2D materials for Spin/Valleytronics
Theoretical Perspective

Stephan Roche ICREA

Pseudomagnetic field
Electron Motion
Spintronics inside!
Spintronics and its industrial/Societal impact

Albert Fert, Peter Grünberg

2007 Physics Nobel Laureates

Magnetic field sensors used to read data in hard disk drives,
Microelectromechanical systems
Minimally invasive surgery

Automotive sensors for fuel handling system,
Anti-skid system, speed control & navigation

\[ MR = \frac{R_{AP} - R_P}{R_P} \]
Data Storage & TMR
Magnetic junctions and MRAM

AEROSPACE
AERONAUTICS
AUTOMOTIVE
RAID SERVERS
FACTORY AUTOMATIZATION
Advanced generation of Spin Transfert Torque MRAM
(proposed by Slonczewski, Berger 1996)

256Mb in production 2018

2016

SAMSUNG In production for 2019
Why Spintronics using 2D Materials?

Proximity effects in 2D Materials-based heterostructures (spin dynamics & relaxation, SHE, weak antilocalization, QSHE)

Generating valley polarized quantum transport (valleytronics)
Spin-based information processing?

Active devices based on Spin manipulation?

- Datta-Das spin transistor
- Spin Hall Effect/QSHE
- Spin torques/pumping

Need for spin information transport on long distance (room T)
Spin injection and detection (ferromagnets/non magnetic materials)

Metals/semiconductors... short spin diffusion length (spin lifetime 0.1-1ns), 1% (or below) of MR signal
What makes graphene attractive

- Ambipolar/tuneable transport
- Linear energy dispersion & Large mobilities (> 100k cm²/V.s at RT, 1M cm²/V.s at 4K)
- Low spin-orbit interaction
- Graphene properties can be tailored by proximity effects

Wang et al., Science (2013)
10 years ago!

N. Tombros, ... Bart J. van Wees
Nature 448, 571-574 (2 August 2007)

"non-local" spin valve geometry + Hanle spin precession measurements

Spin diffusion length $2 \mu m$ (RT)
Spin diffusion length in epitaxial graphene

B. Dluback et al, A. Fert
*Nature Phys. 8,557 (2012)*

2-T magnetoresistance
Spin diffusion length up to $100 \, \mu m (RT)$
Europe has chosen Graphene Flagship as one of only two FET projects, with 1,000 million € over 10 years...

Launch in 2013

“to take graphene and related layered materials from academic laboratories to society, revolutionize multiple industries and create economic growth and new jobs in Europe.”

• 154 partners with in 17 EU countries with an

• Potential applications include:
  – flexible consumer electronics
  – lighter and more energy efficient airplanes
  – optical devices and artificial retinas
  – functional lightweight components
  – advanced batteries
  – spintronics
Experimental partners
Univ. of Groningen [RUG]: Bart van Wees
Univ. of Manchester [UNIMAN]: Irina Grigorieva
Univ. of Aachen [RWTH]: Christoph Stampfer, Bernd Beschoten
Univ. of Basel [UNIBAS]: Christian Schönenerberger
CNRS/Thales [CNRS]: Pierre Seneor and Albert Fert
Chalmers University Technology [CUT]: Saroj Dash
Catalan Inst. Nanoscience & Nanotech [ICN2]: Sergio Valenzuela
NanOSC AB: Johan Åkerman

Theoretical partners:
Catalan Inst. Nanoscience & Nanotech [ICN2]: Stephan Roche
Université Catholique de Louvain [UCL]: Jean Christophe Charlier
University of Regensburg [UREG]: Jaroslav Fabian
Commissariat à l´Energie Atomique [CEA]: Mairbek Chshiev, Xavier Waintal
IMDEA: Paco Guinea
“The global objective of the Graphene Spintronics task force is to establish the ultimate scientific and technological potential of graphene and graphene related materials for spintronics, targeting efficient spin injection, transport and detection but also demonstrating spin gating and spin manipulation in graphene spintronic devices and realizing operational devices for information storage and information processing, by engineering device architecture and material transformations”
Graphene spintronics: the European Flagship perspective

