‘PseudoSpintronics’

Electronic properties and quantum transport in graphene and graphitic bilayers

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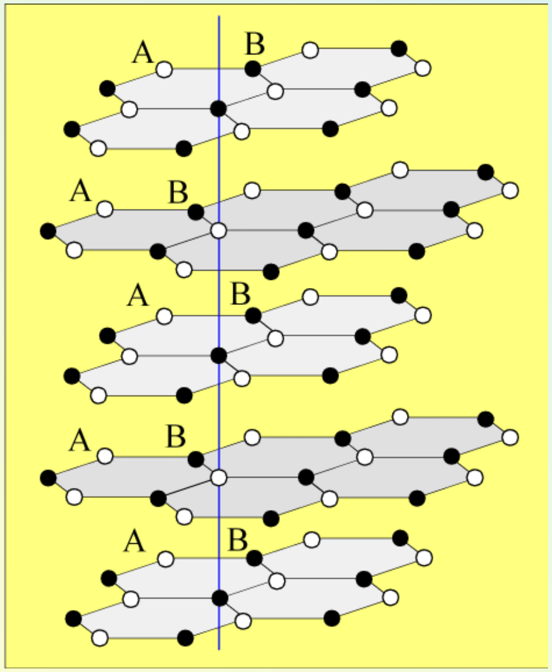
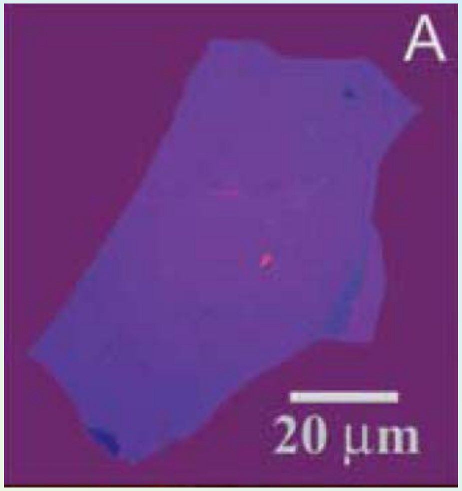
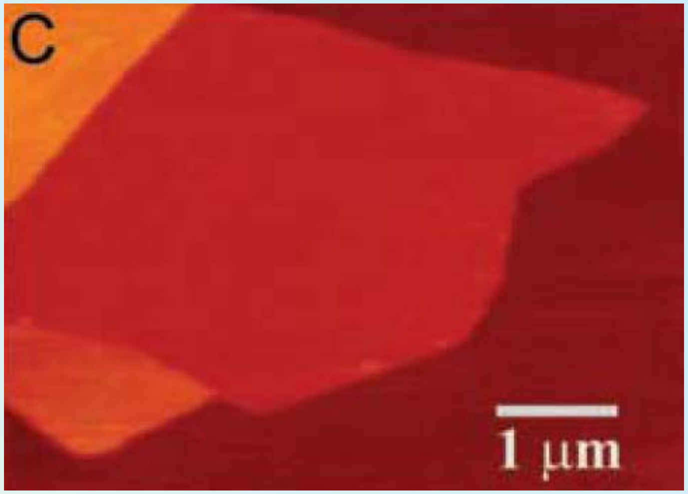
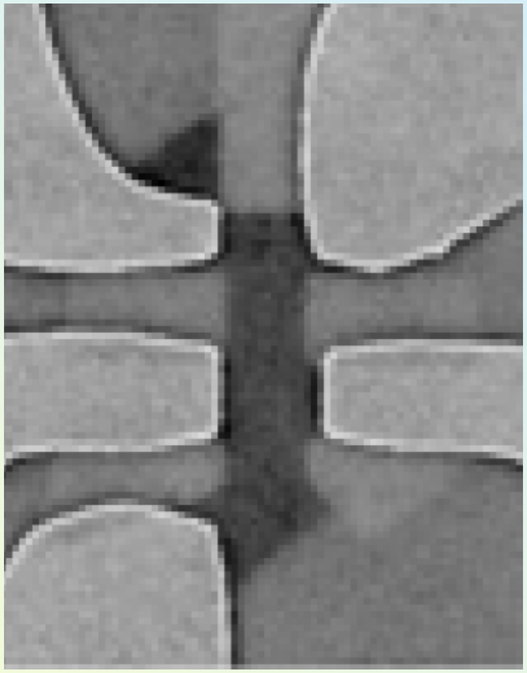
Ultra-thin graphitic films







K. Novoselov et al,
Science 306, 666 (2004)

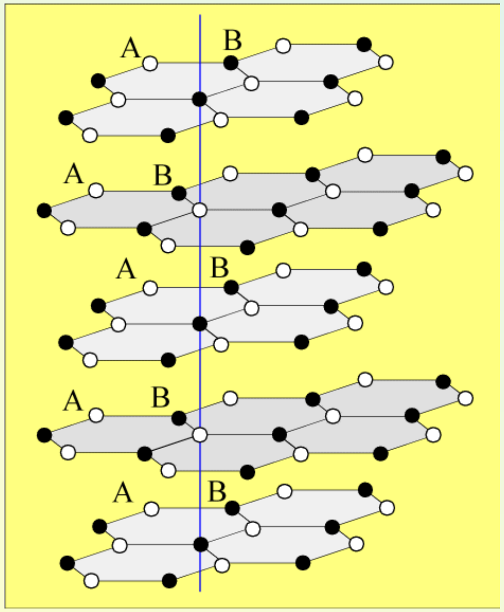


from flakes to micro-devices
(Manchester and Columbia NY)

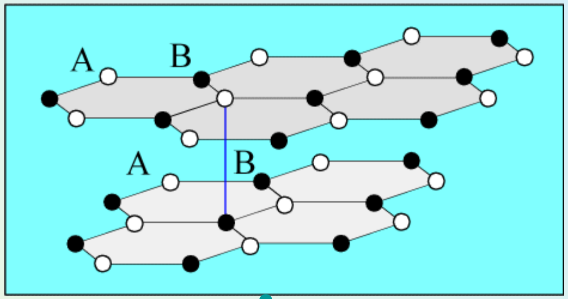
K. Novoselov et al, Nature 438, 197 (2005)
Y. Zhang et al, Phys. Rev. Lett. 94, 176803 (2005)
Y. Zhang et al, Nature 438, 201 (2005)
K. Novoselov et al, Nature Physics 2, 177 (2006)

Content

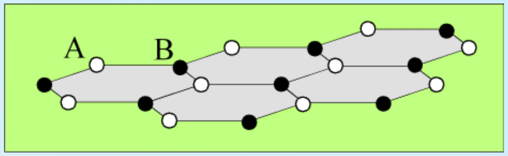
Graphite



Bilayer



Monolayer (graphene)

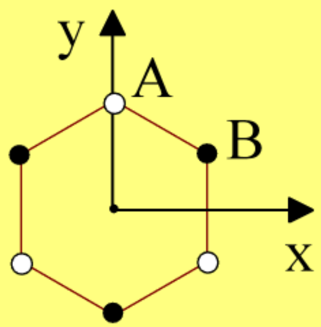


1. **Tight-binding-model analysis showing that electrons (holes) in these materials are chiral and have the Berry phase *J*π**
2. **Transport properties of chiral 2D electrons**
3. **Pseudospin, Berry phase, inter-valley scattering and weak localisation in graphene.**
4. **Quantum Hall effect in monolayers (graphene) and bilayers**

Electronic dispersion of a monolayer

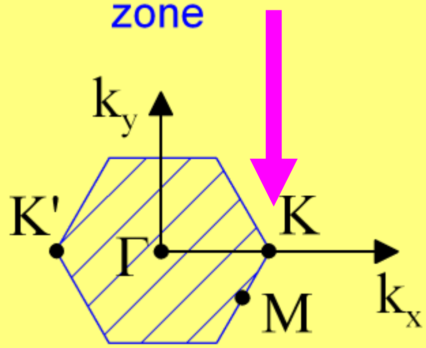
Saito *et al*, "Physical Properties of Carbon Nanotubes" (Imperial College Press, London, 1998)

Symmetrical unit cell

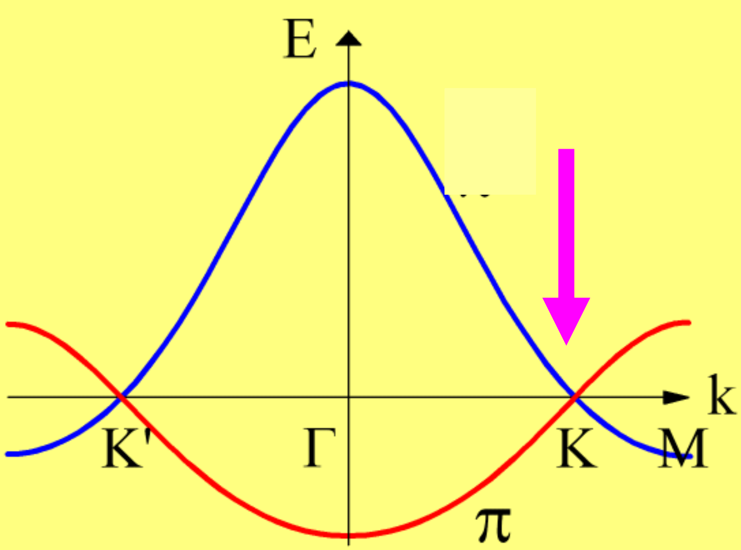


Two non-equivalent carbon positions

Brillouin zone



Two non-equivalent K-points



Two bands: no energy gap at the K-points

Tight binding model of a monolayer

J.Slonczewski and P.Weiss,
Phys. Rev. 109, 272 (1958)

