Two-dimensional semi-conductors: massive Dirac fermions or nothing new?

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Graphene and other 2D crystals

Electronic properties:

• 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

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)

\[
\mathcal{H}_q^{\xi} = \hbar v_F \begin{pmatrix}
0 & \xi q_x - iq_y \\
\xi q_x + iq_y & 0
\end{pmatrix}
\]
Wave functions and winding numbers

Stability of Dirac fermions in 2D condensed matter

→ time-reversal and inversion symmetry

→ topological “charge” of Dirac points (encoded in wave function)

wave function

\[ \psi_{\xi,\lambda; \mathbf{q}} = \frac{1}{\sqrt{2}} \left( \frac{1}{\xi \lambda e^{-i \xi \phi_{\mathbf{q}}}} \right) \tan \phi_{\mathbf{q}} = \frac{q_y}{q_x} \]

winding number (\(\sim\) Berry phase)

\[ W_{\xi,\lambda} = \frac{\xi \lambda}{2\pi} \oint_{C_i} \nabla_{\mathbf{q}} \phi_{\mathbf{q}} \cdot d\mathbf{q} = \xi \lambda \]
Topology of Dirac points in graphene

- 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

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

- gap $2\Delta$, 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

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

- 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
  \[ \rightarrow \text{different onsite energy for boron } \Delta \text{ and nitrogen } -\Delta \]

Low-energy model: \textbf{massive Dirac fermions}

\[
\mathcal{H}(q) = \begin{pmatrix} \Delta & \hbar v_D (q_x - i q_y) \\ \hbar v_D (q_x + i q_y) & -\Delta \end{pmatrix} = \hbar v_D (q_x \sigma^x + q_y \sigma^y) + \Delta \sigma^z
\]
Consequences for 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 $n = 0$, $\epsilon_{n=0} = -\xi \Delta$

⇒ Parity anomaly, independent of gap size [Semenoff, PRL (1984)]
Molybdenum disulfide

- Crystal structure

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

- 3 $p$ orbitals per S, 5 $d$ orbitals per Mo = 11 orbitals
- At $K$ points: $|d_{3t^2-r^2}\rangle$ and $(|d_{xy}\rangle + i\xi|d_{x^2-y^2}\rangle)/\sqrt{2}$
Landau level structure of MoS$_2$ – spin-orbit coupling

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

modelling in terms of massive Dirac fermions

- $\Delta_{so}^v \sim 150$ meV
- $2\Delta \sim 1.66$ eV

Xiao et al., PRL (2012)
Ochoa & Roldán, PRB (2013)
Rose, MOG, Piéchon, PRB (2013)
Infrared transmission spectroscopy on graphene

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

selection rules:
\[ \lambda, n \rightarrow \lambda', n\pm1 \]
Light-matter coupling

- Peierls substitution $q \rightarrow q + \frac{e}{\hbar} [A(r) + A_{\text{rad}}(t)]$

- $\nabla \times A(r) = B$ (magnetic field), $A_{\text{rad}}(t)$ (radiation field)

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

  $\mathcal{H}(q) \rightarrow \mathcal{H}_B + ev \cdot A_{\text{rad}}(t)$

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

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dipolar selection rules:

$\lambda n \rightarrow \lambda'(n + 1)$ for right-handed light

$\lambda n \rightarrow \lambda'(n - 1)$ for left-handed light
Magneto-optical selection rules in MoS$_2$

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

- electronic transition $-0 \rightarrow 1$ (pol. $\bigcirc$) only in valley $K$
- electronic transition $-1 \rightarrow 0$ (pol. $\bigcirc$) only in valley $K'$
Corrections to the model of massive Dirac fermions

- electron-hole asymmetry
- trigonal warping

⇒ Novel optical transitions:  

\[ n \rightarrow n \pm 2 \quad \quad n \rightarrow n \pm 4 \quad \quad n \rightarrow n \]
Mixed Dirac-Schrödinger Character of Electrons in 2D Semiconductors

LPS collaboration with:

Frédéric Piéchon
Gilles Montambaux

EPL 105, 57005 (2014).
**Reminder: Dirac vs. Schrödinger**

Schrödinger fermions

![Schrödinger fermions diagram](image)

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

massive Dirac fermions

![massive Dirac fermions diagram](image)

\[ H(q) = \begin{pmatrix} \Delta & \hbar v_D (q_x - iq_y) \\ \hbar v_D (q_x + iq_y) & -\Delta \end{pmatrix} \]
Reminder: Dirac vs. Schrödinger

\[ \mathcal{H}(q) = \begin{pmatrix} \Delta + \frac{\hbar^2}{2m_0^2}q^2 & \hbar v_D(q_x - iq_y) \\ \hbar v_D(q_x + iq_y) & -\Delta - \frac{\hbar^2}{2m_h^2}q^2 \end{pmatrix} \]