Stephan Roche$^{1,2}$, Johan Åkerman$^{3,4,5}$, Bernd Beschoten$^6$, Jean-Christophe Charlier$^7$, Mairbek Chshiev$^{8,9}$, Saroj Prasad Dash$^{10}$, Bruno Dlubak$^{12}$, Jaroslav Fabian$^{11}$, Albert Fert$^{12}$, Marcos Guimarães$^{13,19}$, Francisco Guinea$^{14,15}$, Irina Grigorieva$^{14}$, Christian Schönberger$^{16}$, Pierre Seneor$^{12}$, Christoph Stampfer$^{17}$, Sergio O Valenzuela$^{1,2}$, Xavier Waintal$^{9,18}$ and Bart van Wees$^{19}$.

2D Mater. 2 (2015) 030202
Graphene/Magnetic insulators

Graphene/EuO and Graphene/Y₃Fe₅O

Spin filtering and exchange splitting Gaps

Exchange splitting (G/YIG) = 40 meV

Yang, Hallal, Waintal, Roche, Chshiev, PRL 110, 046603 (2013)
Hallal et al. 2D materials 4, 025074 (2017)
All-Electrical Spin-FET

Gate control of spin information (switch ON/OFF)

W. Yan, O. Txoperena, R. Llopis, H. Dery, L. E. Hueso & F. Casanova,
*Nature Comm.* 7, 13372 (2016)

A. Dankert & S. P. Dash,
*Nature Comm.* 8, 16093 (2017)
Perpendicular Magnetic Anisotropy in FM/Ox and FM/Graphene interfaces:

Strongly enhanced PMA of Co realized by graphene coating

Layer and orbital resolved contributions unveil the PMA mechanisms

Superlattice structures to obtain Giant PMA

\[ K_{\text{eff}} = \frac{K_s}{t_{\text{Co}}} - E_{\text{demag}} \]

Yang, Coraux/Chshiev et al,
Opportunities “in the valley”

Valley filter and valley valve in graphene

Valleytronics in 2D materials

John R. Schaibley, Hongyi Yu, Genevieve Clark, Pasqual Rivera, Jason S. Ross, Kyle L. Seyler, Wang Yao and Xiaodong Xu

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« Low » Energy Excitations in clean Graphene

No intervalley/spin mixing - (low disorder & SOC)

8-components Matrix

\[
\begin{pmatrix}
0 & p_x - i p_y & 0 & 0 & 0 & 0 & 0 & 0 \\
p_x - i p_y & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -p_x + i p_y & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & p_x - i p_y & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & p_x - i p_y & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -p_x + i p_y & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -p_x + i p_y & 0 \\
\end{pmatrix}
\]

Three internal degrees of freedom
Spin
Valley index
Sublattice pseudospin
Massless Dirac Fermions in 2D graphene

Two valleys \( \rightarrow \) Dirac cones

\[
\mathcal{H}_{K_+} = v_F \hat{\sigma} \cdot \vec{p} = v_F (p_x \sigma_x + p_y \sigma_y)
\]

Pseudo-spinors are eigenstate of the helicity operator

\[
\hat{\mathcal{H}} = \frac{1}{2} \hat{\sigma} \cdot \frac{\vec{p}}{|\vec{p}|}
\]

\[
\Psi_{\vec{p}} = \frac{1}{\sqrt{2}} \begin{pmatrix}
\Psi_{\vec{p}}(A) & 1 \\
0 & 1
\end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix}
se^{i\theta_p/2} \\
e^{-i\theta_p/2}
\end{pmatrix}
\]

"pseudospin" = sublattice index: up (on A) / down (on B) 

\[
\tan \theta_p = \frac{p_y}{p_x}
\]
Transition Metal dichalcogenides (monolayer)

**Broken inversion symmetry**

\[ \mathcal{H} = at(\tau_z k_x \hat{\sigma}_x + k_y \hat{\sigma}_y) + \frac{\Delta}{2} \sigma_z + \lambda_{SO} \tau_z \hat{s}_z \]