Bloch function

$$\Phi_j(\mathbf{k},\mathbf{r}) = \frac{1}{\sqrt{N}}\sum_{\mathbf{R}_j}^{N} e^{i\mathbf{k}.\mathbf{R}_j}\,\phi_j(\mathbf{r}-\mathbf{R}_j)$$

sum over N atomic positions

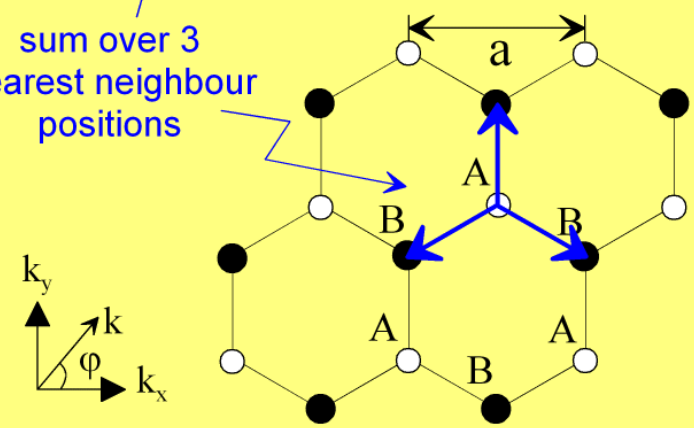
j^{th} atomic orbital: j = A or B

Transfer integral on a hexagonal lattice

$$\mathcal{H}_{AB} = \langle\Phi_A|H|\Phi_B\rangle$$

$$\mathcal{H}_{AB} = \frac{1}{N}\sum_{\mathbf{R}_A}^{N}\sum_{\mathbf{R}_B}^{N} e^{i\mathbf{k}.(\mathbf{R}_B-\mathbf{R}_A)}\underbrace{\langle\phi_A(\mathbf{r}-\mathbf{R}_A)|H|\phi_B(\mathbf{r}-\mathbf{R}_B)\rangle}_{\gamma_0}$$

sum over 3 nearest neighbour positions



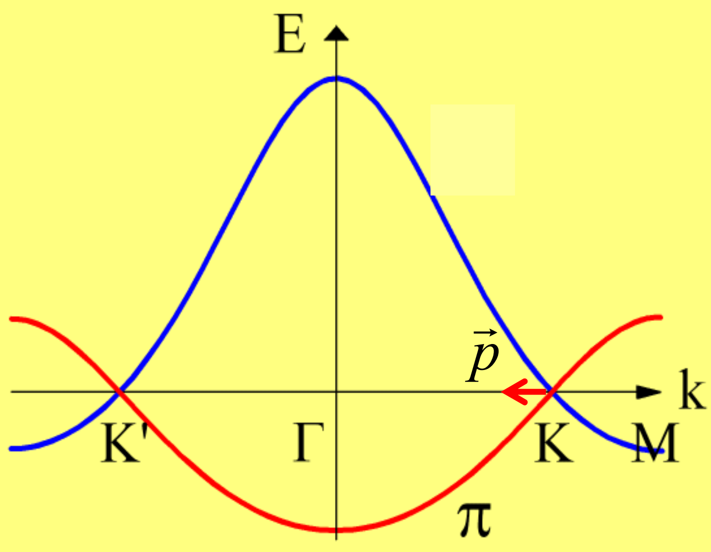
Dirac Hamiltonian of a monolayer

written in a 2 component basis of A and B sites

B to A hopping given by $\pi^{+} = p_x - ip_y$

$$H = v\xi \begin{pmatrix} 0 & \pi^{+} \\ \pi & 0 \end{pmatrix} = v\xi(\sigma_x p_x + \sigma_y p_y)$$

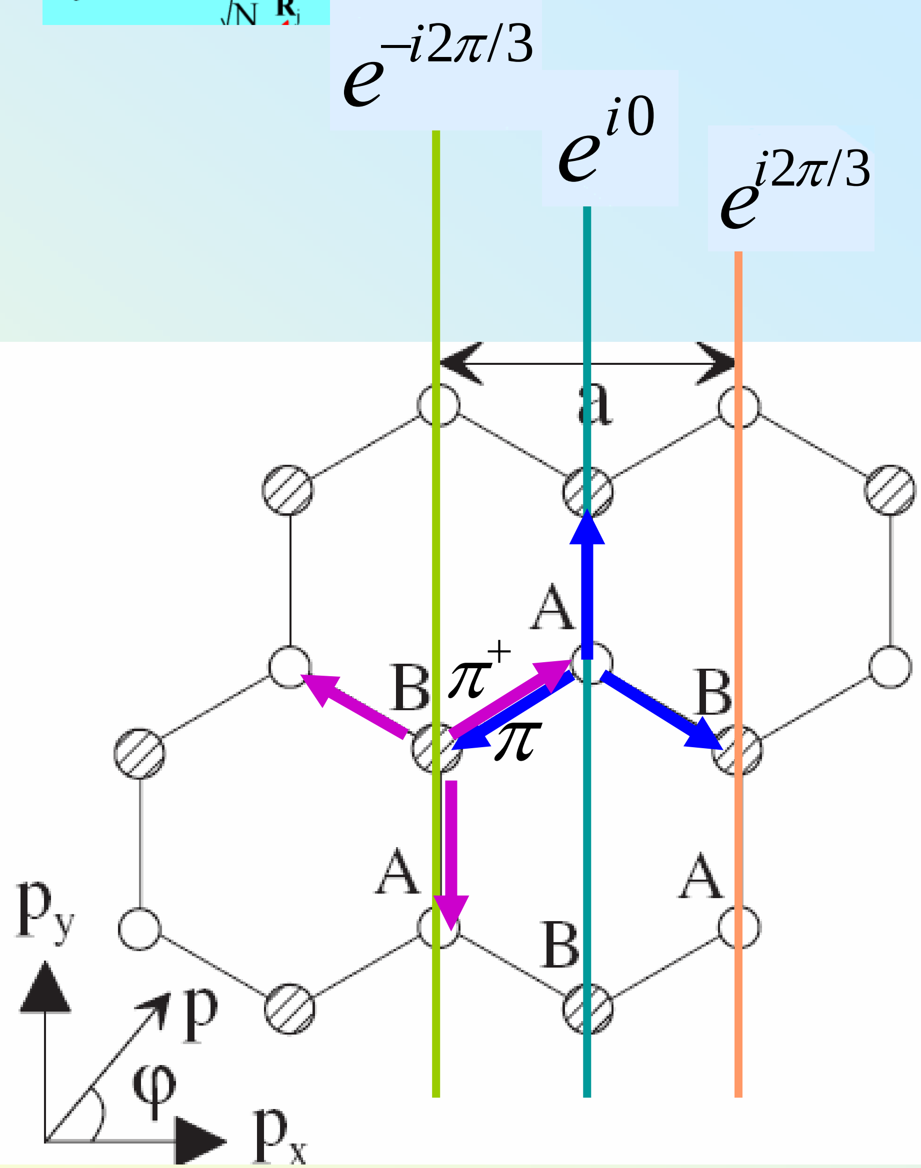
A to B hopping given by $\pi = p_x + ip_y$



Two bands: no energy gap at the K-points

$$\sum_{\mathbf{R}_B}^{N} e^{i\mathbf{k}.(\mathbf{R}_B - \mathbf{R}_A)} \underbrace{\langle \phi_A(\mathbf{r}-\mathbf{R}_A)|H|\phi_B(\mathbf{r}-\mathbf{R}_B)\rangle}_{\gamma_0}$$

$$\Phi_j(\mathbf{k}, \mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}_j}^{N} e^{i\mathbf{k}.\mathbf{R}_j} \phi_j(\mathbf{r}-\mathbf{R}_j)$$



Bloch function amplitudes on the AB sites ('pseudospin') mimic spin components of a relativistic Dirac fermion.

$$\pi = p_x + ip_y = pe^{i\varphi}$$

$$\pi^+ = p_x - ip_y = pe^{-i\varphi}$$

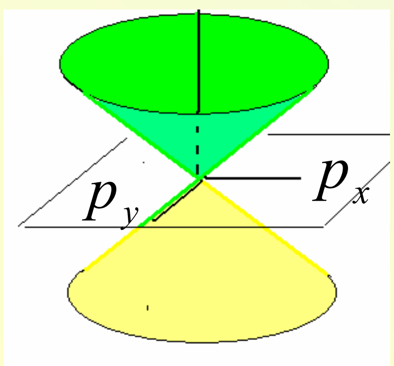
$$\psi = \begin{pmatrix} \varphi_{(A)} \\ \varphi_{(B)} \end{pmatrix}$$

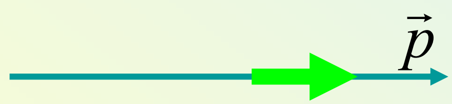
$$H_1 = v \begin{pmatrix} 0 & \pi^+ \\ \pi & 0 \end{pmatrix} = v\vec{\sigma} \cdot \vec{p} = vp\ \vec{\sigma} \cdot \vec{n}$$

Chiral electrons

pseudospin direction is linked to the axis determined by the electron momentum.

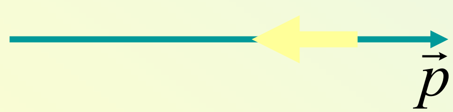
$$\varepsilon = vp$$





For conduction band electrons,

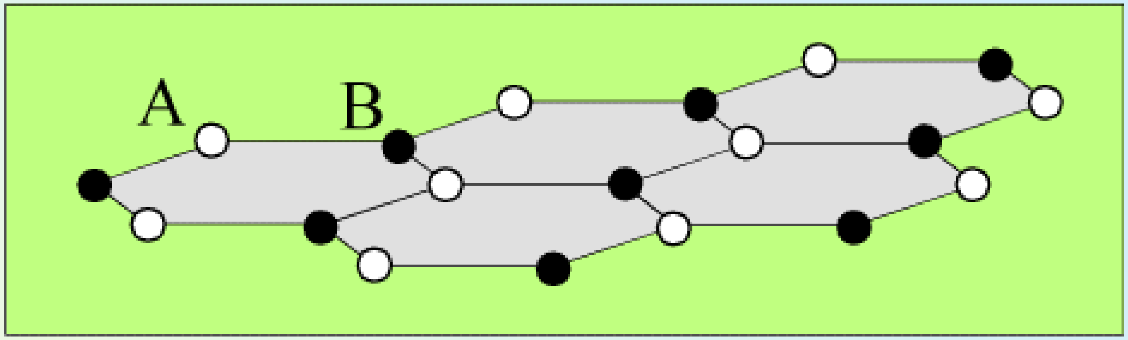
$$\vec{\sigma} \cdot \vec{n} = 1$$



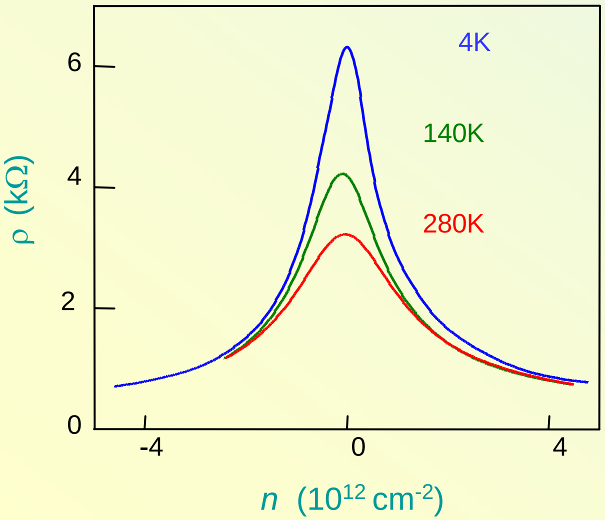
$$\vec{\sigma} \cdot \vec{n} = -1$$

Valence band ('holes')

