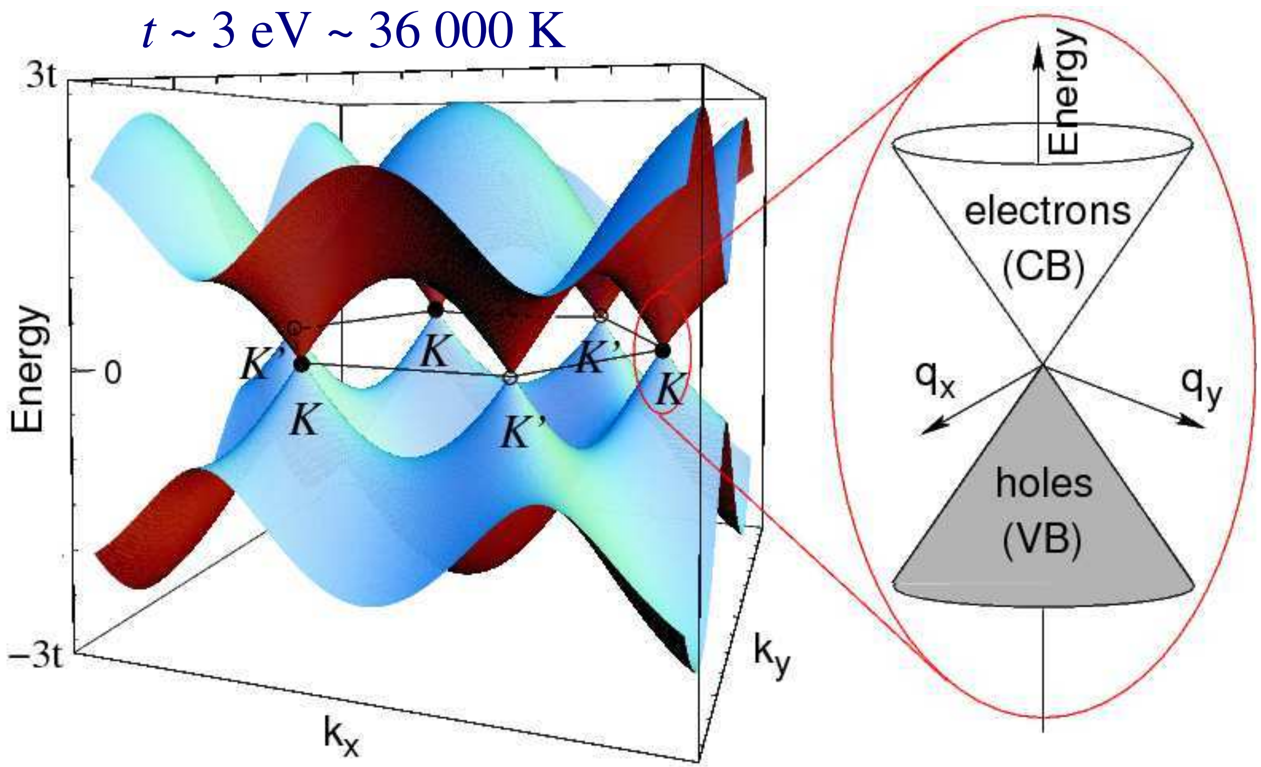
"Quantum mechanics meets relativity in condensed matter"
(electrons behave as 2D massless Dirac fermions)

Band structure of graphene

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



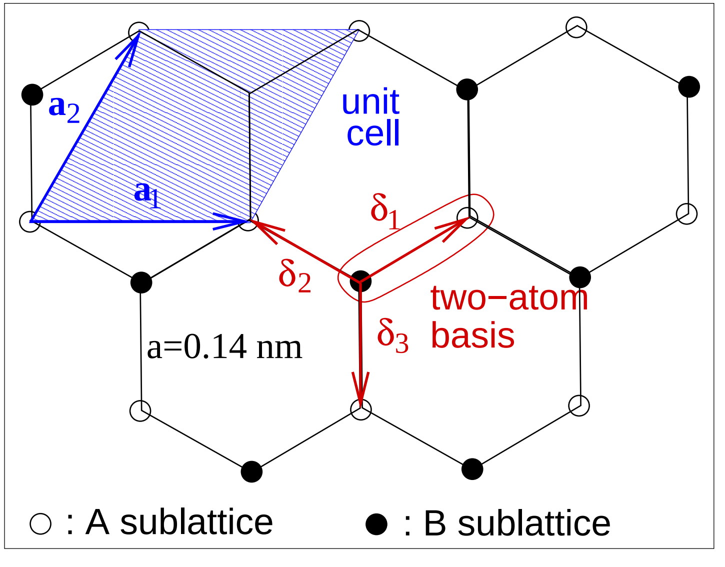
Massless Dirac fermions in Nature

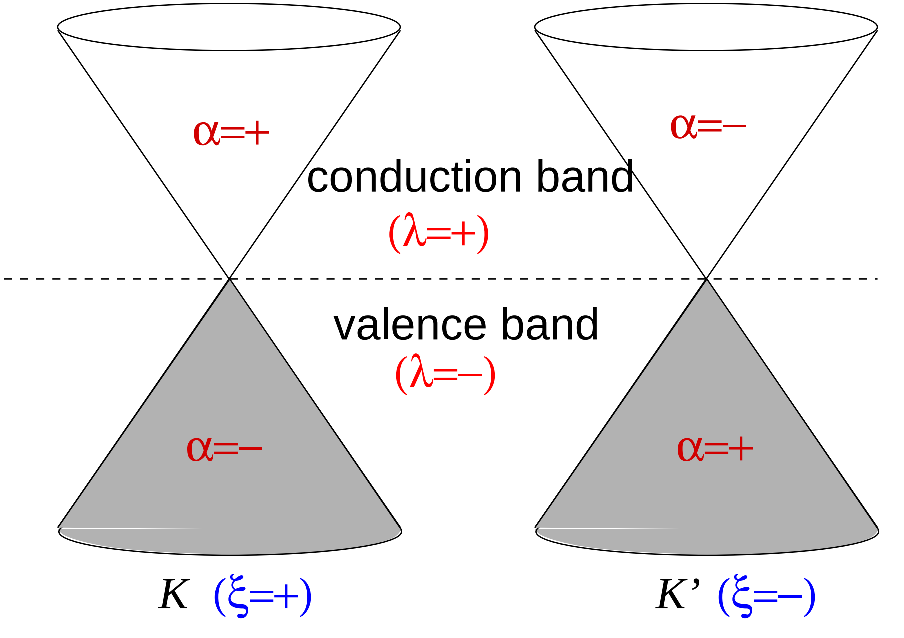
High-E phys. (neutrinos)

- tiny mass
- 3-dimensional space
- no electric charge
- true spin $s = 1/2$

Low-E CM phys. (graphene)

- zero *effective* mass
- 2-dimensional space
- electric charge $-e$
- sublattice isospin $1/2$

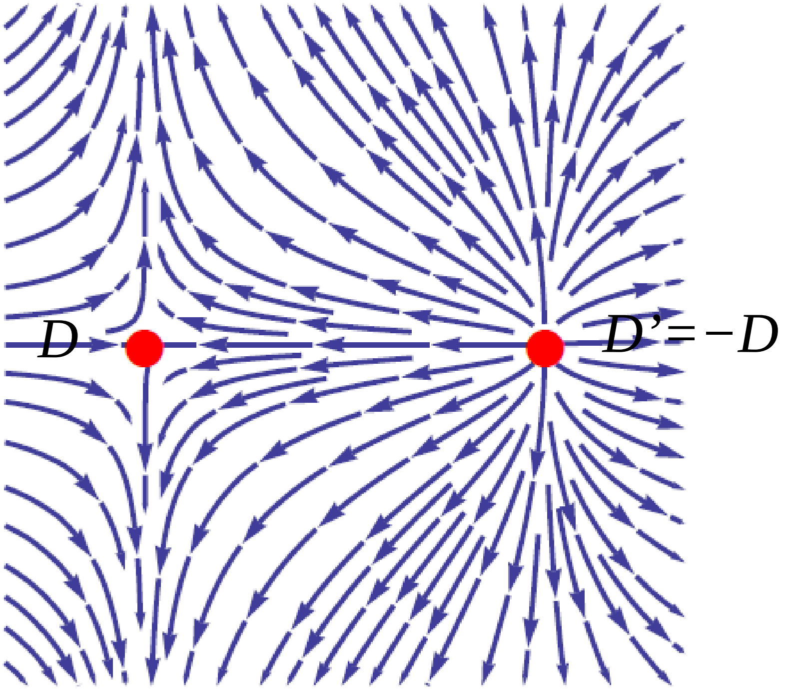




chirality $\alpha = \boldsymbol{\sigma} \cdot \boldsymbol{\kappa}/|\boldsymbol{\kappa}| = \pm$