D. Xiao et al.
PRL 108, 196802 (2012)

**Massive Dirac Fermion model**
Partially filled d-orbitals (metal)

**Gap** \( \sim 2 \text{ eV} \)

**Spin-Split vbands** \( \sim 150 - 400 \text{ meV} \)

**Valley pseudospin** \( \pm K (\tau = \pm 1) \)

**Spin-valley locking**
Interlinking optics with Valleytronics & Spintronics

Opto-Valleytronic Spin Injection in Monolayer MoS$_2$/Few-Layer Graphene Hybrid Spin Valves

Yunqiu Kelly Luo,† Jinsong Xu,† Tiancong Zhu,† Guanzhong Wu,† Elizabeth J. McCormick,† Wenbo Zhan,† Mahesh R. Neupane,† and Roland K. Kawakami*†,‡

Multifunctional 2D spintronic/valleytronic devices
Why Spintronics using 2D Materials?

Proximity effects in 2D Materials-based heterostructures (spin dynamics & relaxation, SHE, weak antilocalization, QSHE)

Generating valley polarized quantum transport (valleytronics)
Experimental spin lifetime features

Graphene on SiO₂

Suspended Graphene

Epitaxial graphene on SiC

Graphene on BN

charge mobility $\mu \sim 100 - 100.000 \text{cm}^2 \text{V}^{-1} \text{s}^{-1}$

Room temperature

$\tau_s \sim 0.1 - 10 \text{ ns}$

Avsar et al, Nano Lett. 11, 2363 (2011)
Drögeler et al. Nano Lett. 16 (6), 3533 (2016)
Tight-binding Modelling

\[ \mathcal{H} = -\gamma_0 \sum_{ij} c_i^+ c_j + \sum_i V_i c_i^+ c_i + iV_R \sum_{ij} c_i^+ \vec{z} \cdot (\vec{s} \times \vec{d}_{ij}) c_j \]

**Screened Coulomb potential**

**Long range (Gaussian) potential**

\[ V_i = \sum_{\alpha=1}^{N_\alpha} \varepsilon_\alpha \exp\left(-|\vec{r}_\alpha - \vec{r}_i|^2/(2\xi^2)\right) \]

Shaffique Adam et al *Phys. Rev. B* 84, 235421 (2011)

\[ Rashba SOC \]

\[ V_R \sim 20\mu eV \]

Graphene on SiO₂

\[ \tau_{p}^{\text{SiO₂}} / T_\Omega \ll 1 \]

Graphene on hBN

\[ \tau_{p}^{\text{hBN}} / T_\Omega \geq 1 \]

Onsite energy distribution of the π–orbitals with standard deviation for hBN (5meV) & SiO₂ (56meV)
Spin dynamics of propagating wavepacket

\[ |\Psi_{\perp}(0)\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} |\varphi_{RP}\rangle \quad |\Psi(t)\rangle = e^{-i\hat{H}t/\hbar} |\Psi(0)\rangle \]

\[ s_i(t) = |\Psi_i^\dagger(t)|^2 - |\Psi_i(t)|^2 \] (time-dependent)

Local spin density in real space

\[ \langle \Psi(t) | \sigma_z \delta(E - \hat{H}) + \delta(E - \hat{H}) \sigma_z | \Psi(t) \rangle \]

\[ 2 \langle \Psi(t) | \delta(E - \hat{H}) | \Psi(t) \rangle \]

\[ S_z(t) \sim \cos \left( \frac{2\pi t}{T_\Omega} \right) e^{-t/\tau_s} \]
Graphene on **SiO₂**

Electron-hole puddles drive the relaxation

\[ \tau_{p}^{\text{SiO₂}} / T_{Ω} \ll 1 \]

\[ \tau_{S} \sim \frac{1}{n_{i}} \]

\[ \tau_{S}^{\perp} / \tau_{S}^{\parallel} \rightarrow 0.5 \]

**Dyakonov-Perel relaxation mechanism**

Graphene on **hBN**

Electron-hole puddles drive the relaxation

\[ \tau_{p}^{\text{hBN}} / T_{Ω} \geq 1 \]

\[ \tau_{S}(E) \approx 4T_{Ω} \approx 4 \frac{\pi \hbar}{\lambda_{R}} \]

\[ \tau_{S} \approx 1 - 10 \text{ ns} \]