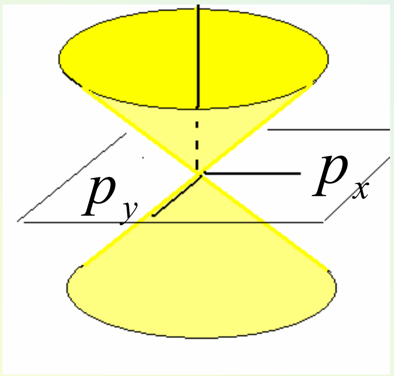
Monolayer (graphene)

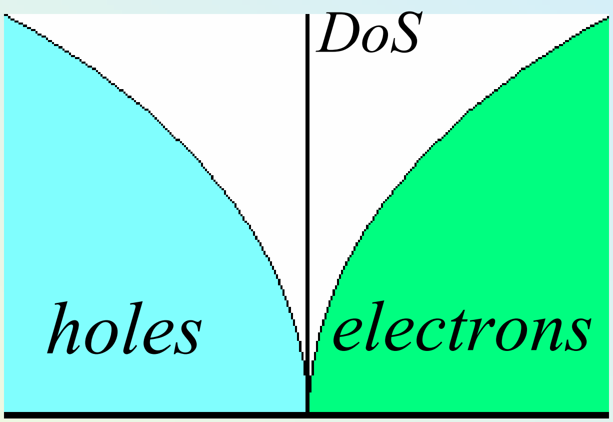


Two dimensional zero-gap semiconductor with Dirac spectrum of electrons



$|\varepsilon| = vp$

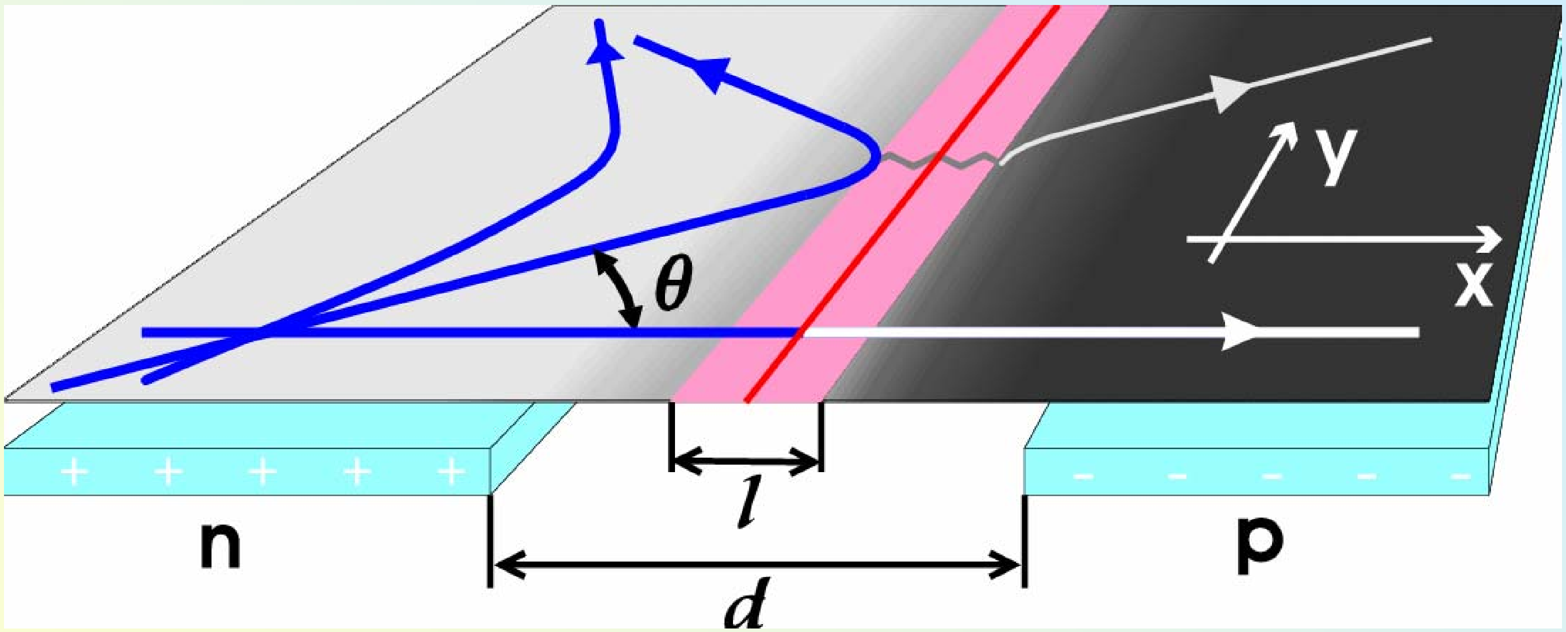




$n_{carriers} \propto V_{gate}$

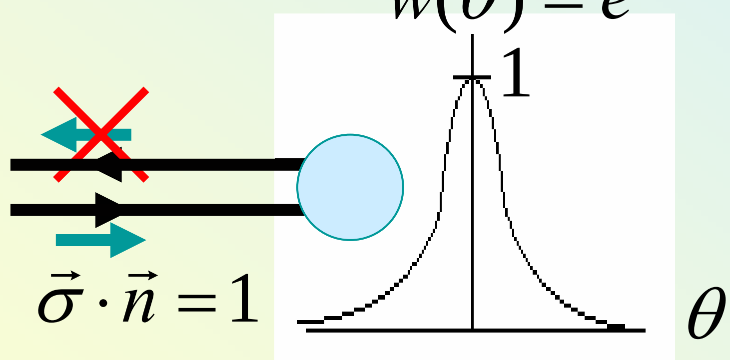
K. Novoselov et al., Science 306, 666 (2004)

Suppressed backscattering of chiral quasiparticles from a potential step leads to a selective transmission properties of an *n-p* junction



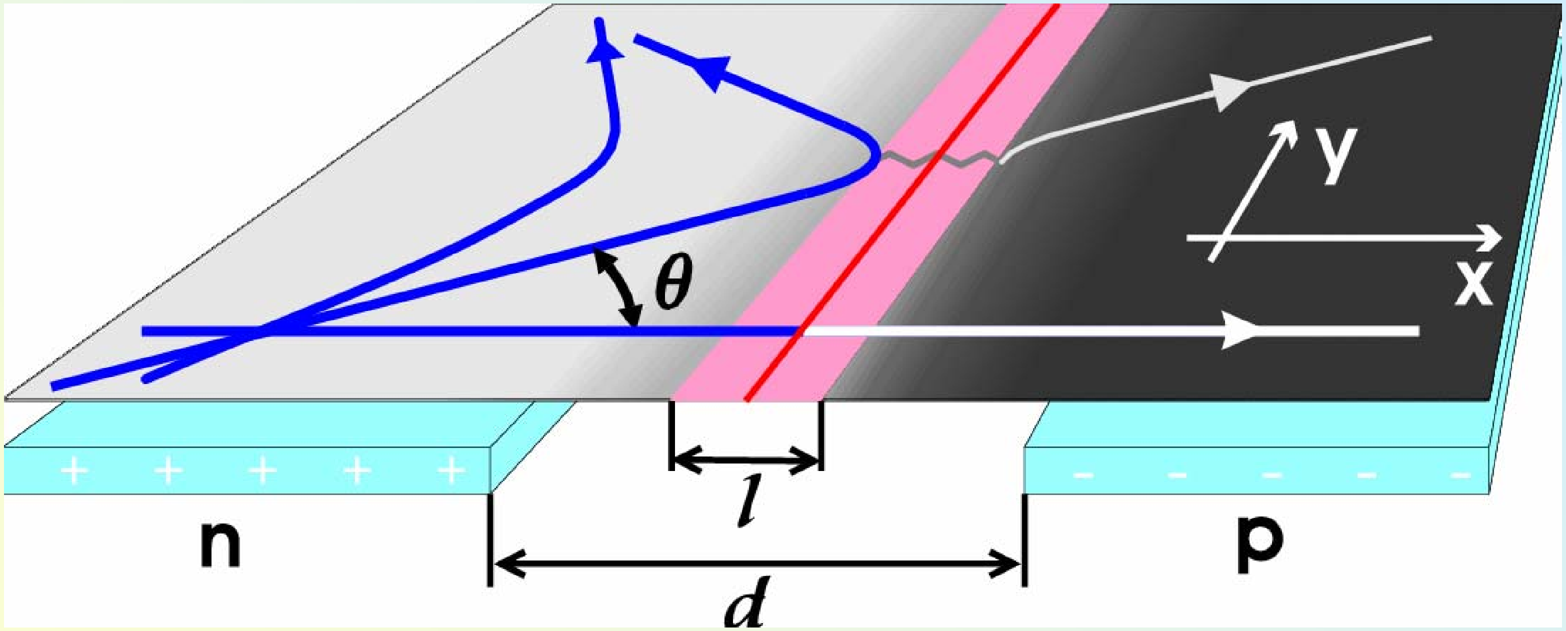
Due to the pseudospin conservation, electrostatic potential cannot scatter a chiral fermion in a backward direction.

$$w(\theta) = e^{-\pi d k_F \sin^2 \theta}$$



T.Ando, T.Nakanishi, R.Saito,
J. Phys. Soc. Japan 67, 2857 (1998)
V.Cheianov, V.Fal'ko, cond-mat/0603624

Suppressed backscattering of chiral quasiparticles from a potential step leads to a selective transmission properties of an *n-p* junction



Due to selective transmission of electrons with a small incidence angle, an *n-p* junction in graphene would display a finite conductance per unit length and a characteristic Fano factor in the shot noise

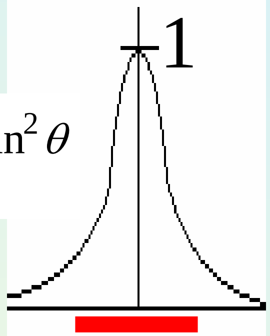
$$g_{np} = \frac{2e^2}{\pi h}\sqrt{\frac{k_F}{d}}$$

$$\langle I \cdot I \rangle = \left(1-\sqrt{\tfrac{1}{2}}\right)\ eI$$

V.Cheianov, V.Fal'ko, cond-mat/0603624

selective transmission in an *n-p* junction

$$w(\theta) = e^{-\pi k_F d \sin^2\theta}$$



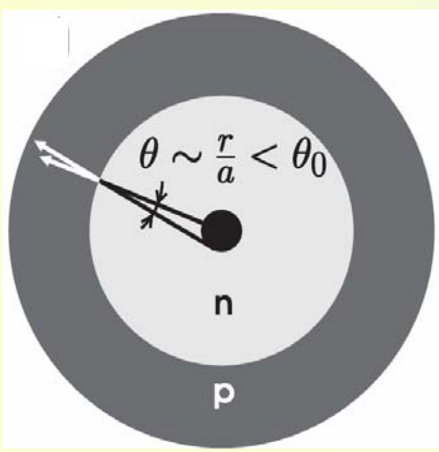
$$|\theta| < \theta_0 = \sqrt{\pi k_F d}$$