Wave functions and winding numbers

Phase of wave function
(TRS−related Dirac points)



wave function

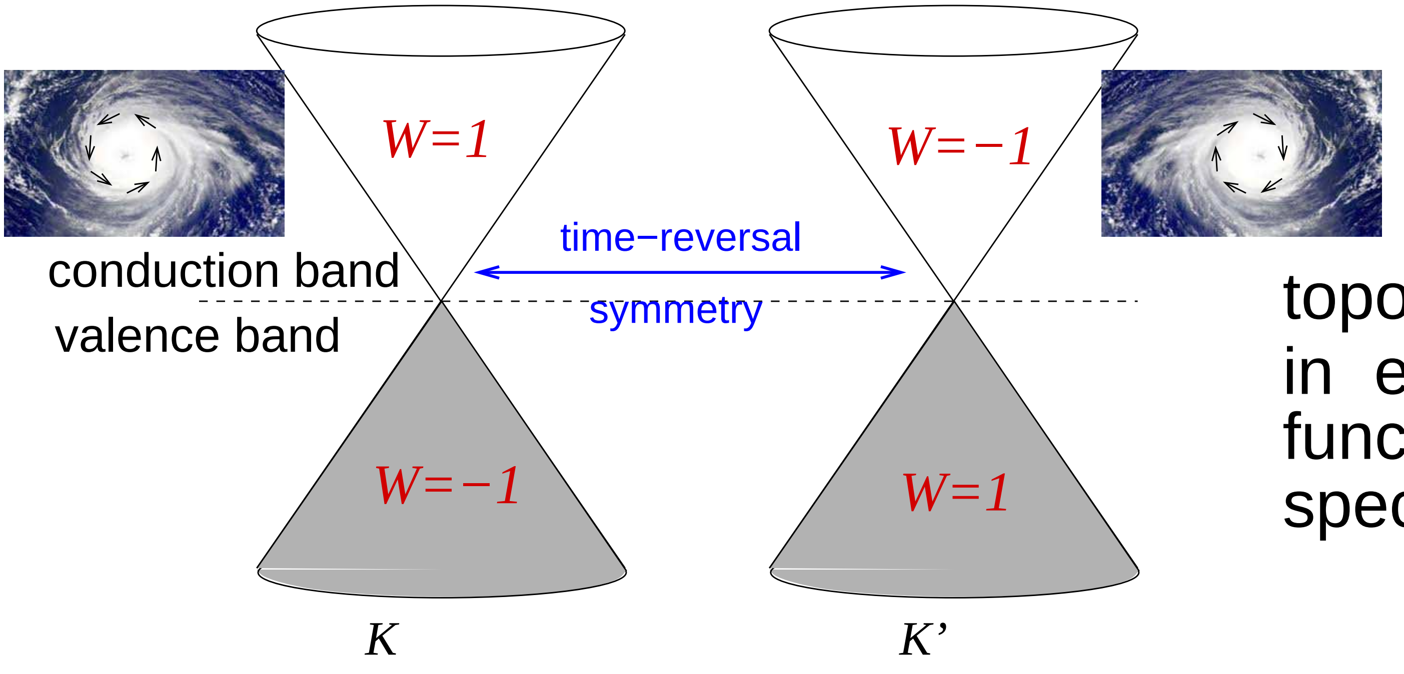
$$\psi_{\xi,\lambda;\mathbf{q}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \xi\lambda e^{-i\xi\phi_{\mathbf{q}}} \end{pmatrix} \qquad \tan\phi_{\mathbf{q}} = \frac{q_y}{q_x}$$

winding number ($\sim$ topol. charge)

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

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

Topology of Dirac points in graphene



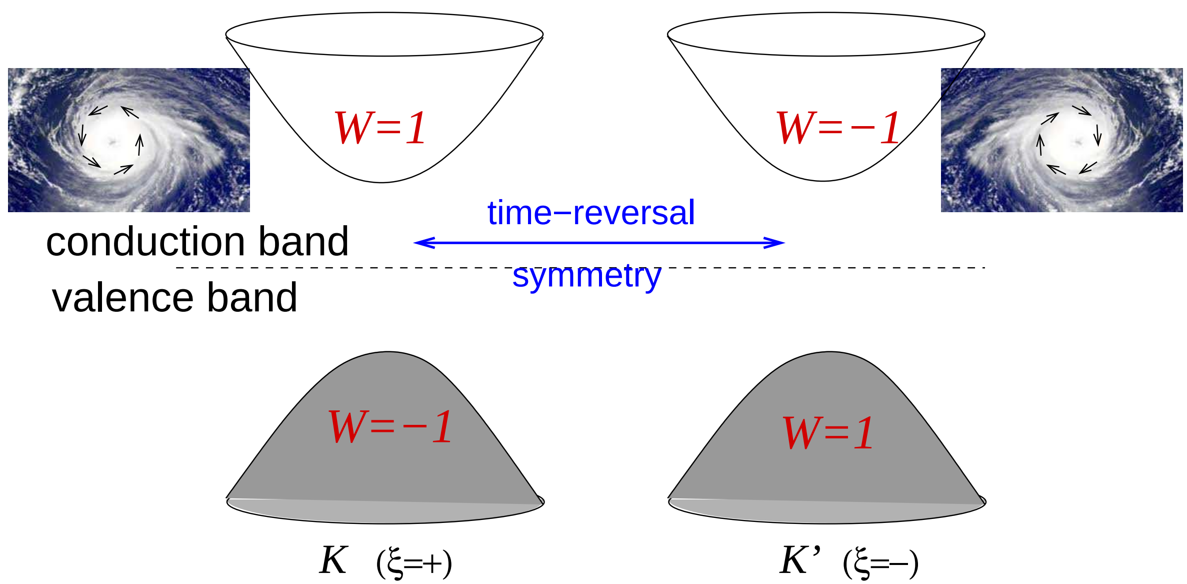
topology encoded in electronic wave function, *not* in spectrum

- topological invariant ("charge"): winding W of wave function

⇒ protects Dirac points (together with time-reversal and inversion symmetry)

2D semiconductors: massive Dirac vs. Schrödinger fermions

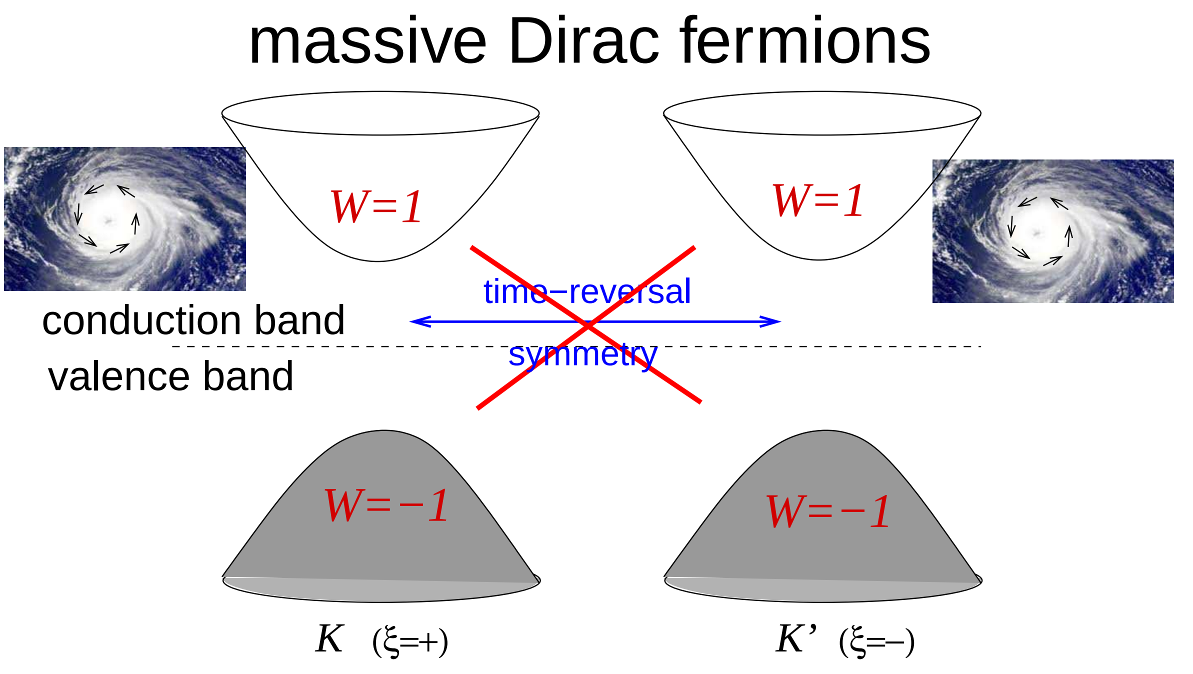
massive Dirac fermions



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

- gap 2Δ, velocity v_D *plays role of* speed of light
- $W = \pm 1$: topological part of Berry phase [Fuchs et al., EPJB (2010)]

2D semiconductors: massive Dirac vs. Schrödinger fermions



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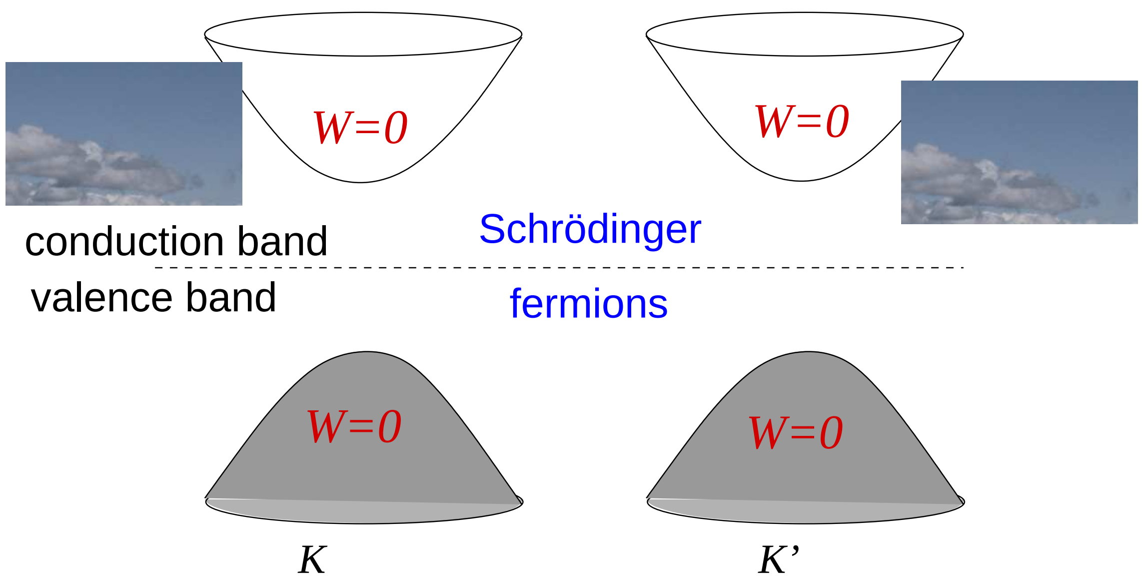
2D semiconductors: massive Dirac vs. Schrödinger fermions