(for \( \lambda_{R} \rightarrow 5 \mu \text{eV} \))

**Dephasing relaxation mechanism**
Pseudospin-driven spin relaxation mechanism in graphene

Dinh Van Tuan¹,², Frank Ortmann¹,³,⁴, David Soriano¹, Sergio O. Valenzuela¹,⁵ and Stephan Roche¹,⁵*
Hybrid devices of graphene and other 2D materials

Martin Gmitra and Jaroslav Fabian
Realistic Model of Graphene/TMDC
with interface disorder

DFT-TB model from
M. Gmitra, D. Kochan, P. Högl, & J. Fabian
PRB 93, 155104 (2016)

\[ H_0 = -t \sum_{\langle i,j \rangle} \left( a_i^\dagger b_j + b_i^\dagger a_j \right) + \frac{\Delta}{2} \sum_i \left( a_i^\dagger a_i - b_i^\dagger b_i \right) \]

\[ H_{so} = \frac{2i}{3} \sum_{\langle i,j \rangle,\sigma} \left( \hat{s} \times \mathbf{d}_{i,j} \right)_{z,\sigma,\bar{\sigma}} \lambda_R a_{i,\sigma}^\dagger b_{j,\bar{\sigma}} + h.c \]

\[ + \frac{2i}{3} \sum_{\langle \{i,j\} \rangle,\sigma} \left( \hat{s} \times \mathbf{D}_{i,j} \right)_{z,\sigma,\bar{\sigma}} \left( \lambda_{PIA}^{(A)} a_{i,\sigma}^\dagger a_{j,\bar{\sigma}} + \lambda_{PIA}^{(B)} b_{i,\sigma}^\dagger b_{j,\bar{\sigma}} \right) \]

\[ + \frac{i}{3\sqrt{3}} \sum_{\langle \{i,j\} \rangle,\sigma} \nu_{i,j} \left( \hat{s}_z \right)_{\sigma,\sigma} \left( \lambda_I^{(A)} a_{i,\sigma}^\dagger a_{j,\sigma} - \lambda_I^{(B)} b_{i,\sigma}^\dagger b_{j,\sigma} \right) \]

Random distribution of \( n_p \) electron-hole puddles
S. Adam et al. PRB 84, 235421 (2011)

\[ U_n(r) = u_n \exp \left( -\frac{(r-R_n)^2}{2\xi_p^2} \right) \]

\[ \xi_p = \sqrt{3}a \quad \text{Puddle range} \]

\[ u_n \in [-U_p, U_p] \quad R_n \text{ is the position of the center of the Gaussian pot.} \]
Spin dynamics (Graphene/TMDC+ el-h puddles)

Intravalley scattering

Strong valley mixing

\[ S_\alpha \simeq \exp\left(-\frac{t}{\tau_{s,\alpha}}\right) \cos(\omega_z t) \]
High-quality Graphene/TMDC

Absence of valley mixing (Dyakonov-Perel)

\[
\frac{\tau_{S, \perp}}{\tau_{S, \parallel}} = 1/2
\]

Weak anisotropy as in conventional Rashba disordered systems

Dyakonov-Perel regime (single valley approximation)
Giant spin lifetimes anisotropy in low quality Graphene/TMDs (strong valley mixing)

Symbols:
- Effective spin-orbit fields arising from the SOC terms
- Equation of motion of density matrix

\[ H = H_0 + \frac{1}{2} \hbar \vec{\omega}(t) \cdot \vec{s} \]

\[ \frac{d\rho_I(t)}{dt} = \left( \frac{1}{i\hbar} \right)^2 \int_0^{t \gg \tau_c} [V_I(t), [V_I(t'), \rho_I(t)]] dt', \]

\[ V_I(t) = \frac{1}{2} \hbar \vec{\omega}(t) \cdot \vec{s}_I(t) \text{ and } \vec{s}_I(t) = e^{iH_0t/\hbar} \vec{s} e^{-iH_0t/\hbar} \]

\[ \frac{\tau_{s, \perp}}{\tau_{s, \parallel}} = 10 - 100 \]