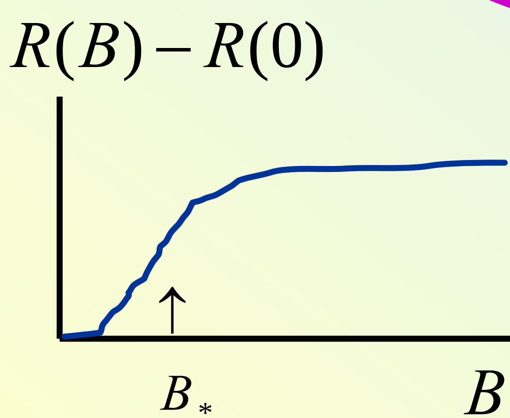
$$\theta' \approx \frac{r}{r_c(B_*)} = \theta_0$$

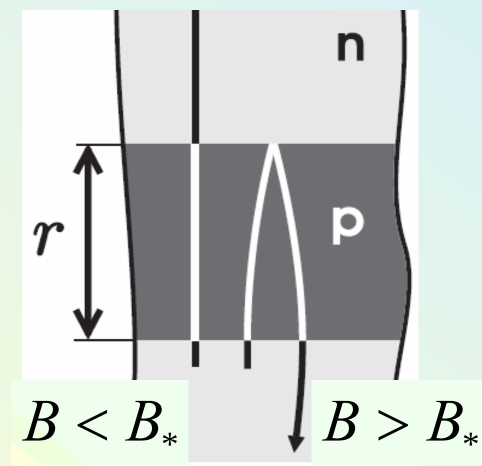
weak-field magnetoresitance of ballistic *n-p* junctions

$$R(B) = R_{cont} + \frac{2\pi a}{g_{np}} f\left(\frac{B}{B_*}\right)$$

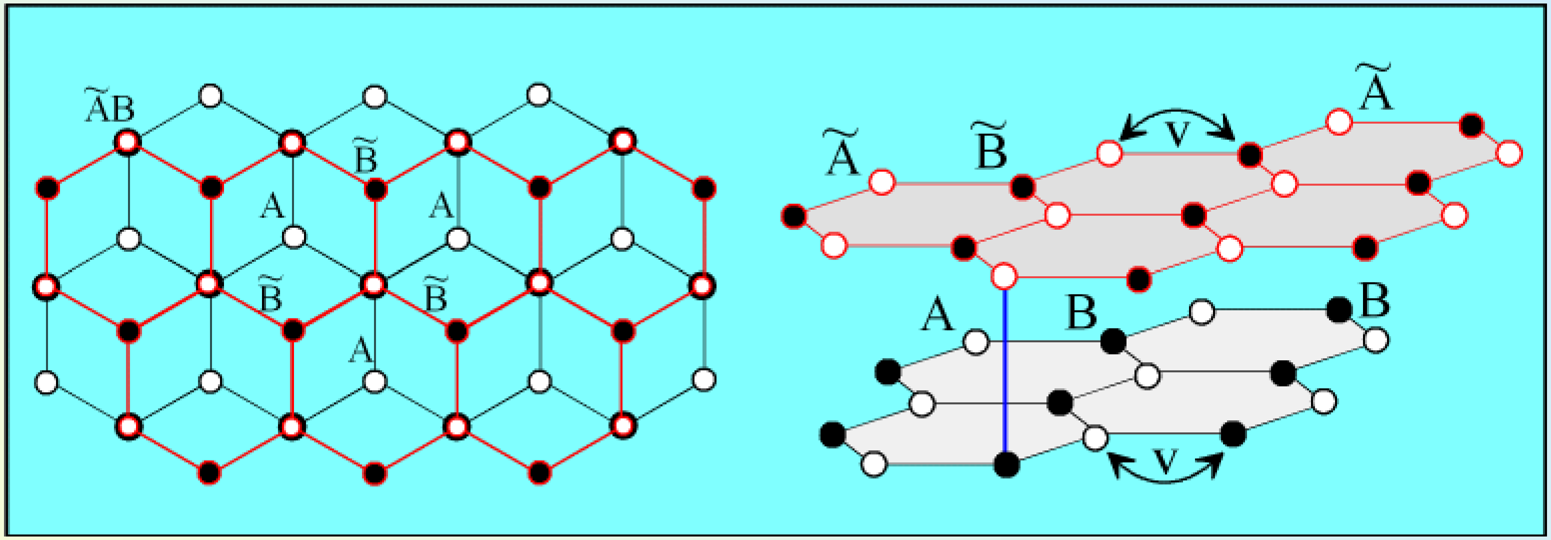
$$g_{npn} = \frac{g_{np}}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{dz}{e^{z^2} + e^{(z+B/B_*)^2} - 1}$$







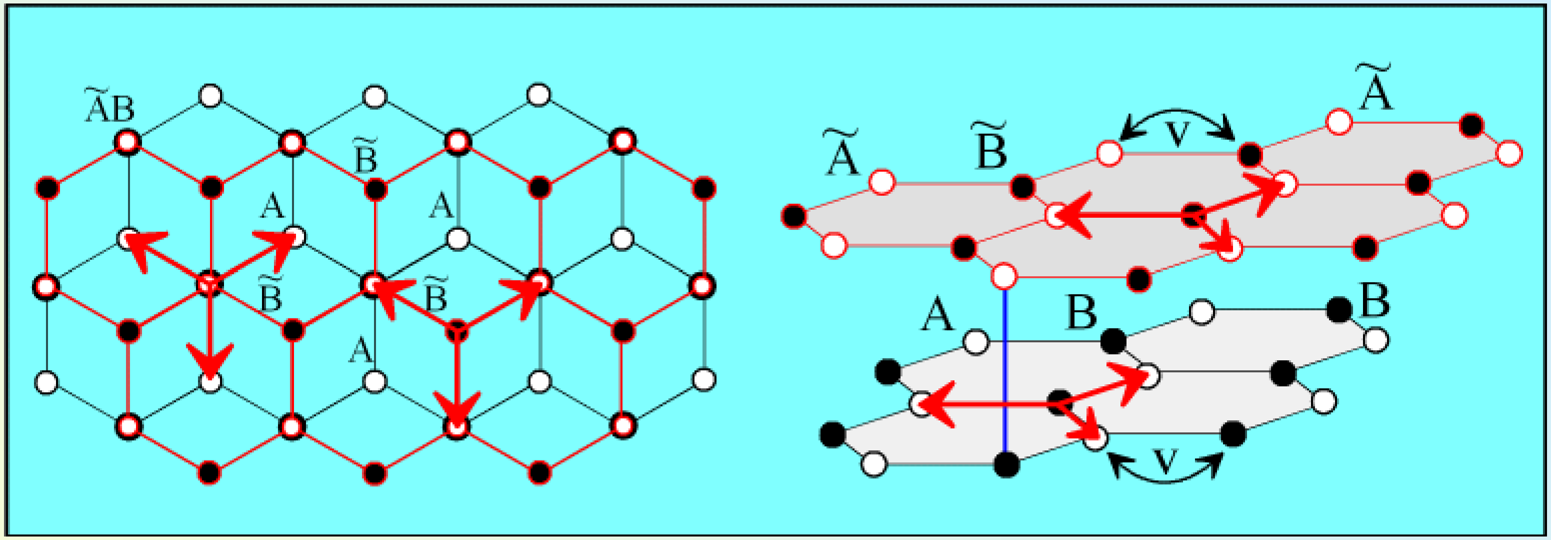
Bilayer [Bernal (AB) stacking]



4 atoms
per unit cell

$$\mathcal{H}=\begin{array}{c} \begin{array}{cccc} A & \tilde{B} & \tilde{A} & B \end{array} \\ \left(\begin{array}{cccc} & & & \\ & & & \\ & & & \\ & & & \end{array}\right) \end{array} \begin{array}{c} A \\ \tilde{B} \\ \tilde{A} \\ B \end{array}$$

Bilayer [Bernal (AB) stacking]

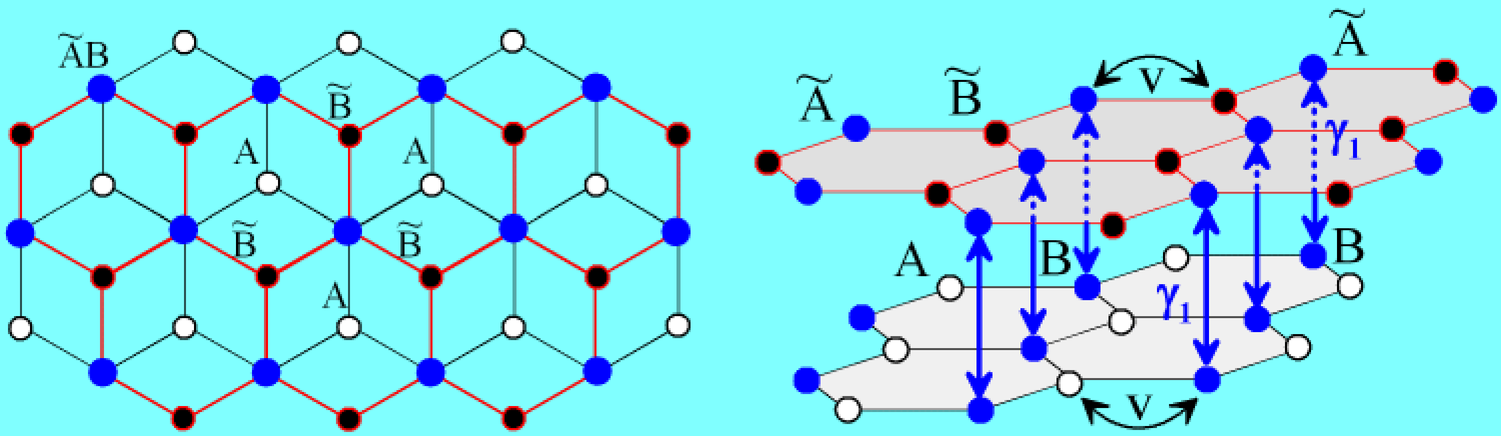


(B to A) and ($\tilde{B}$ to $\tilde{A}$) hopping given by $\pi^{+} = p_x - ip_y$

$$
H = \begin{array}{c} \\ \\ \\ \\ \end{array}
\begin{array}{cccc}
A & \tilde{B} & \tilde{A} & B \\
\end{array}
$$

$$
H = \left(\begin{array}{cccc}
 & & & v\pi^{+} \\
 & & v\pi & \\
 & v\pi^{+} & & \\
v\pi & & &
\end{array}\right)
\begin{array}{c} A \\ \tilde{B} \\ \tilde{A} \\ B \end{array}
$$