Schrödinger fermions



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

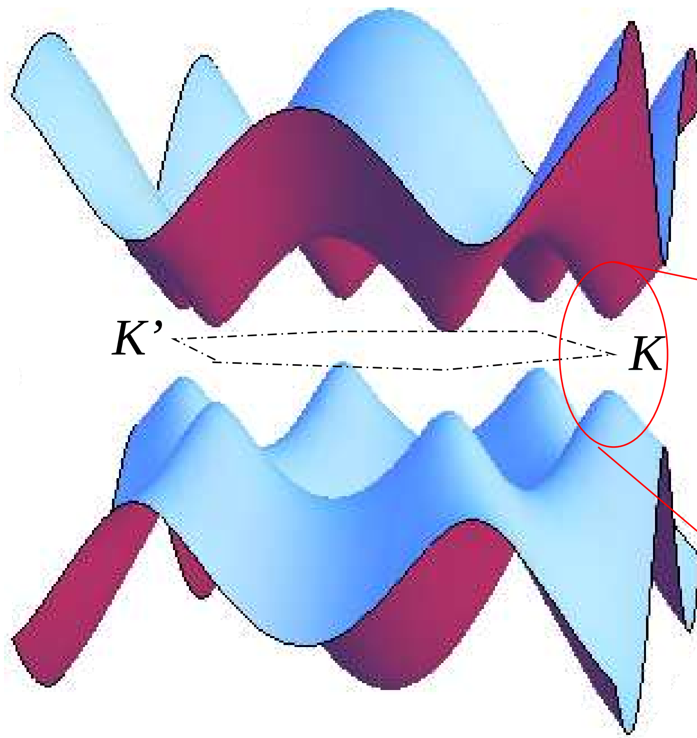
- same parabolicity if $m \to \Delta / v_D^2$ (Dirac mass)

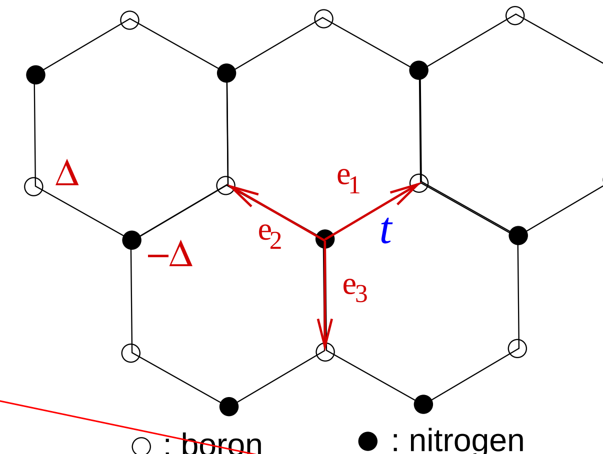
Physical consequences of difference between massive Dirac and Schrödinger fermions ?

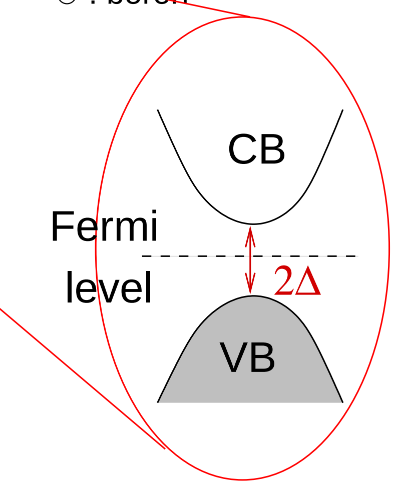
Tight-binding model of boron nitride/gapped graphene

- only nn hopping t
- same model as for graphene

$\rightarrow$ different onsite energy for boron Δ and nitrogen $-\Delta$







Low-energy model: massive Dirac fermions

$$\mathcal{H}(\mathbf{q}) = \begin{pmatrix} \Delta & \hbar v_D(q_x - iq_y) \\ \hbar v_D(q_x + iq_y) & -\Delta \end{pmatrix} = \hbar v_D(q_x\sigma^x + q_y\sigma^y) + \Delta\sigma^z$$

2D Electrons in the Presence of a Magnetic Field

Landau-Level Quantisation

Dirac fermions in a magnetic field

- Magnetic field $(B\mathbf{e}_z = \nabla \times \mathbf{A})$ via Peierls substitution:

$$\hbar\mathbf{q} \to -i\hbar\nabla + e\mathbf{A}$$

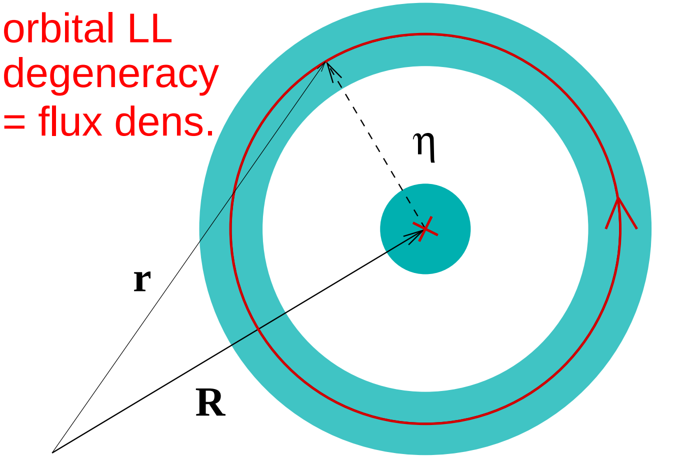
(semi-cl.: $\varepsilon(\mathbf{q}) \to \varepsilon(\sqrt{2n}/l_B)$, $l_B = \sqrt{\hbar/eB} \gg$ latt. spacing)

- Schrödinger fermions:

$$\varepsilon_n = \hbar\omega_C\left(n + \frac{1}{2}\right)$$

(Landau levels $\sim$ harmonic oscillator)

$\omega_C = eB/m$: cyclotron frequency



η : energy quantisation

R : constant of motion (degeneracy)

Dirac fermions in a magnetic field

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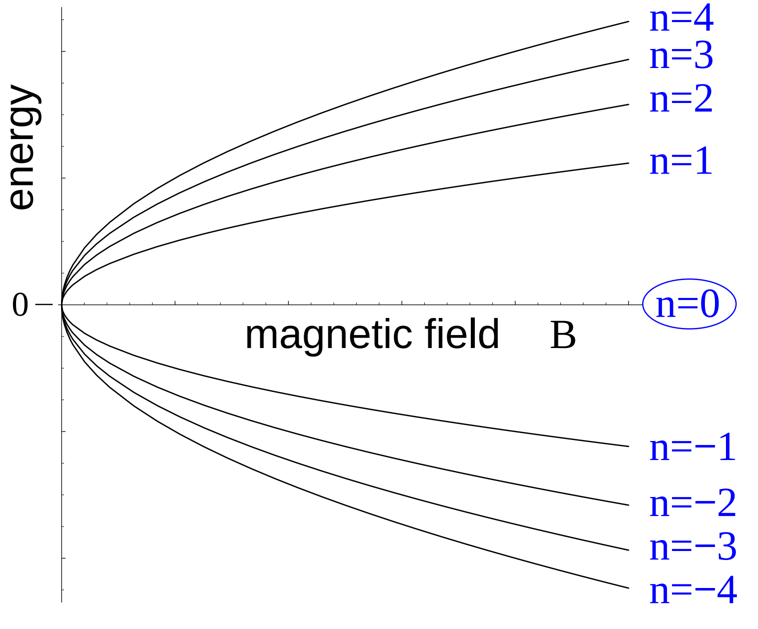
- Massless Dirac fermions (graphene):

$$\varepsilon_{\lambda,n} = \lambda\hbar\frac{v_F}{l_B}\sqrt{2|n|} \propto \sqrt{B|n|}$$

(Relativistic Landau levels)



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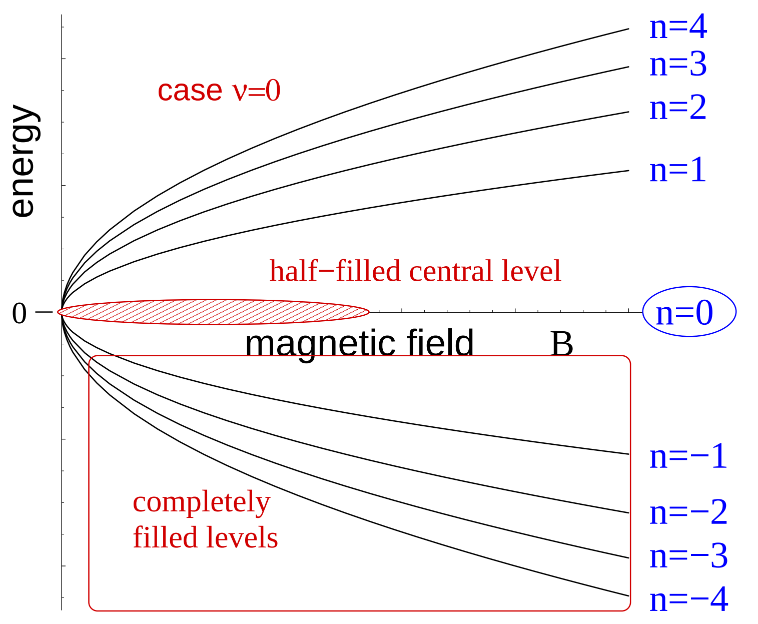
- Quantum Hall effect in graphene at