Lifetime values
\[ \tau_{s, \perp} \in [10, 1000] \text{ps} \]
\[ \tau_{s, \parallel} \in [1, 10] \text{ps} \]

Dyakonov-Perel mechanism
\[ \tau_{s, \perp} \& \tau_{s, \parallel} \sim \frac{1}{n_p} \]

\[ \omega_\alpha(t)\omega_\beta(t') = \delta_{\alpha\beta} \omega_\alpha^2 e^{-|t-t'|/\tau_{c,\alpha}} \]
Theoretical prediction confirmed !!!

AW. Cummings, J.H. García, J. Fabian, S. Roche,

Large Proximity-Induced Spin Lifetime Anisotropy in Transition-Metal Dichalcogenide/Graphene Heterostructures
Talieh S. Ghiasi, Josep Ingla-Aynés, Alexey A. Kaverzin, and Bart J. van Wees
Physics of Nanodevices, Zernike Institute for Advanced Materials, University of Groningen, Groningen, 9747 AG, The Netherlands

Strongly anisotropic spin relaxation in graphene-transition metal dichalcogenide heterostructures at room temperature
L. Antonio Benítez, Juan F. Sierra, Williams Savero Torres, Aloís Arrighi, Frédéric Bonell, Marius V. Costache and Sergio O. Valenzuela

GRAPHENE FLAGSHIP
Tunable spin lifetimes in Graphene/Bi$_2$Se$_3$

K. Song  D. Soriano, A. W. Cummings, R. Robles, P. Ordejón, and S. Roche
Nano Lett. Article ASAP- DOI: 10.1021/acs.nanolett.7b05482
SOC-proximity effect & Weak antilocalization


From the fits the scaling of spin scattering times versus Momentum scattering time yields
DYAKONOV PEREL mechanism

Spin Hall Effect

M.I. Dyakonov and V.I. Perel (1971)

Appearance of spin accumulation on the lateral surfaces of an electric current-carrying sample (signs of the spin directions being opposite on the opposing boundaries)

Strong spin-orbit coupling materials ("effective magnetic field")

Direct electronic measurement of the spin Hall effect

Graphene acquires spin–orbit coupling up to 17 meV, three orders of magnitude higher than its intrinsic value, without modifying the structure of the graphene. The proximity SOC leads to the spin Hall effect even at room temperature, and opens the door to spin field effect transistors.

\[ \tau_s \approx 5 - 10 \text{ps} \]
Localization effects for graphene/WS$_2$ + el-h puddles

Scaling theory of localization

$$\sigma_{xx}(\varepsilon_F) = \sigma_{sc}(\varepsilon_F) + \delta\sigma(\varepsilon_F)$$

$$\tau_p = \frac{\sigma_{sc}(\varepsilon_F)}{v_F^2 \rho(\varepsilon_F)}$$

Case of strong scatterers (puddles) and large intervalley scattering

Weak localization
Localization effects for graphene/WS2 + el-h puddles

Scaling theory of localization

\[ \sigma_{xx}(\varepsilon_F) = \sigma_{sc}(\varepsilon_F) + \delta\sigma(\varepsilon_F) \]

\[ \delta\sigma = +\frac{2e^2}{\pi\hbar} \log\left(\frac{L}{\ell_e}\right) \]

Weak Antilocalization

Case of strong scatterers (puddles) and large intervalley scattering

SOC switch ON

No valley mixing

Spin Hall Effect for Graphene /TMDC heterostructures

**Intrinsic mechanism**

Driven by the translational invariant spin-orbit coupling fields (effective B fields)
Rashba+ intrinsic + Pseudospin Inversion
Asymmetry terms...