Bilayer [Bernal (AB) stacking]



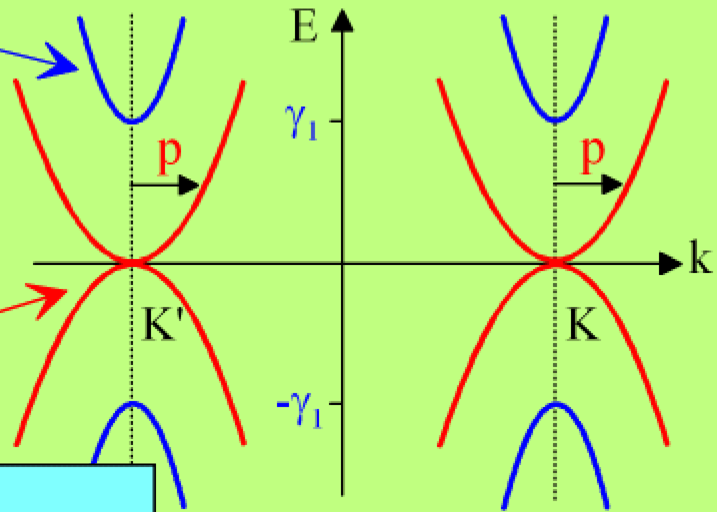
Bilayer Hamiltonian

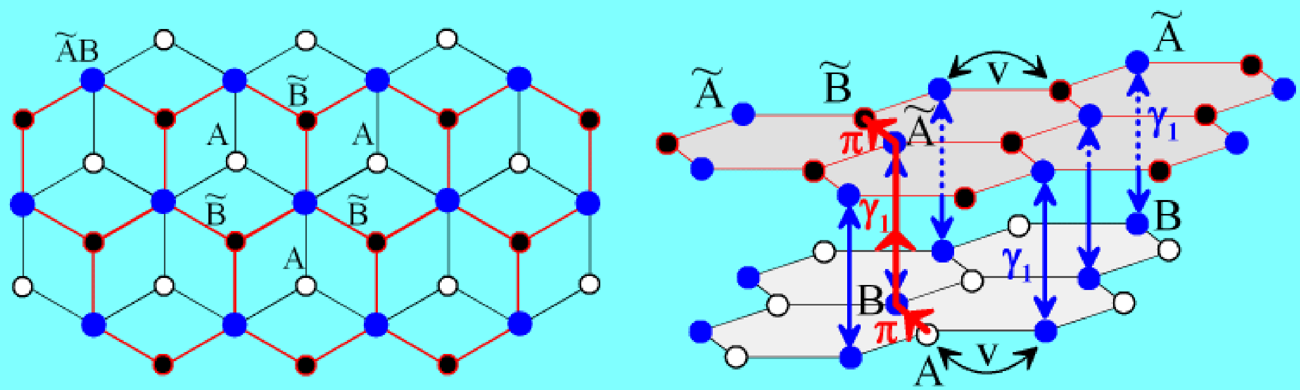
$$
H = \begin{array}{c}
\begin{array}{cccc} A & \tilde{B} & \tilde{A} & B \end{array} \\
\left(\begin{array}{cccc}
0 & 0 & 0 & v\pi^{+} \\
0 & 0 & v\pi & 0 \\
0 & v\pi^{+} & 0 & \gamma_1 \\
v\pi & 0 & \gamma_1 & 0
\end{array} \right)
\end{array}
\begin{array}{c} \\ A \\ \tilde{B} \\ \tilde{A} \\ B \end{array}
$$

$\tilde{A}B$ orbitals form dimers with energy $|E| \gtrsim \gamma_1$

Quadratic dispersion at low energy:

$$E = \pm \frac{p^2}{2m}$$





Bilayer Hamiltonian written in a 2 component basis of A and $\tilde{B}$ sites

$$H = \frac{-1}{2m}\begin{pmatrix} 0 & (\pi^+)^2 \\ \pi^2 & 0 \end{pmatrix}$$

mass

$m = \gamma_1 / v^2$

A to $\tilde{B}$ hopping

- bottom layer A → B (factor π)
- switch layers via dimer $B\tilde{A}$ (γ_1^{-1})
- top layer $\tilde{A}$ → $\tilde{B}$ (factor π)

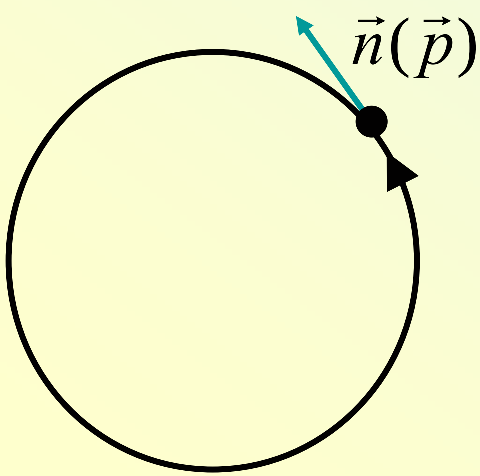
$$\pi = p_x + i p_y$$

General case: $$H = g\begin{pmatrix} 0 & (\pi^+)^J \\ \pi^J & 0 \end{pmatrix}$$

$$\pi = p_x + ip_y = pe^{i\varphi} \qquad \pi^+ = p_x - ip_y = pe^{-i\varphi}$$

$$H = g\,|p|^J \begin{pmatrix} 0 & e^{-iJ\varphi} \\ e^{iJ\varphi} & 0 \end{pmatrix} = g\,|p|^J\,(\sigma_x \cos J\varphi + \sigma_y \sin J\varphi)$$

$$H = g\,|p|^J\,(\boldsymbol{\sigma}.\mathbf{n}) \qquad \boldsymbol{\sigma} = (\sigma_x, \sigma_y) \qquad \mathbf{n} = (\cos J\varphi, \sin J\varphi)$$



$$\psi \to e^{J2\pi\frac{i}{2}\sigma_3}\psi = e^{iJ\pi}\psi$$

Berry phase $J\pi$

(for a monolayer π

for a bilayer 2π **)**

$$H_1 = v\begin{pmatrix} 0 & \pi^+ \\ \pi & 0 \end{pmatrix}$$

Berry phase π
suppressed backscattering
weak anti-localisation ?

H. Suzuura, T. Ando, Phys. Rev. Lett. 89, 266603 (2002)
D. Khveshchenko, cond-mat/0602398

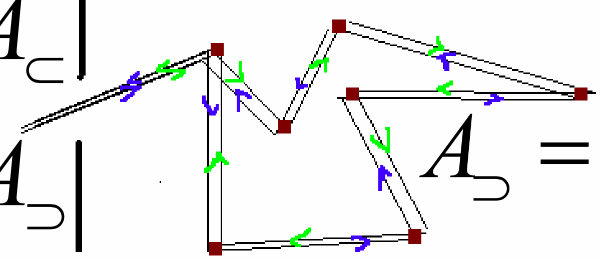
Berry phase romantics

$$H_2 = \frac{1}{2m}\begin{pmatrix} 0 & (\pi^+)^2 \\ \pi^2 & 0 \end{pmatrix}$$

Berry phase 2π
weak localisation ?

Weak localisation *vs* anti-localisation

$$w \sim |A_{\subset} + A_{\supset}|^2 = |A_{\subset}|^2 + |A_{\supset}|^2 + [A_{\subset}^* A_{\supset} + A_{\subset} A_{\supset}^*]$$



$A_{\subset}|$ $A_{\supset}|$ $A_{\supset} = A_{\subset}$

$$A_{\subset}^* A_{\supset} = |A_{\subset}|^2 > 0$$

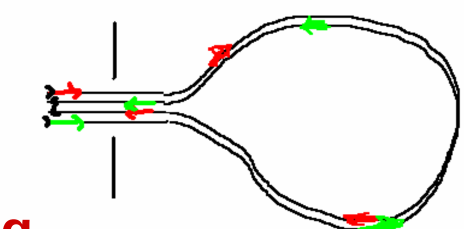
WL = enhanced backscattering in time-reversal symmetric systems

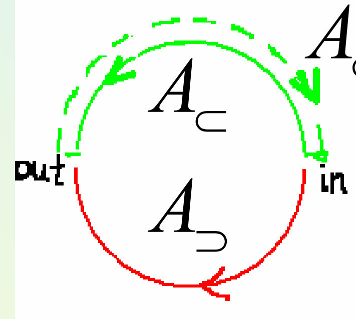
chiral electrons with $\vec{\sigma} \cdot \vec{p} = 1$

$$A_{\subset} A_{\supset}^* = e^{-i2\pi(\sigma_z/2)} |A_{\subset}|^2$$

$$= -|A_{\subset}|^2 < 0$$

$$\psi_{out} = e^{-i\phi(\sigma_z/2)} \psi_{in}$$





$A_{\subset}^*$ $A_{\subset}$ $A_{\supset}$

WAL = suppressed backscattering

higher order expansion

$$H_1 = \varsigma v\begin{pmatrix} 0 & \pi^+ \\ \pi & 0 \end{pmatrix} + \mu\begin{pmatrix} 0 & \pi^2 \\ (\pi^+)^2 & 0 \end{pmatrix} + \hat{V}(\vec{r}) \qquad \begin{pmatrix} A \\ B \\ B \\ A \end{pmatrix} \begin{matrix} \varsigma=+1 \\ \\ \varsigma=-1 \end{matrix}$$

'trigonal warping': symmetry of wave vector K is lower than the hexagonal symmetry

valley

$$H_2 = \frac{1}{2m}\begin{pmatrix} 0 & (\pi^+)^2 \\ \pi^2 & 0 \end{pmatrix} + \varsigma v_3\begin{pmatrix} 0 & \pi \\ \pi^+ & 0 \end{pmatrix} + \hat{V}(\vec{r}) \qquad \begin{pmatrix} A \\ B \\ \tilde{B} \\ \tilde{A} \end{pmatrix} \begin{matrix} \varsigma=+1 \\ \\ \varsigma=-1 \end{matrix}$$

off-diagonal $A\tilde{B}$ interlayer hopping

Weak localisation

$\varepsilon_F \tau >> 1$ **High electron (hole) density and remote Coulomb scatterers**