$$\nu = \frac{n_{el}}{eB/h} = \pm 2, \pm 6, \pm 10, \ldots$$



Dirac fermions in a magnetic field

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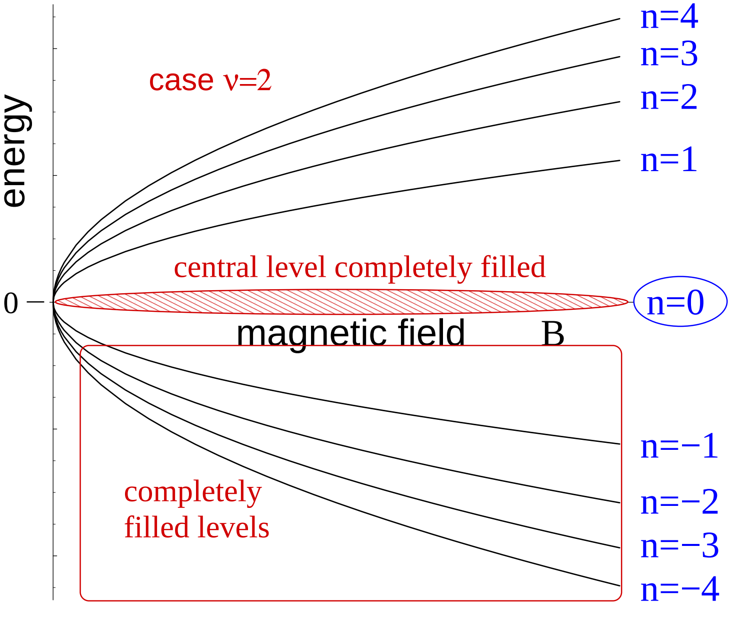
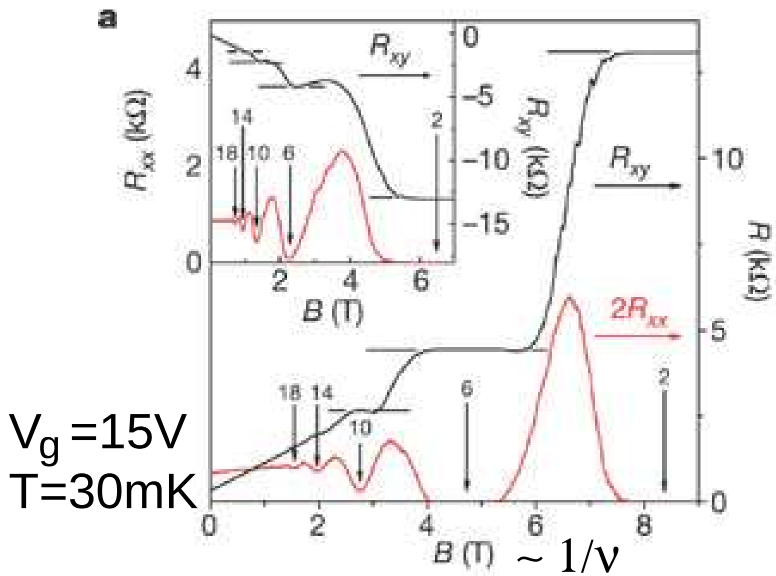
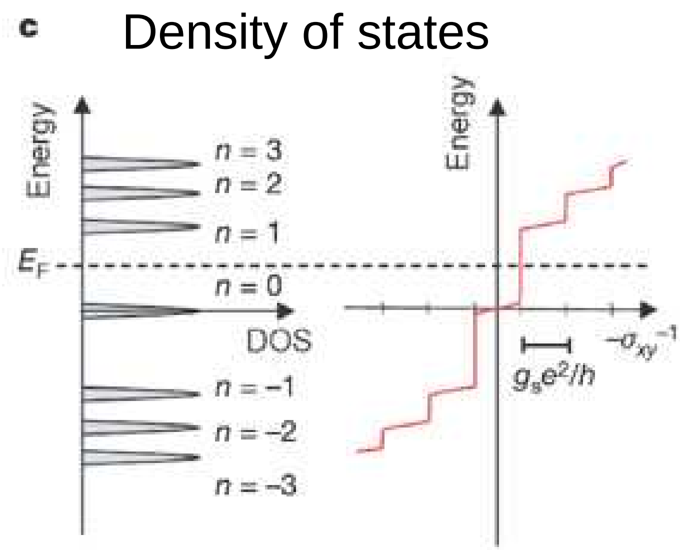


IQHE in graphene

Novoselov et al., Nature 438, 197 (2005)

Zhang et al., Nature 438, 201 (2005)

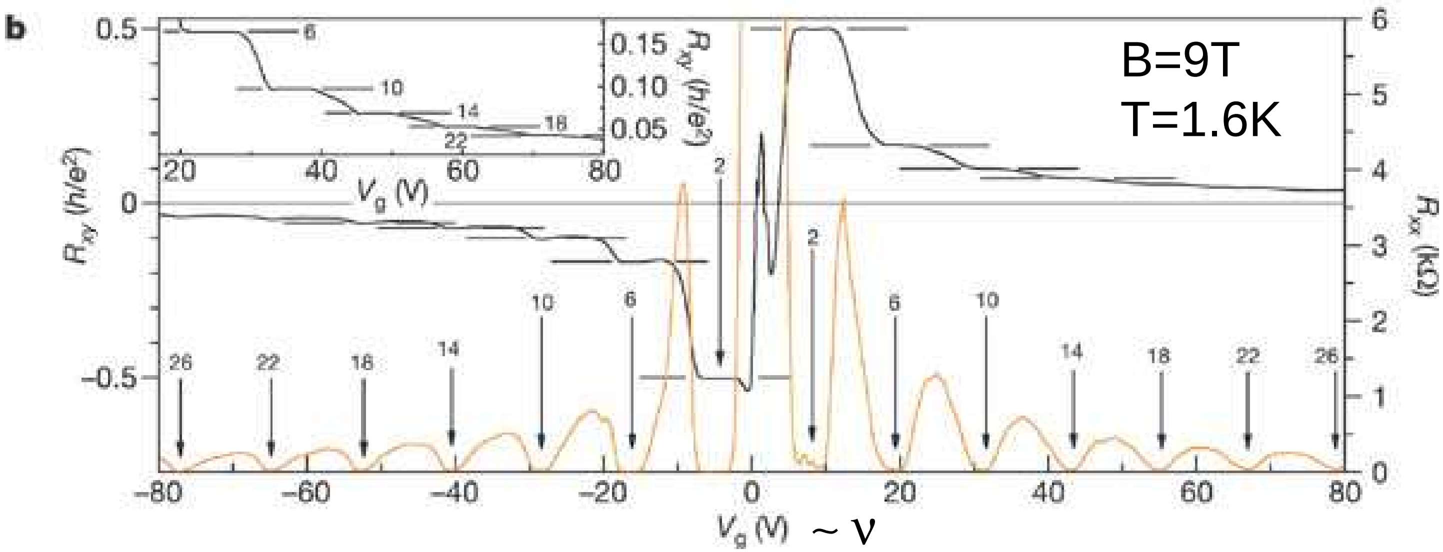




Graphene IQHE:

$R_H = h/e^2\nu$

at $\nu = 2(2n+1)$

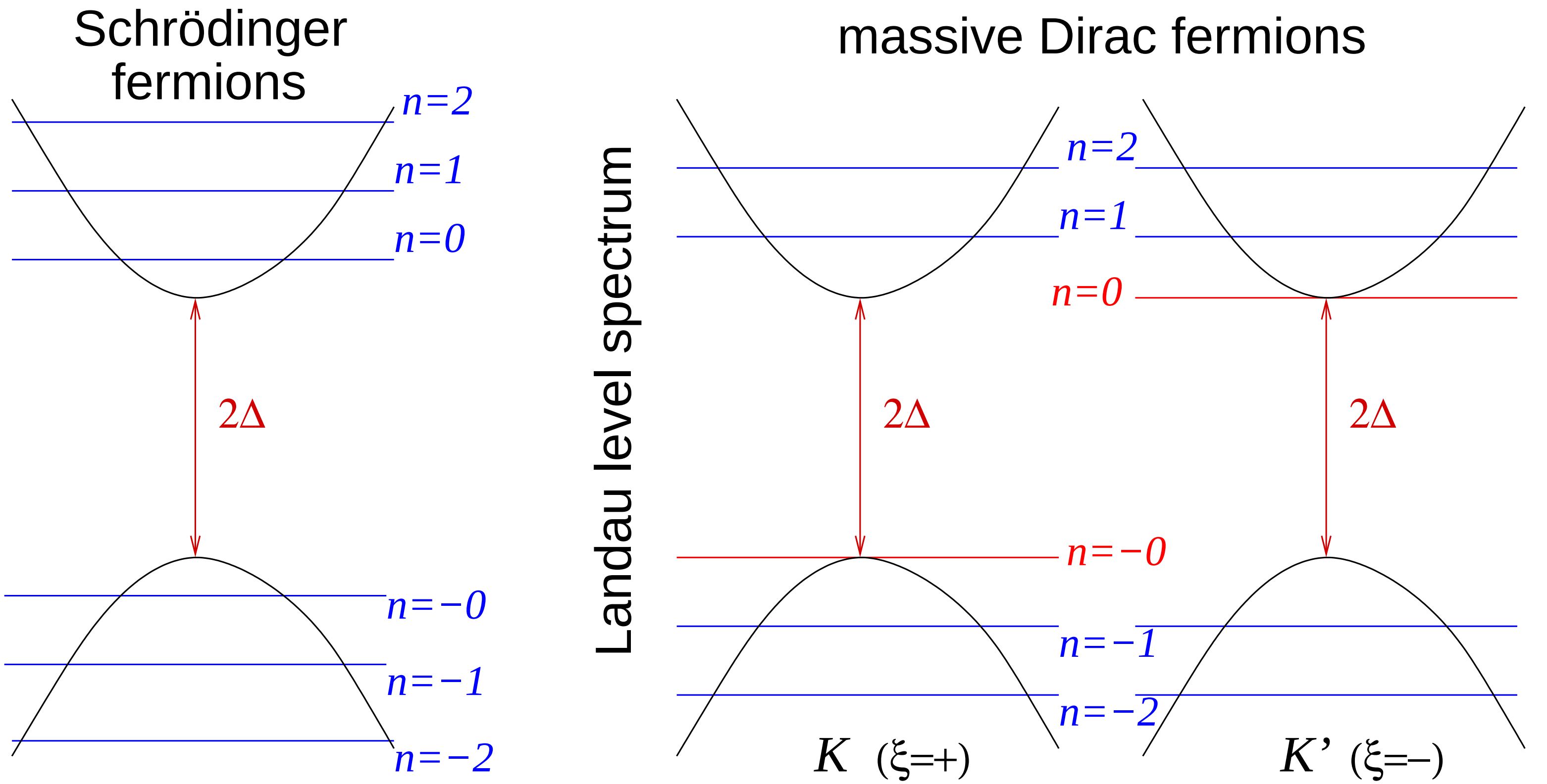


Usual IQHE:

at $\nu = 2n$

(no Zeeman)