**Extrinsic mechanism**

If impurities introduce local changes of SOC here  **electron-hole puddles** (disorder)
Spin Hall Kubo conductivity in clean graphene/TMDC interfaces

\[ \theta_{SH} \]

Spin Hall angle measures the efficiency of converting charge current to spin current

\[ \theta_{SH} = \frac{|J^z_s|}{|J^c|} \]

Dissipative SHE

\[ \theta_{SH} = \frac{\sigma^z_{xy}}{\sigma_{xx}} \]
Spin Hall Kubo conductivity

in large scale disordered graphene models

\[ \sigma_{\text{sH}} = \frac{\hbar e}{\Omega} \sum_{m,n} \frac{f(E_m) - f(E_n)}{E_m - E_n} \text{Im}[\langle m | J^z_x | n \rangle \langle n | \nu_y | m \rangle \frac{E_m - E_n + i\eta}{E_m - E_n + i\eta}], \]

\[ J^z_x = \frac{\hbar}{4} \{ \sigma_z, \nu_x \} \]

is the spin current operator

dc-Kubo conductivity

real-space formalism

\[ \sigma_{\text{sH}} = \frac{e\hbar}{\Omega} \int dudv \frac{f(u) - f(v)}{(u - v)^2 + \eta^2} j(u, v), \]

\[ j(u, v) = \sum_{m,n} \text{Im}[\langle m | J^z_x | n \rangle \langle n | \nu_y | m \rangle \delta(u - E_m)\delta(v - E_n)] \]

\[ = \sum_{m,n} (4\mu_{mn}g_m g_n T_m(\hat{u})T_n(\hat{v}))/((1 + \delta_{m,0})(1 + \delta_{n,0})\pi^2 \sqrt{(1 - \hat{u}^2)(1 - \hat{v}^2)}), \]

\[ \mu_{mn} = \frac{4}{\Delta E^2} \text{Im}[\text{Tr}[J^z_x T_n(\hat{H})\nu_y T_m(\hat{H})]] \]

The trace in \( \mu_{mn} \) is computed by the average on a small number \( R \ll N \) of random phase vectors \( \varphi \)

\[ \sigma_{xx} = \frac{2\hbar e^2}{\pi \Omega} \sum_{m,n=0}^{M} \text{Im}[g_m(\epsilon + i\eta)] \text{Im}[g_n(\epsilon + i\eta)] \mu_{mn} \]
Spin Hall Kubo conductivity in clean graphene/TMDC interfaces

\[ \theta_{SH} \]

measures the efficiency of converting charge current to spin current

\[ \theta_{SH} = \frac{|J^z_s|}{|J^z_c|} \]

Dissipative SHE

\[ \theta_{SH} = \frac{\sigma^z_{xy}}{\sigma_{xx}} \]

Clean case: “intrinsic SHE”

WS\textsubscript{2} leads to larger Spin Hall conductivity (larger SHA)
Spin Hall Effect
in disordered graphene/TMDC interfaces

\[ \theta_{SH}(\%) \approx 4\% \]

\[ \theta_{SH}(\%) \ll 1\% \]
Weak antilocalization vs Spin Hall Effect

\[ \frac{\tau_{S, \perp}}{\tau_{S, \parallel}} = 10 - 100 \]

\[ \frac{\tau_{S, \perp}}{\tau_{S, \parallel}} = \frac{1}{2} \]
OUTLINE

Why Spintronics using 2D Materials?

Proximity effects in 2D Materials-based heterostructures (spin dynamics & relaxation, SHE, weak antilocalization, QSHE)

Generating valley polarized quantum transport (valleytronics)
Strained superlattices
Gap opening & QHE

\[ \mathbf{B}_{\text{strain}} = \nabla \times \mathbf{A} \]

The strain-induced, pseudomagnetic field (idem for gauge-field vector potential) **has opposite signs for graphene’s two valleys \( K \) and \( K' \) (no TRS breaking)**

Distribution of strain (triangular symmetry) results in a **strong uniform pseudomagnetic field**

Strain of 10%
\[ B_{\text{field}} = 40 \text{ Tesla} \]
Lattice deformation strain & pseudomagnetic fields


Signature of the pseudomagnetic field is a local sublattice symmetry breaking observable as a redistribution of the local density of states

Engineering strain fields in graphene

Strain Superlattices in graphene induced by corrugated substrates
A. Reserbat-Planteay et al, 
Nano Lett. 14 (9), 5044 (2014)