Berry phase π

$$\delta g_1 = - C_{KK'-symm} + C_{KK'-antisymm} \quad \cancel{+ C_{KK} + C_{K'K'}}$$

can be suppressed only by decoherence

may be suppressed by the intervalley scattering τ_i due to atomically sharp scatterers or edges

killed by trigonal warping reflecting the asymmetry

$$H(-\vec{p}) \neq H(\vec{p})$$

in each valley

$$\delta g_2 = - C_{KK'-symm} + C_{KK'-antisymm} \quad \cancel{- C_{KK} - C_{K'K'}}$$

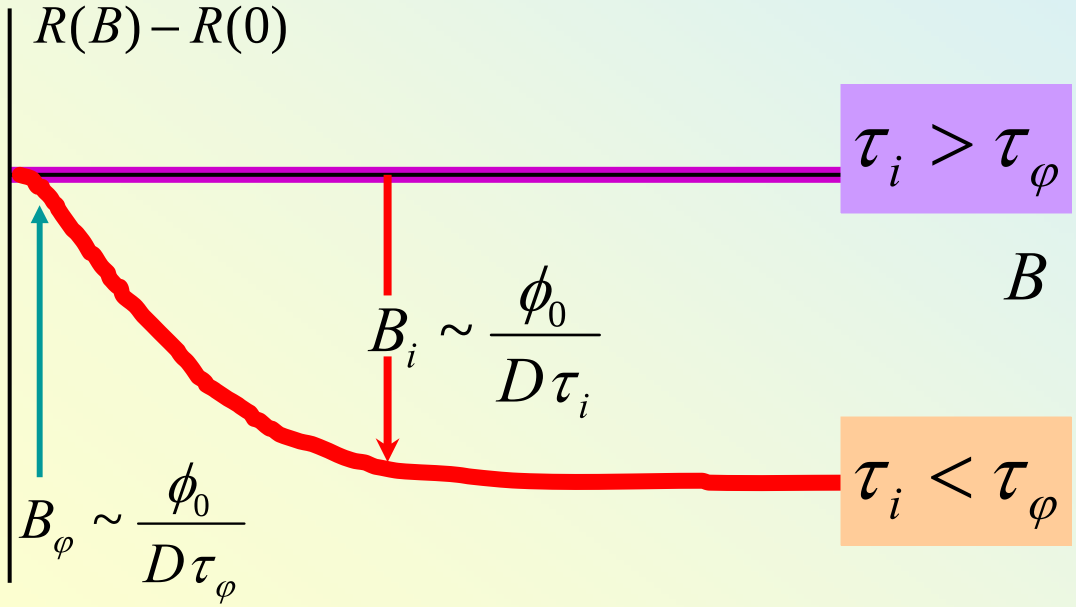
Berry phase 2π

Weak localisation magnetoresistance

$$\varepsilon_F \tau >> 1$$

$$\boxed{\delta g_1 = - \ C_{KK'-symm} \ + \ C_{KK'-antisymm}}$$

E. McCann, K.Kechedzhi, V.Falko, H.Suzuura, T.Ando, B.Altshuler
cond-mat/0604015



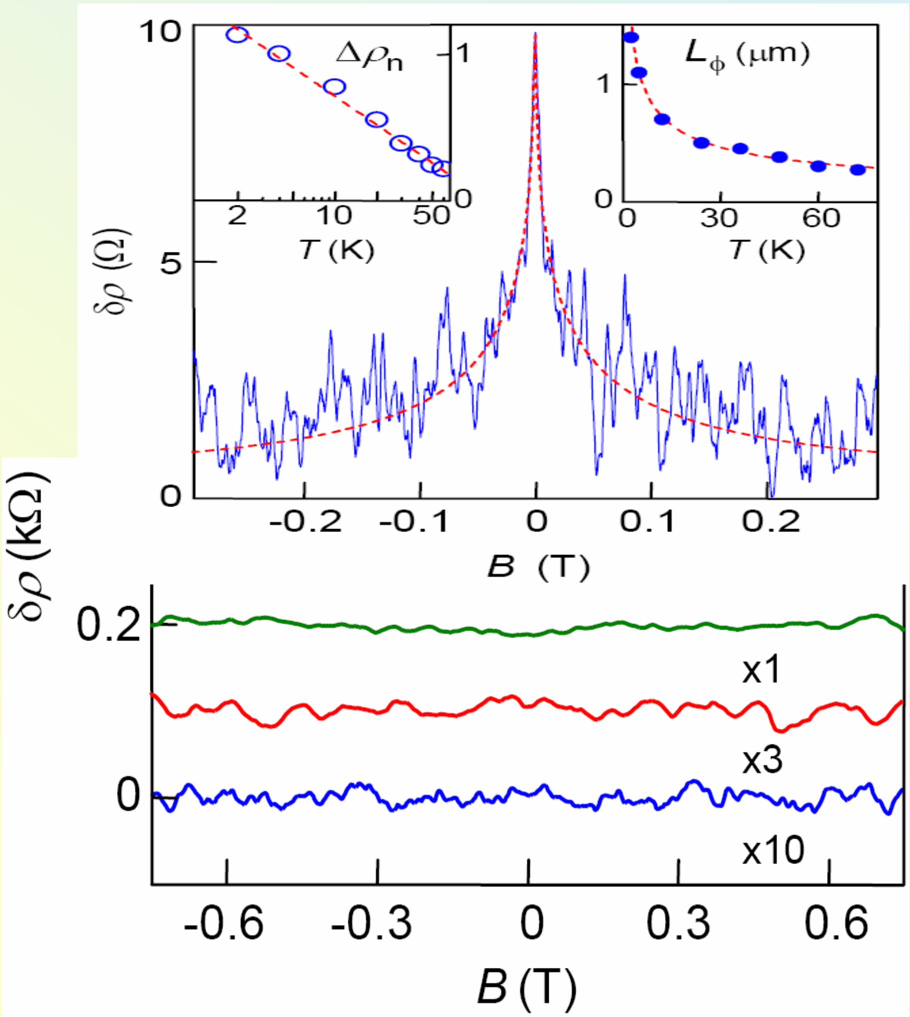
'slow' inter-valley scattering: neither WL nor WAL

'fast' inter-valley scattering: usual WL magnetoresistance cut at B_i

$$\boxed{\delta g_2 = - \ C_{KK'-symm} \ + \ C_{KK'-antisymm}}$$

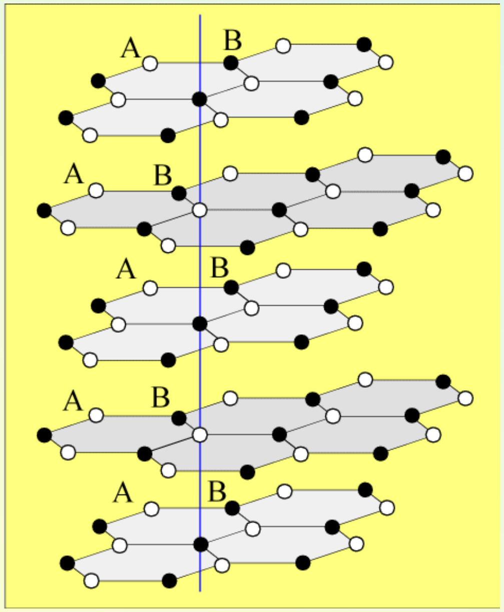
E. McCann, K.Kechedzhi, V.Falko, B.Altshuler, 2006

Weak localisation magnetoresistance in graphene

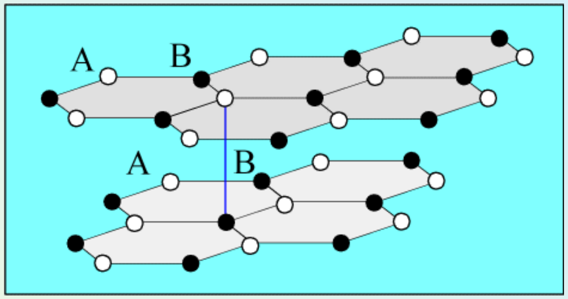


S.V. Morozov et al, cond-mat/0603826
(Manchester group)

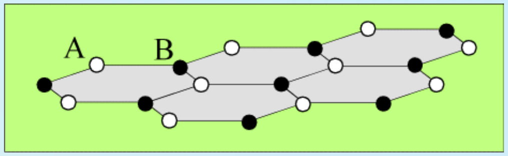
Graphite



Bilayer



Monolayer



1. **Tight-binding-model analysis showing that electrons (holes) in these materials are chiral and have the Berry phase $J\pi$.**
2. **Ballistic transport of chiral electrons.**
3. **Weak localisation in graphene.**
4. **Landau levels and the quantum Hall effect in monolayers and bilayers.**

2D Landau levels

$$\vec{p} = -i\hbar\nabla - \tfrac{e}{c}\vec{A}, \quad rot\vec{A} = B\vec{l}_z$$

$$\pi = p_x + ip_y; \quad \pi^+ = p_x - ip_y$$

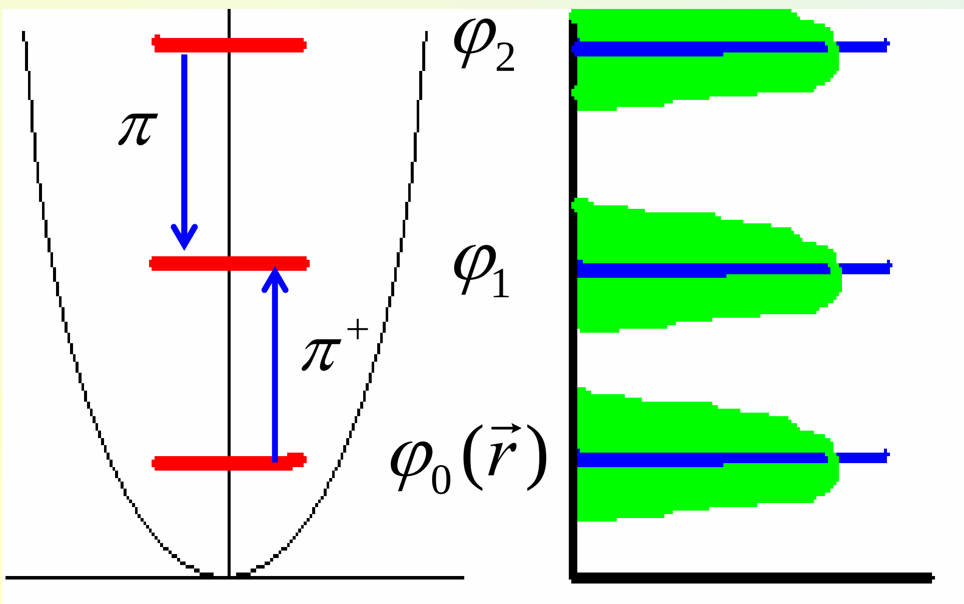
semiconductor
QW / heterostructure
(GaAs/AlGaAs)