Massive Dirac vs. Schrödinger: Landau levels

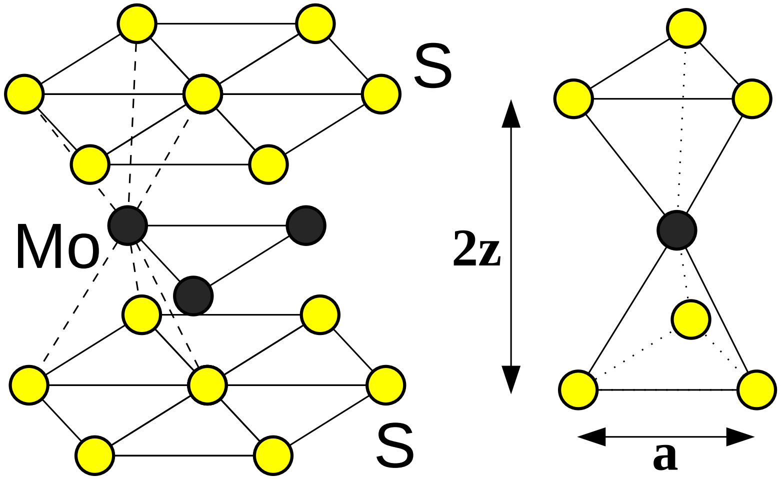


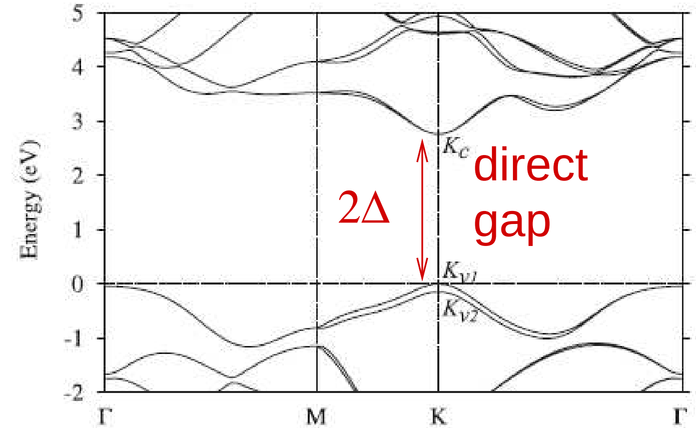
- Schrödinger fermions: $\epsilon_{\pm n} = \pm\hbar\omega_C(n + 1/2)$
- Dirac fermions: electron-hole symmetry broken in single Dirac point for LL $n = 0$, $\epsilon_{n=0} = -\xi\Delta$

$\Rightarrow$ Parity anomaly, independent of gap size [Semenoff, PRL (1984)]

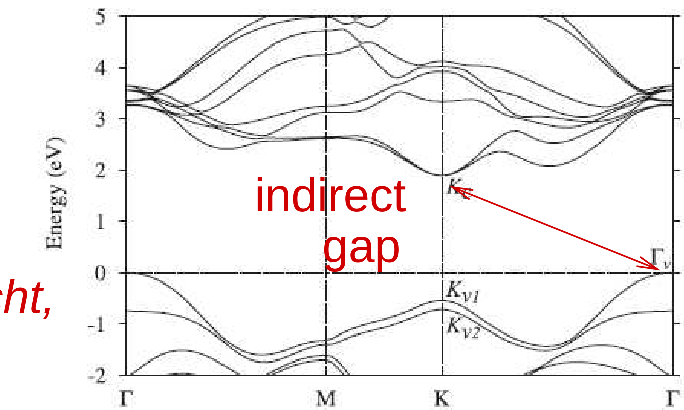
Molybdenum disulfide

crystal structure





monolayer

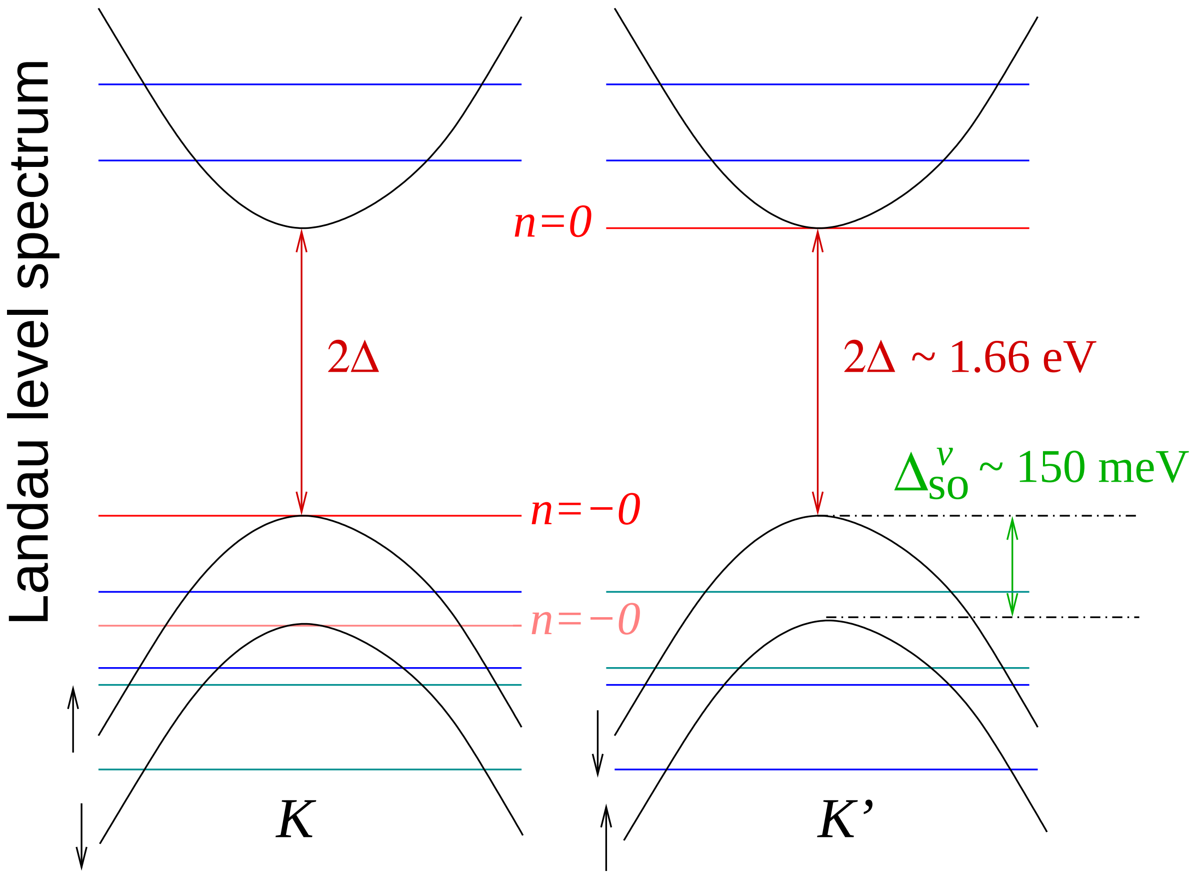


bilayer (~bulk)

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 $(|d_{\mathrm{xy}}\rangle + i\xi|d_{\mathrm{x}^2-\mathrm{y}^2}\rangle)/\sqrt{2}$

Landau level structure of MoS_2 – spin-orbit coupling



modelling in terms of massive Dirac fermions

Xiao et al., PRL (2012)