Landau level spectrum

fermions

Schrödinger massive Dirac fermions

\[ n = 0 \]
\[ n = 1 \]
\[ n = 2 \]
\[ n = -1 \]
\[ n = -2 \]

\[ n = 0 \]
\[ n = 1 \]
\[ n = 2 \]
\[ n = -1 \]
\[ n = -2 \]

K (\(\xi = +\))

K' (\(\xi = -\))

Band masses: \(1/m_\lambda = 1/m_\lambda^0 + 1/m_D\), 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: \( \Omega = eB/M \), \( \delta \omega = eB/\mu \), \( \omega' = \sqrt{2v_D/l_B} \)

bare electron mass: \( 1/m_e^0 = 1/M + 1/\mu \)

bare hole mass: \( 1/m_h^0 = 1/M - 1/\mu \)

\[ \text{spectrum in parabolic approximation:} \]

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

\[ \rightarrow \text{Phase offset} \ \gamma_\lambda \ \text{no longer quantised!} \]

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

(pure Schrödinger: \( \gamma = 1/2 \), pure Dirac: \( \gamma = 0 \))
Landau level spectrum

increasing "Diracness"

energy levels (in a magnetic field)

Conduction Band

Valence Band

Energy

0

non-relativistic carriers

mixed-type carriers

massive Dirac carriers

\[ \gamma = \frac{1}{2} \quad \gamma = \frac{1}{4}(\frac{3}{4}) \quad \gamma = 0 \]
A measure of Diracness

MOG, Montambaux, Piéchon, EPL (2014)

Phase offset encodes Diracness

\[ \gamma_\lambda = \frac{1}{2} (1 + \lambda \delta_\lambda) \]

Diracness:

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

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

→ measurable in Shubnikov-de-Haas oscillations (experimentally)

→ extractable from Berry curvature at gap \( \mathcal{B}_\lambda(q = 0) \) (*ab initio* calculations)
General 2D direct-gap semiconductors

General model (Luttinger-Kohn representation):

\[ H = \begin{pmatrix}
\Delta + \frac{\hbar^2}{2m^e_{ij}} q_i q_j & \hbar (v_1 \cdot q - i v_2 \cdot q) \\
\hbar (v_1 \cdot q + i v_2 \cdot q) & -\Delta - \frac{\hbar^2}{2m^h_{ij}} q_i q_j
\end{pmatrix} \]

- Landau levels:

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

- Diracness:

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

in terms of Dirac mass

\[ m_D = \frac{\Delta}{v_1 \wedge v_2} \]
Relevance of mixed Dirac/Schrödinger fermions

Where to look for them?

• 2D semiconductors with a direct gap
  → 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?
  → electronic transport
**Isospin quantum numbers in graphene**

- Valley isospin $\xi = \pm$: two-fold degeneracy
- Band index $\lambda = \pm$: valence band (VB) or conduction band (CB)
- Chirality $\alpha = \sigma \cdot q/|q| = \pm$ (sublattice spin projected on wave vector)
- (True spin $s = \uparrow, \downarrow$)

**Band index = Valley Isospin \times Chirality**
**Absence of backscattering – Klein tunneling**

Slowly varying obstacle (elastic scatterer): $H_{\text{diff}} = V(r) \mathbb{1}$

$\Rightarrow$ no sublattice-isospin coupling

$\Rightarrow$ no valley coupling + elastic $\Rightarrow$ chirality conservation

Chirality conservation $\Rightarrow$ **absence of backscattering**
Absence of backscattering – Klein tunneling

Slowly varying obstacle (elastic scatterer): $H_{diff} = V(r) \mathbb{1}$

$\Rightarrow$ no sublattice-isospin coupling

$\Rightarrow$ no valley coupling + elastic $\Rightarrow$ chirality conservation

Klein tunneling at a potential barrier vs. qm tunneling
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
Evolution of Diracness at high energy (I)

• Semi-classical treatment of model

\[ \mathcal{H}(q) = \begin{pmatrix} \Delta + \frac{\hbar^2}{2m_0}q^2 & \hbar v_D(q_x - iq_y) \\ \hbar v_D(q_x + iq_y) & -\Delta - \frac{\hbar^2}{2m_0^h}q^2 \end{pmatrix} \]

• 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 \( \Gamma \) and curvature \( \mathcal{A} \)

\[ \Gamma = \int_{C(\epsilon_\lambda)} d\mathbf{q} \cdot \hat{\mathcal{A}}_\lambda(\mathbf{q}) \quad \rightarrow \quad \delta_\lambda = -\frac{\lambda}{\pi \frac{d(\epsilon \Gamma)}{d|\epsilon_\lambda|}} \]
Evolution of Diracness at high energy (II)

• Energy-dependent Diracness [with $M = (m_{e_1}^0 + m_{h_1}^0)/2$]

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

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