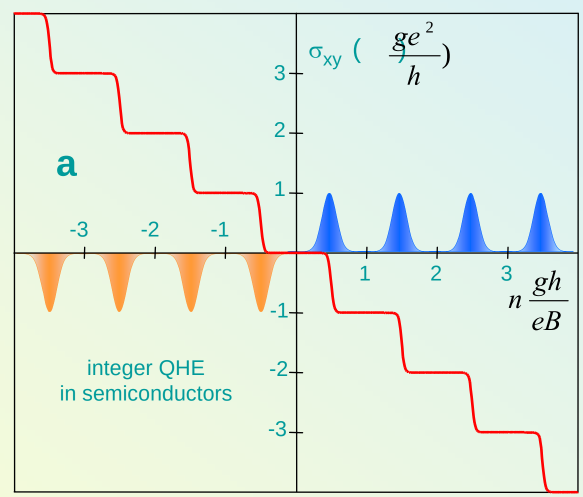
$$\pi\varphi_0 = 0$$

$$\varphi_{n+1} = \tfrac{1}{\sqrt{n+1}}\pi^+\varphi_n$$

$$H = \frac{\vec{p}^{\,2}}{2m} = \frac{\pi\pi^+ + \pi^+\pi}{4m} \Rightarrow (n+\tfrac{1}{2})\hbar\omega_c$$

Landau levels / wave functions





Monolayer:

$$H = v\xi \begin{pmatrix} 0 & \pi^+ \\ \pi & 0 \end{pmatrix}$$

Bilayer:

$$H = \frac{-1}{2m} \begin{pmatrix} 0 & (\pi^+)^2 \\ \pi^2 & 0 \end{pmatrix}$$

In a perpendicular magnetic field B:

$$\left.\begin{array}{l} \pi \longrightarrow \text{lowering operator} \\ \pi^+ \longrightarrow \text{raising operator} \end{array}\right\} \begin{array}{c} \text{of magnetic oscillator} \\ \text{eigenstates } \phi_n \end{array}$$

We are able to determine the spectrum of discrete Landau levels

States at zero energy are determined by

monolayer: $\pi\phi_0 = 0$

bilayer: $\pi^2\phi_0 = \pi^2\phi_1 = 0$

2D Landau levels of chiral electrons

$$g \begin{pmatrix} 0 & (\pi^{+})^{J} \\ \pi^{J} & 0 \end{pmatrix} \psi = \varepsilon \psi$$

$$\pi^{J} \varphi_0 = \ldots = \pi^{J} \varphi_{J-1} = 0 \qquad \begin{pmatrix} \varphi_0 \\ 0 \end{pmatrix}, \ldots, \begin{pmatrix} \varphi_{J-1} \\ 0 \end{pmatrix} \Rightarrow \quad \varepsilon = 0$$

valley index

$$\begin{pmatrix} 0 & (\pi^{+})^{J} & & \\ \pi^{J} & 0 & & \\ & & 0 & (-\pi^{+})^{J} \\ & & (-\pi)^{J} & 0 \end{pmatrix} \begin{pmatrix} A & + \\ \tilde{B} & + \\ \tilde{B} & - \\ A & - \end{pmatrix}$$

also, two-fold real spin degeneracy

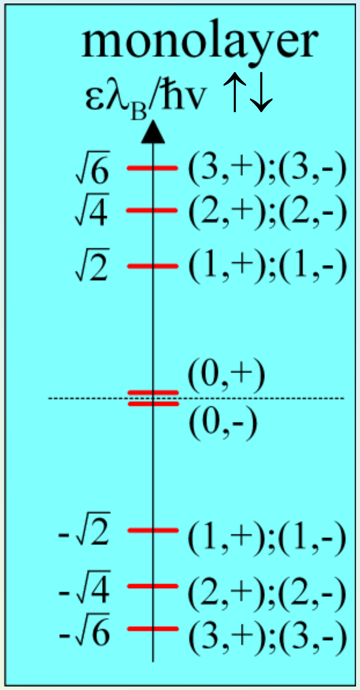
monolayer:

energy scale $\hbar v/\lambda_B$

where $\lambda_B = \sqrt{\dfrac{\hbar}{eB}}$

state at zero energy:

$$\pi\phi_0 = 0$$



J.McClure, Phys. Rev. 104, 666 (1956)

F.Haldane, Phys.Rev.Lett. 61, 2015 (1988)

Y.Zheng, T.Ando
Phys. Rev. B 65, 245420 (2002)

$$g \begin{pmatrix} 0 & (\pi^+)^J \\ \pi^J & 0 \end{pmatrix} \psi = \varepsilon\psi$$

bilayer:

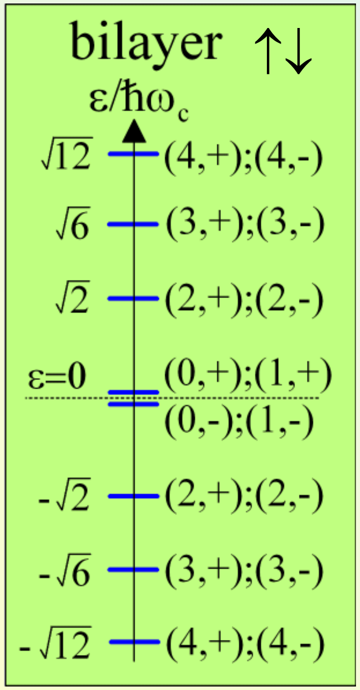
energy scale $\hbar\omega_c$

where $\omega_c = \dfrac{eB}{m}$

states at zero energy:

$$\pi^2\phi_0 = 0$$

$$\pi^2\phi_1 = 0$$



E.McCann, V.Fal'ko
Phys. Rev. Lett. 96, 086805 (2006)

4J*-degenerate zero-energy Landau level for electrons with degree of chirality *J

$$\hat{H}_2 = -\frac{1}{2m}\left[\sigma_x\left(p_x^2 - p_y^2\right) + \sigma_y\left(p_x p_y + p_y p_x\right)\right]$$

$$+ v_3\left(\sigma_x p_x - \sigma_y p_y\right)$$

'trigonal warping'

weak magnetic field

$$\lambda_B^{-1} \sim p < mv_3$$

strong magnetic field

$$\lambda_B^{-1} \sim p >> mv_3$$

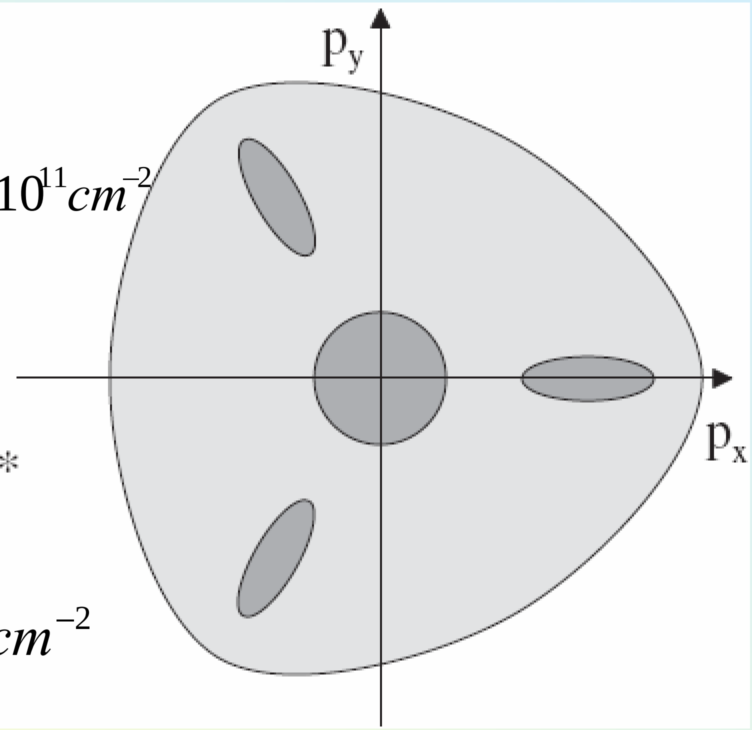
$$0 < \varepsilon < \frac{\gamma_1}{2}\left(\frac{v_3}{v}\right)^2$$