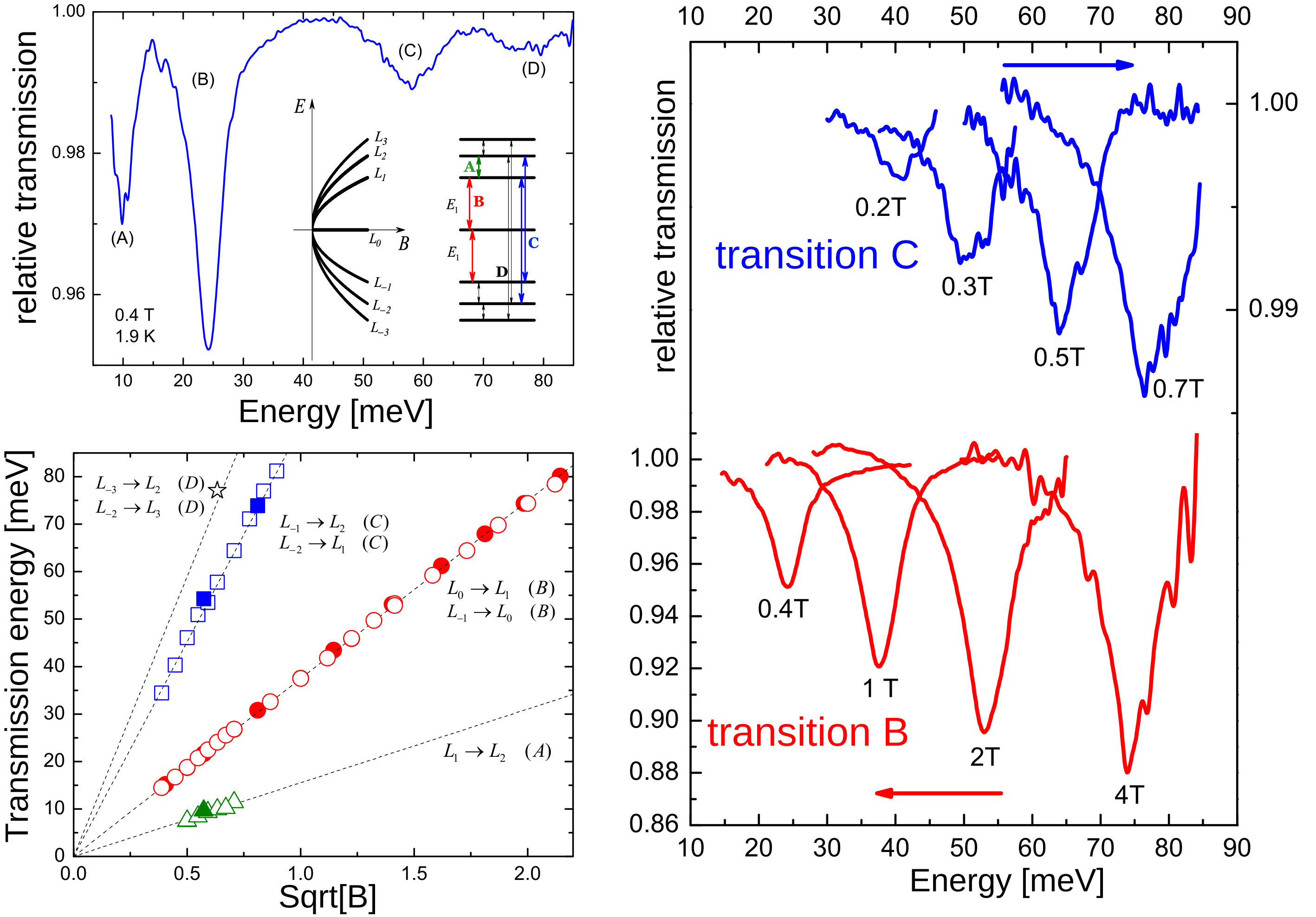
Ochoa & Roldán, PRB (2013)

Rose, MOG, Piéchon, PRB (2013)

- spin-orbit coupling Δ_{so} most prominent in valence band
- $\Delta_{so}^{v} \simeq 150$ meV $\gg \Delta_{so}^{c} \simeq 3$ meV

Magneto-Optical Spectroscopy as a Probe of Landau Levels

Infrared transmission spectroscopy on graphene



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

selection rules :

$$\lambda, n \to \lambda', n \pm 1$$

Light-matter coupling

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

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

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

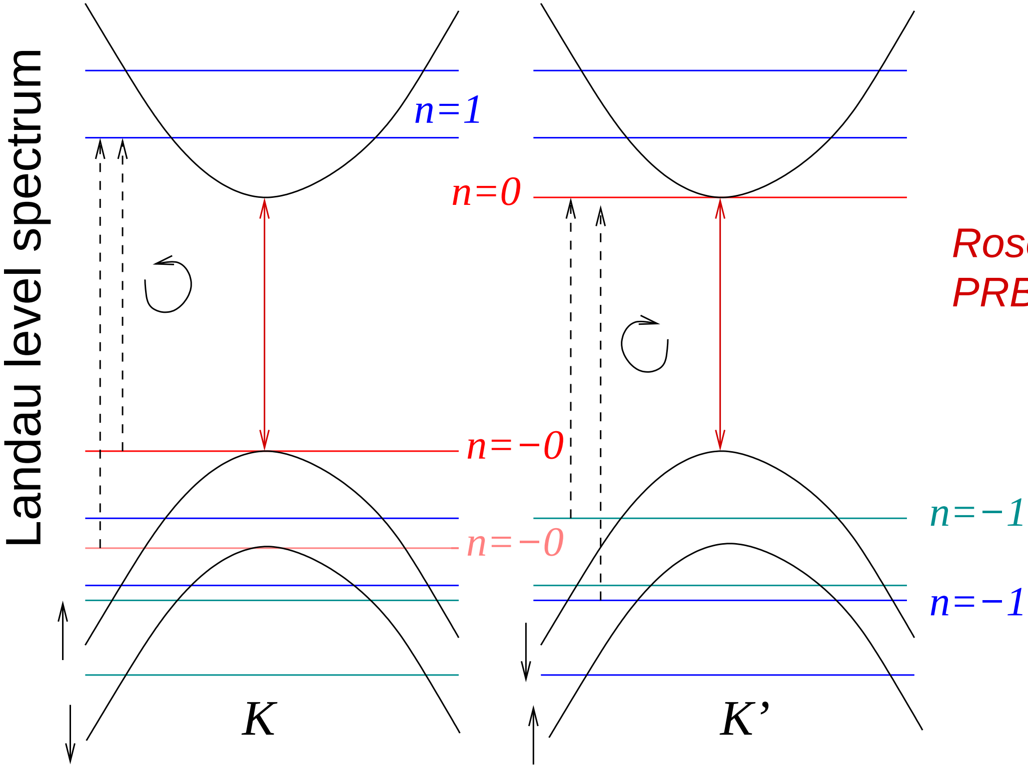
- $\mathcal{H}_B \rightarrow$ Landau levels, velocity operator $\mathbf{v} = \nabla_{\mathbf{q}}\mathcal{H}/\hbar$

<u>dipolar selection rules:</u>

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

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

Magneto-optical selection rules in MoS_2

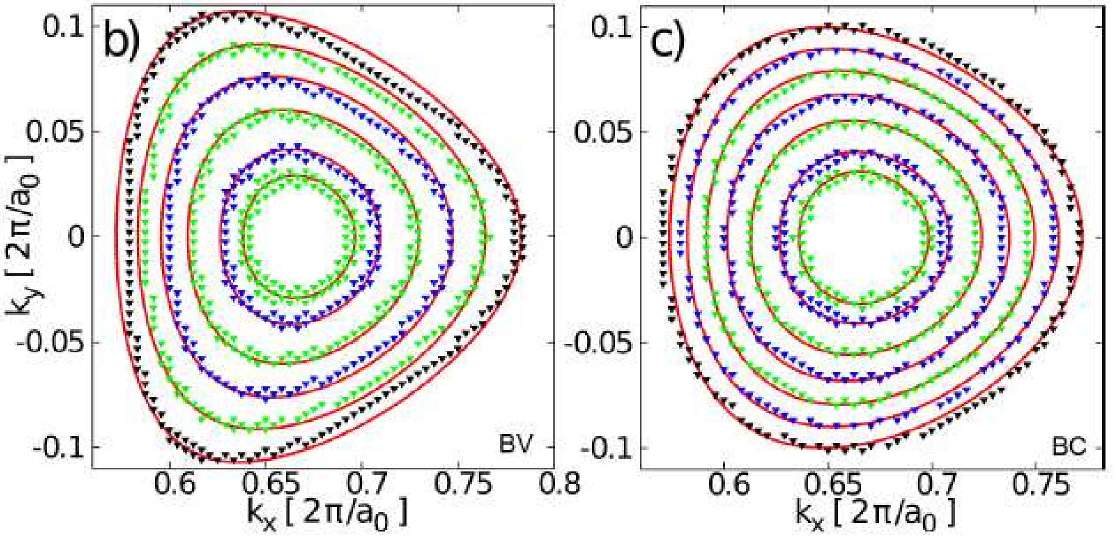


Rose, MOG, Piéchon, PRB (2013)

selective spin-valley excitation of electrons, via polarisation and frequency

- electronic transition $-0 \to 1$ (pol. ↺) only in valley K
- electronic transition $-1 \to 0$ (pol. ↻) only in valley K'

Corrections to the model of massive Dirac fermions



[Kormányos et al., PRB (2013)]

- electron-hole asymmetry
- trigonal warping

$\Rightarrow$ Novel optical transitions: [Rose, MOG, Piéchon, PRB (2013)]

$$n \to n \pm 2 \qquad\qquad n \to n \pm 4$$

$$n \to n$$

Mixed Dirac-Schrödinger Character of Electrons in 2D Semiconductors

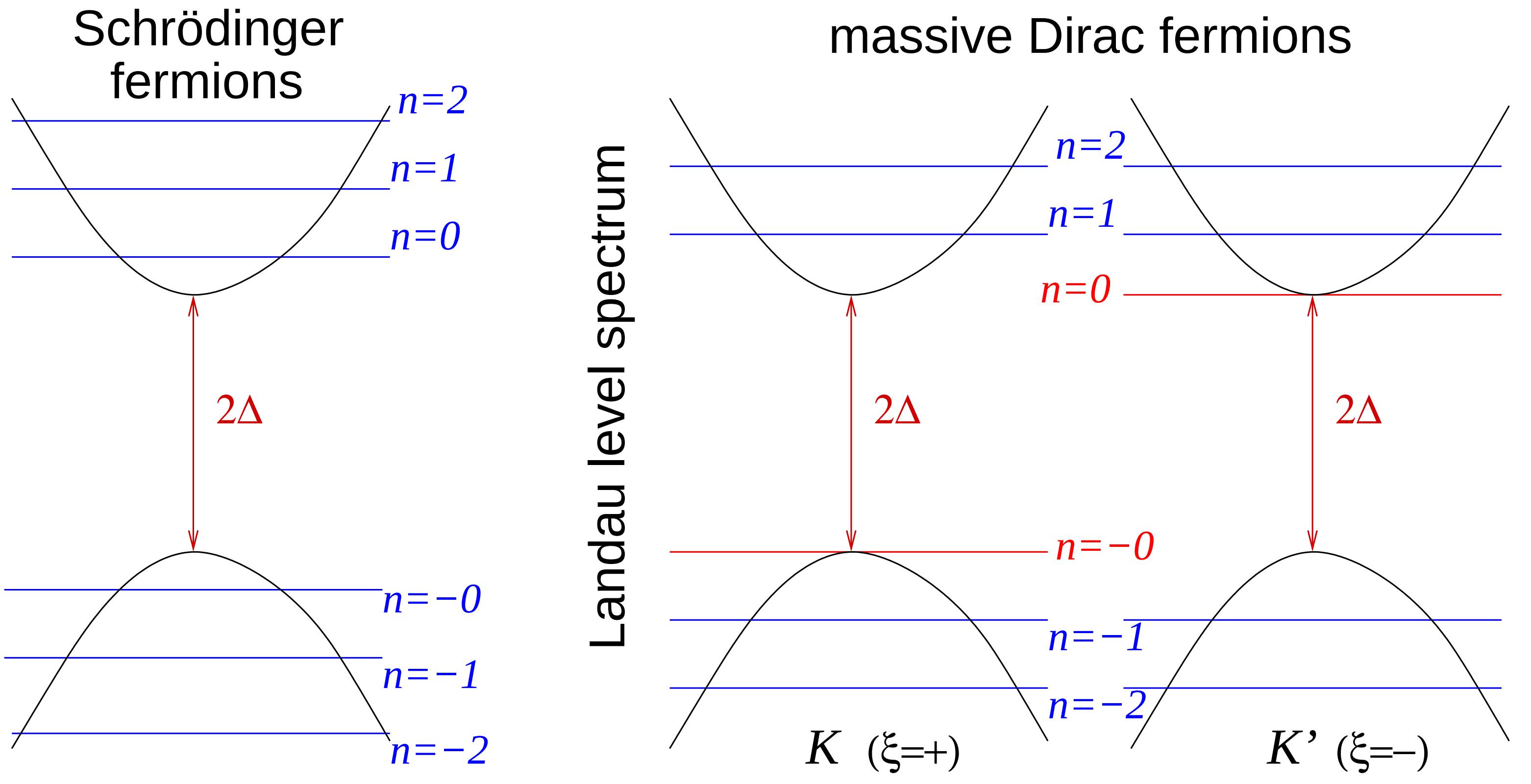
LPS collaboration with:

Frédéric Piéchon

Gilles Montambaux

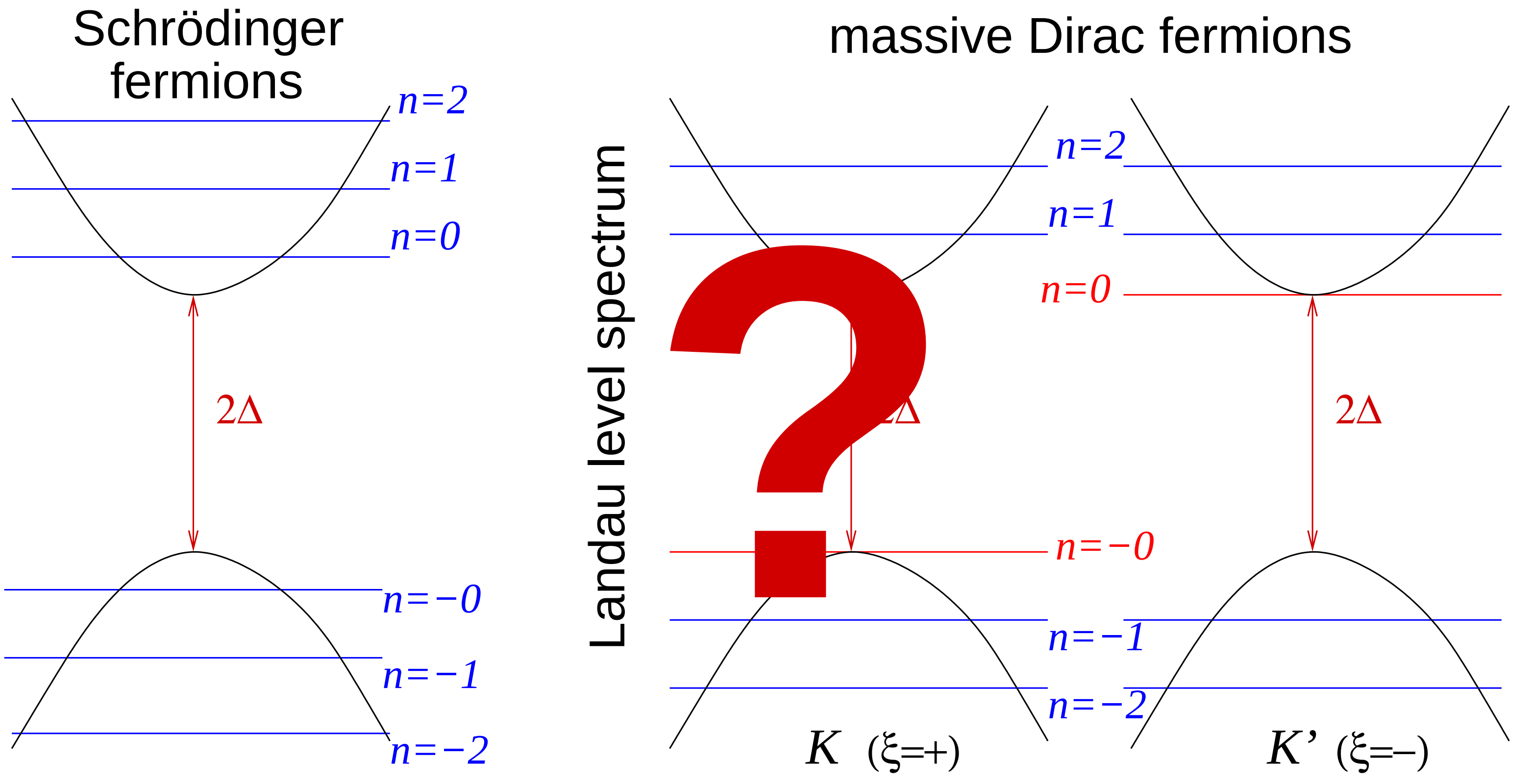
EPL **105**, 57005 (2014).

Reminder: Dirac vs. Schrödinger



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

Reminder: Dirac vs. Schrödinger



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

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

Landau-level spectrum

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

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

spectrum in parabolic approximation:

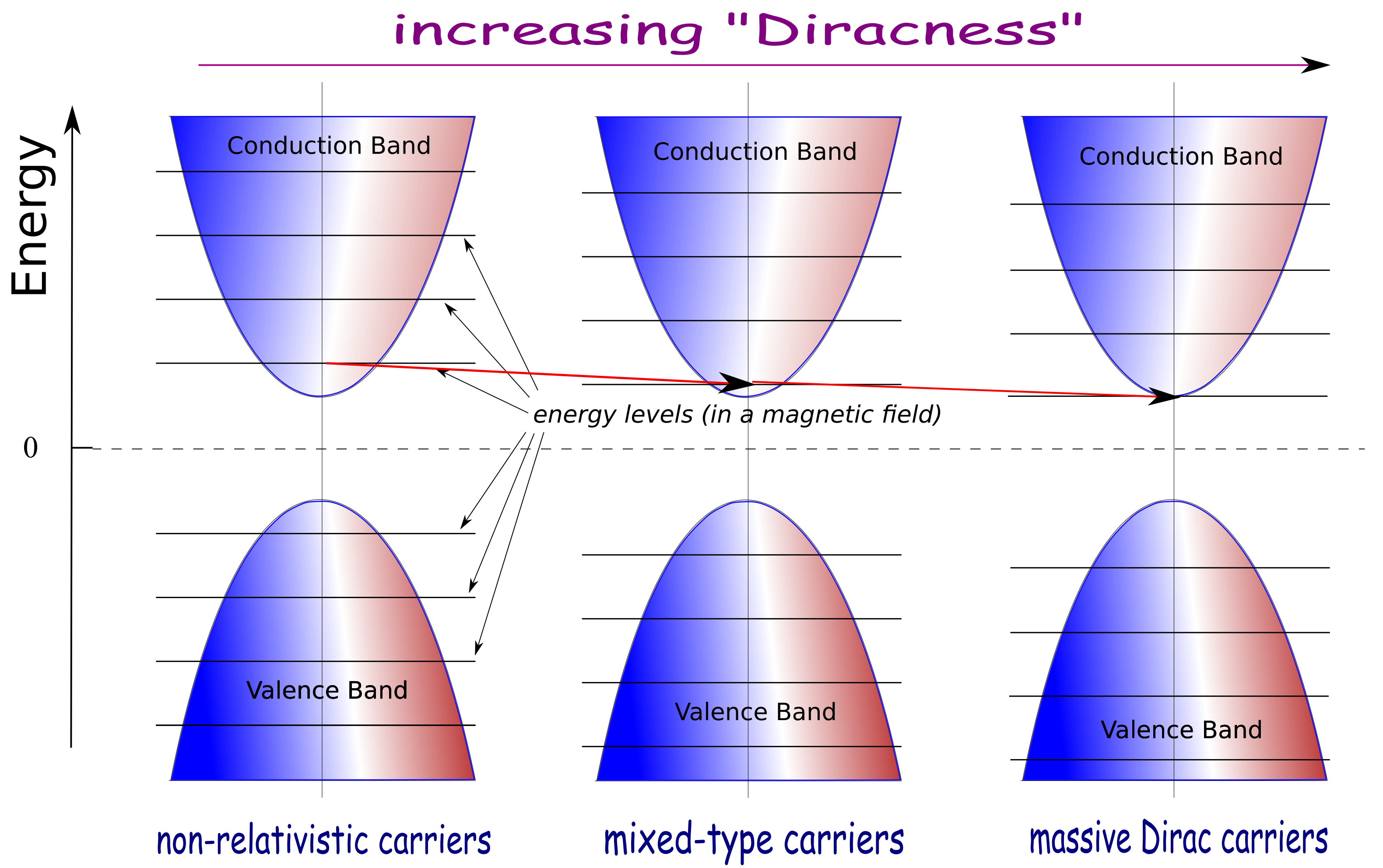
$$\epsilon_{\lambda,n} = \lambda\left[\Delta + \hbar\omega_\lambda(n + \gamma_\lambda)\right], \qquad \omega_\lambda = eB/m_\lambda$$

$\rightarrow$ 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 level spectrum



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

A measure of Diracness

MOG, Montambaux, Piéchon, EPL (2014)

Phase offset encodes Diracness

$$\gamma_\lambda = \frac{1}{2}\left(1 + \lambda\delta_\lambda\right)$$

Diracness:

$$\delta_\lambda = \frac{m_\lambda}{m_D} = \frac{2m_\lambda\Delta|\mathcal{B}_\lambda(\mathbf{q}=0)|}{\hbar^2}$$

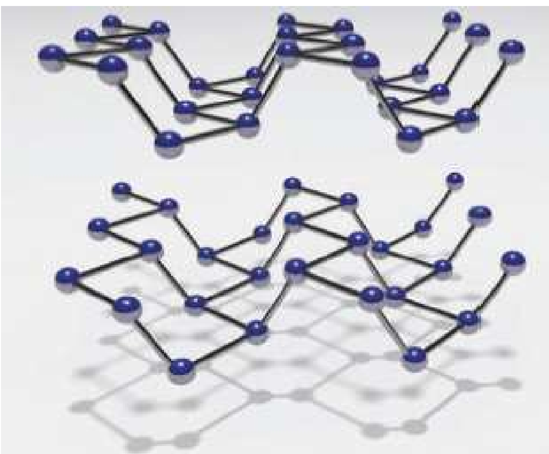
- varies between $\delta_\lambda = 0$ (Schrödinger) and 1 (Dirac)
- not measurable from band dispersion alone !