Evolution of graphene Moiré blisters towards geometrically well-defined graphene nanobubbles
Jiong Lu, A.H. Castro Neto & Kian Ping Loh 
Nature Communications 3, 823 (2012)
Pseudomagnetic fields for an array of nanobubbles

DoS of a strain array (blue) with local $B_s=450$ Tesla (dashed : unstrained) (red: inner part of the strained region)

$E_n = \hbar \omega^{\text{Dirac}} \text{sgn}(n) \sqrt{|n|}$

$\omega^{\text{Dirac}} = v_F \sqrt{\frac{2eB}{\hbar c}}$

M. Settnes, J.H. Garcia, S. Roche
2D Mater. 4, 031006 (2017)

$\pm \vec{A}_S$ Valley-dependent strain-induced gauge

$\vec{A}_S \propto (\epsilon_{xx} - \epsilon_{yy}, -2\epsilon_{xy})$ strain tensor - triaxial deformation-

M. Settnes et al. 2D Mater. 3, 034005 (2016)

Real magnetic field
$\mathbf{B}_M = \nabla \times \mathbf{A}$

Pseudomagnetic field
$\mathbf{B}_S = \nabla \times \mathbf{A}_S$

Valley $K'$
Total effective field $=2B_0$

Valley $K$
Total effective field $=0$
Charge and valley Hall Kubo conductivity

\[ \sigma_{\alpha\beta} = \frac{i e^2 \hbar}{\Omega} \int_{-\infty}^{\infty} d\epsilon f(\epsilon) \text{Tr} \left[ \nu_\alpha \delta(\epsilon - H) \nu_\beta \frac{dG^r(\epsilon)}{d\epsilon} \right. \
- \left. \nu_\alpha \frac{dG^a(\epsilon)}{d\epsilon} \nu_\beta \delta(\epsilon - H) \right], \quad \nu_\beta \equiv P_{K'} \nu_\beta P_{K'} - P_{K} \nu_\beta P_{K}, \]

\[ P_{K} (P_{K'}) \text{ is the valley projection operator} \]

Valley Hall effect

But valley Hall conductivities are NOT observables
Charge and valley Hall Kubo conductivity

Total charge Hall current \( \sigma_{xy} = \sigma_{xy}^{K'} \neq 0 \)

Valley polarization \( \zeta = (\sigma_{xx}^{K} - \sigma_{xx}^{K'}) / (\sigma_{xx}^{K} + \sigma_{xx}^{K'}) \approx 1 \)

Robust with respect to disorder

M. Settnes, J.H. Garcia, S. Roche 2D Mater. 4, 031006 (2017)
Valleytronics and Valley currents

Recent claims of VHE measurements in Graphene/hBN in non-local transport geometries

(large non-local resistance at the Dirac point)

Gorbachev et al. Science 346, 448 (2014)

Gapped Dirac fermions + electric field
An anomalous perpendicular velocity is generated by the “Berry curvature” Valley Hall effect

\[ \mathbf{v} = \frac{1}{\hbar} \frac{\partial \varepsilon_{nk}}{\partial \mathbf{k}} - \partial_t \mathbf{k} \times \Omega_{nk} \]
Valleytronics and Valley currents?

Problems!!

Semiclassical argument of gap-induced Berry’s curvature is not enough for generating topologically protected edge states.


Exact calculations of bulk transport coefficients (Kubo) of non-local resistance (multiterminal Landauer-Büttiker)

\[ R_{NL} \propto (\sigma_{xy}^v)^2 \rho_{xx}^3 \]

Gapped G/hBN leads to quantized valley Hall conductivity, and zero \( R_{NL} \) + disorder broadening invalidates the formula
Origin of nonlocal resistance in multiterminal G/hBN heterostructures

J. M. Marmolejo-Tejada et al
(PRL, arXiv:1706.09361)
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Theoretical & Computational Nanoscience

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Marc Vila (PhD la Caixa – 10/2016)
Bruna Gabrielly (PhD 09/2017)
And now dancing with the stars...
In Memoriam