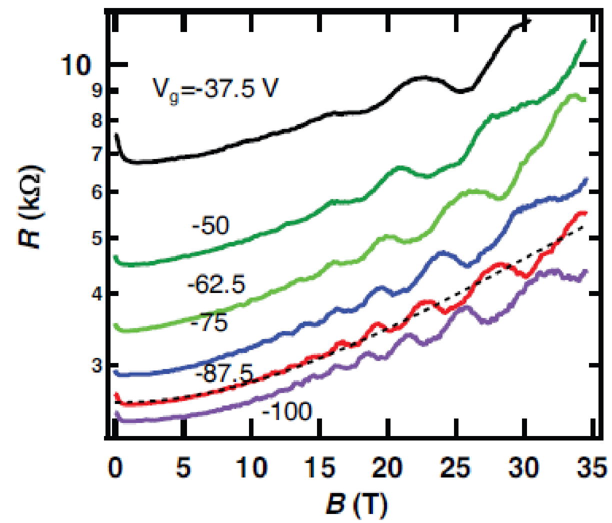
$\rightarrow$ measurable in Shubnikov-de-Haas oscillations (experimentally)

$\rightarrow$ extractable from Berry curvature at gap $\mathcal{B}_\lambda(\mathbf{q}=0)$ (*ab initio* calculations)

SdH oscillations in 2D black phosphorus – experiment

Tayari et al., arXiv:1412.0259 (Skopek-Gervais group, McGill Montréal)

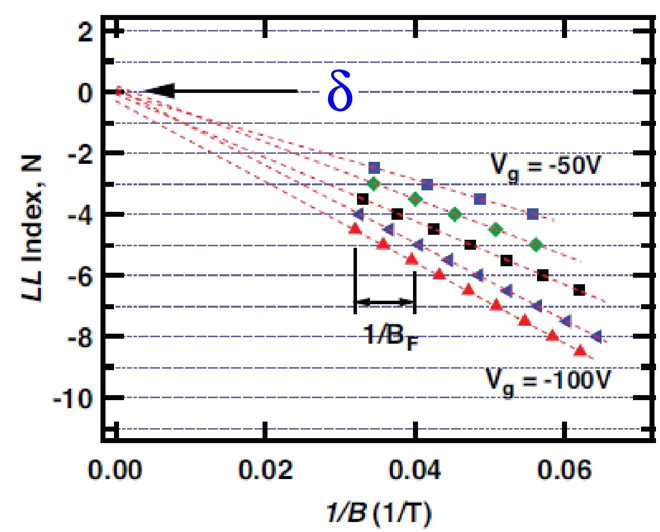




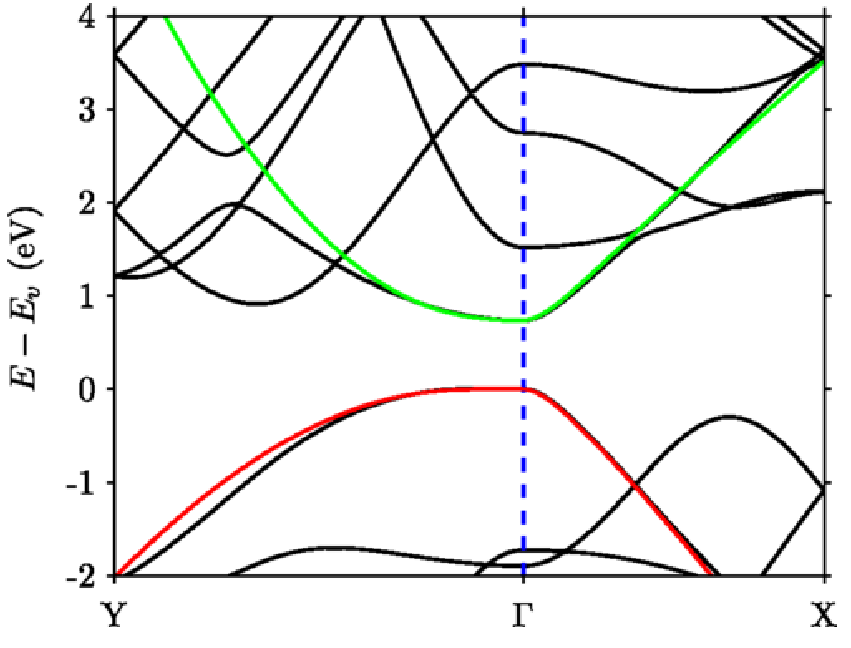
$$\Delta R \propto \cos\left[2\pi\left(\frac{B_F}{B}+\frac{1}{2}(1\pm\delta)\right)\right]$$

$B_F = \frac{h n_{el}}{ge}$: magnetic frequency

$\delta = 0 \;\Rightarrow$ Schrödinger fermions !



SdH oscillations in 2D black phosphorus – theory



Rodin et al., PRL (2014)

- direct-gap 2D semiconductor

- Direct gap at the Γ point (TR-invariant)

- anti-symmetric Berry curvature around a TRIM :

$$B(\mathbf{q}) = -B(-\mathbf{q})$$

$\Rightarrow$ $B(\mathbf{q} = \Gamma) = 0$

$\Rightarrow$ vanishing Diracness:
$\delta \propto B(\mathbf{q} = \Gamma) = 0$

$\Rightarrow$ “trivial” Berry phase

Possibly interesting evolution under strain !

Conclusions

Second-generation of 2D crystals (beyond graphene):
playground for (massive) Dirac physics

- electrons may have mixed Dirac-Schrödinger character

$\rightarrow$ measure of Diracness (physical quantity)

  - measurable experimentally via SdH oscillations
  - extractable from ab initio calculations (information beyond band dispersion)

- Dirac fermions in MoS_2 (?)
  - parity anomaly in $n = 0$ Landau level

  $\rightarrow$ spin-valley selection via polarisation & frequency of light
  - corrective terms: novel optically active transitions

Relevance of mixed Dirac/Schrödinger fermions

Where to look for them ?

- 2D semiconductors with a direct gap

$\longrightarrow$ What happens in 3D ? (yet to be done)

- direct gap must be at points in 1BZ that are *not* time-reversal invariant momenta (mainly at K and K')

Other physical consequences of massive Dirac fermions ?

- Klein tunneling and electrostatic confinement ?

$\longrightarrow$ electronic transport at $B = 0$?

- orbital magnetism

General 2D direct-gap semiconductors

General model (Luttinger-Kohn representation):

$$H = \begin{pmatrix} \Delta + \frac{\hbar^2}{2m^{\mathrm{e}}_{ij}} q_i q_j & \hbar(\mathbf{v}_1 \cdot \mathbf{q} - i\mathbf{v}_2 \cdot \mathbf{q}) \\ \hbar(\mathbf{v}_1 \cdot \mathbf{q} + i\mathbf{v}_2 \cdot \mathbf{q}) & -\Delta - \frac{\hbar^2}{2m^{\mathrm{h}}_{ij}} q_i q_j \end{pmatrix}$$

- Landau levels:

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

- Diracness:

$$\delta_\lambda = \frac{m^C_\lambda}{m_D} = \frac{2m^C_\lambda \Delta |\mathcal{B}_\lambda(\mathbf{q}=0)|}{\hbar^2}$$

in terms of Dirac mass

$$m_D = \frac{\Delta}{\mathbf{v}_1 \wedge \mathbf{v}_2}$$

Evolution of Diracness at high energy (I)

- Semi-classical treatment of model

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

- Onsager quantisation rule:

$$S(\epsilon_\lambda)l_B^2 = 2\pi(n + \gamma_\lambda) \quad \text{with} \quad \gamma_\lambda = \frac{1}{2}(1 + \lambda\delta_\lambda)$$

- Diracness expressed in terms of Berry phase Γ and curvature $\mathcal{A}$

$$\Gamma = \int_{\mathcal{C}(\epsilon_\lambda)} d\mathbf{q} \cdot \vec{\mathcal{A}}_\lambda(\mathbf{q}) \quad \rightarrow \quad \delta_\lambda = -\frac{\lambda}{\pi}\frac{d(\epsilon\Gamma)}{d|\epsilon_\lambda|}$$

Evolution of Diracness at high energy (II)

- Energy-dependent Diracness [with $M = (m_{\rm el}^0 + m_{\rm h}^0)/2$]

$$\delta_\lambda(\epsilon) = 1 - \frac{\epsilon}{\sqrt{\epsilon^2 + M^2 v_D^4 + 2\Delta M v_D^2}}.$$

- phase offset as a function of energy and $\delta = \delta(E = 0)$