$$0 < N < 2\left(\frac{v_3}{v}\right)^2 N^* \sim 10^{11}\, cm^{-2}$$

$$\frac{\gamma_1}{2}\left(\frac{v_3}{v}\right)^2 < \varepsilon < \gamma_1$$

$$2\left(\frac{v_3}{v}\right)^2 N^* < N < 8N^*$$

$$N^* = \frac{\gamma_1^2}{4\pi\hbar^2 v^2} \sim 4\times 10^{12}\, cm^{-2}$$



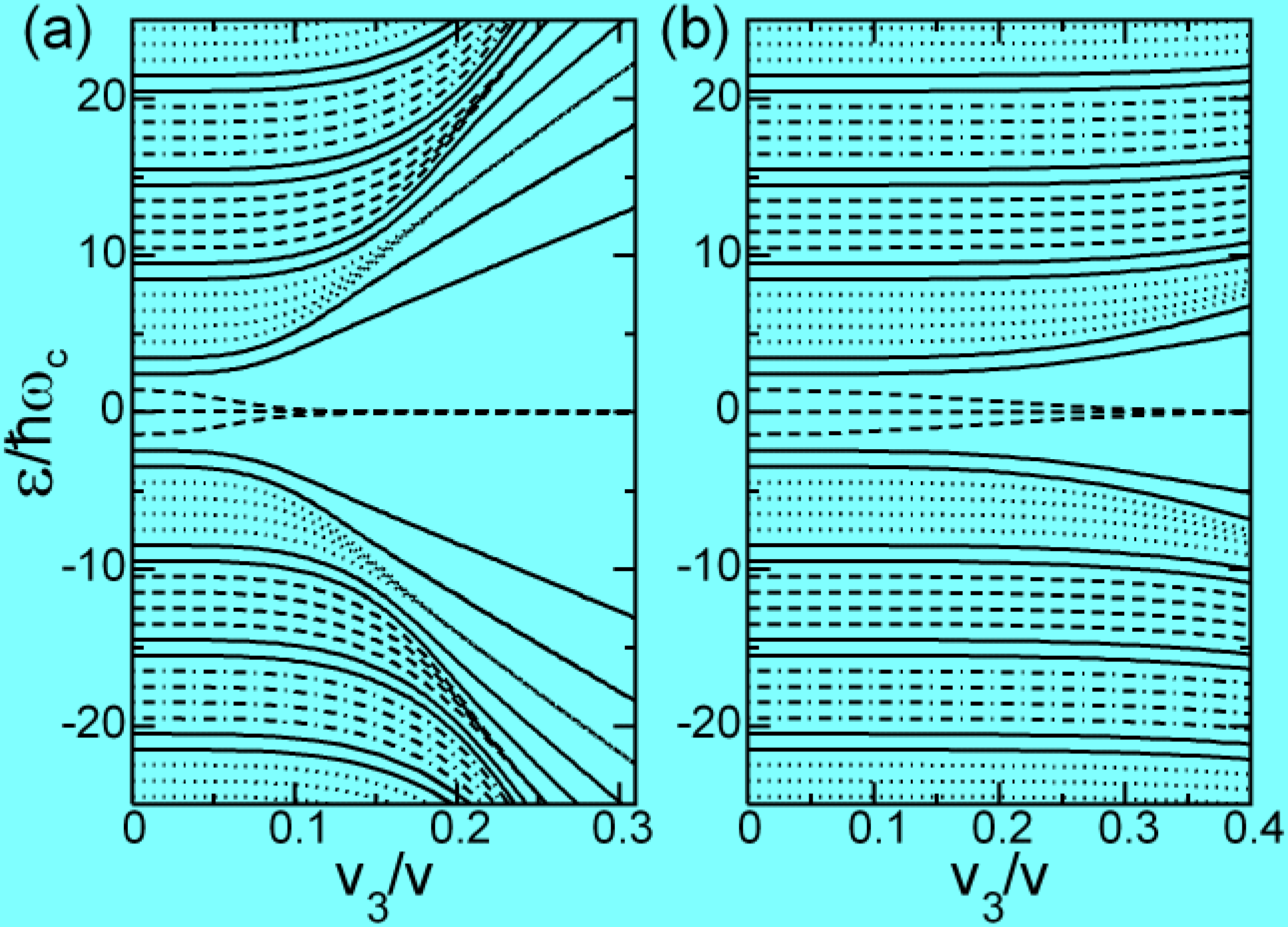
$$-\frac{v^2}{\gamma_1}\begin{pmatrix} 0 & \left(\pi^\dagger\right)^2 \\ \pi^2 & 0 \end{pmatrix} + \xi v_3 \begin{pmatrix} 0 & \pi \\ \pi^\dagger & 0 \end{pmatrix}$$

$$\pi = p_x + i p_y,$$
$$\mathbf{p} = -i\hbar\nabla - e\mathbf{A}$$
$$\left[\pi, \pi^\dagger\right] = 2\hbar e B.$$

Landau wavefunctions

$$e^{iky}\phi_n(x)$$

$$\pi^\dagger \phi_n = i(\hbar/\lambda_B)\sqrt{2(n+1)}\phi_{n+1}$$



B = 0.1 T
$\hbar\omega_c$ = 0.216 meV
λ_B = 0.0812 μm

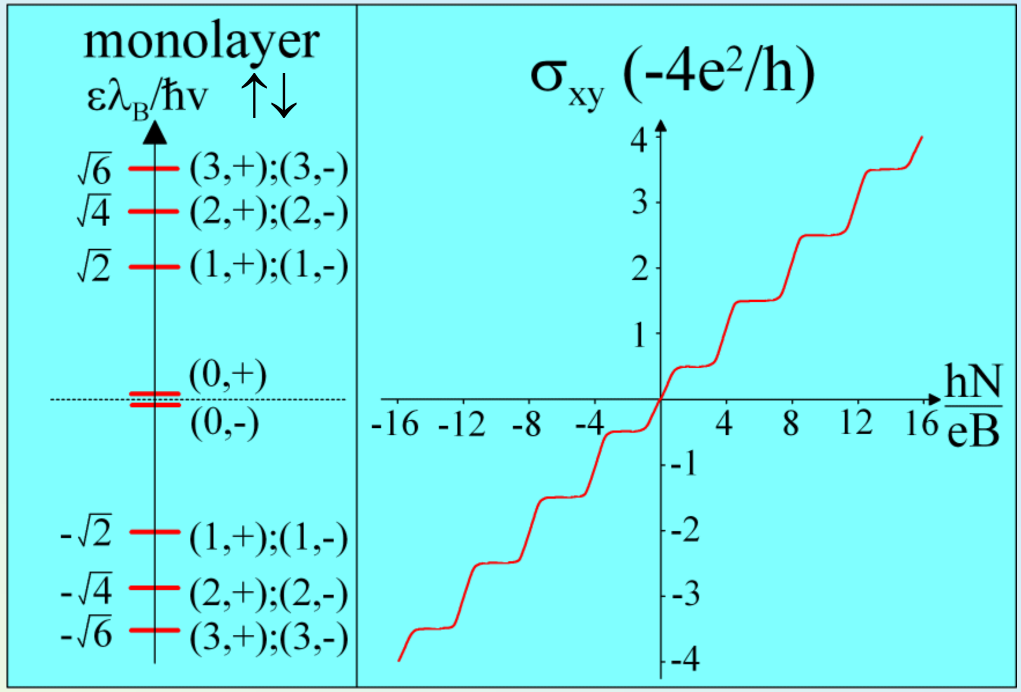
B = 1 T
$\hbar\omega_c$ = 2.16 meV
λ_B = 0.0257 μm

monolayer:

$$H = v\xi \begin{pmatrix} 0 & \pi^{+} \\ \pi & 0 \end{pmatrix}$$

state at zero energy:

$$\pi\phi_0 = 0$$



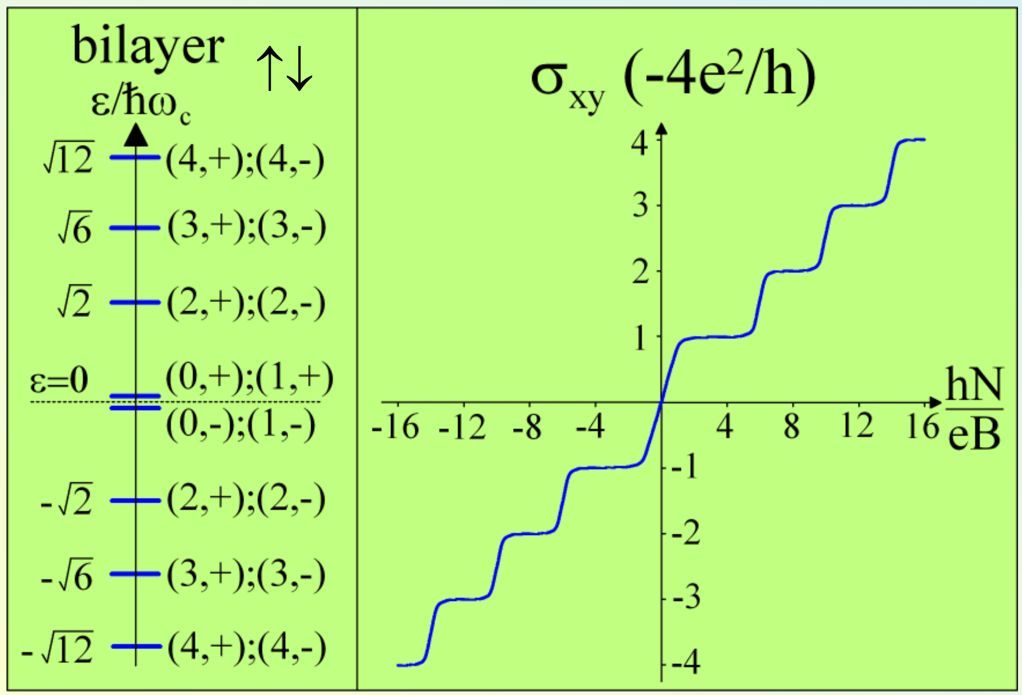
bilayer:

$$H = \frac{-1}{2m} \begin{pmatrix} 0 & (\pi^{+})^2 \\ \pi^2 & 0 \end{pmatrix}$$

states at zero energy:

$$\pi^2\phi_0 = 0$$

$$\pi^2\phi_1 = 0$$



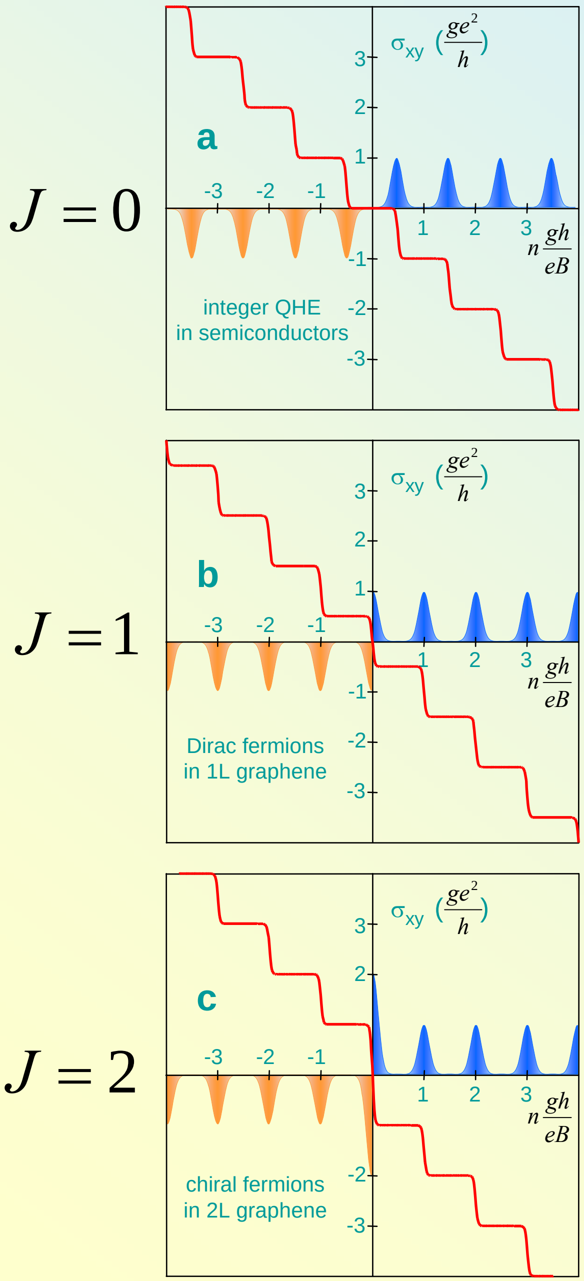


Figure 1

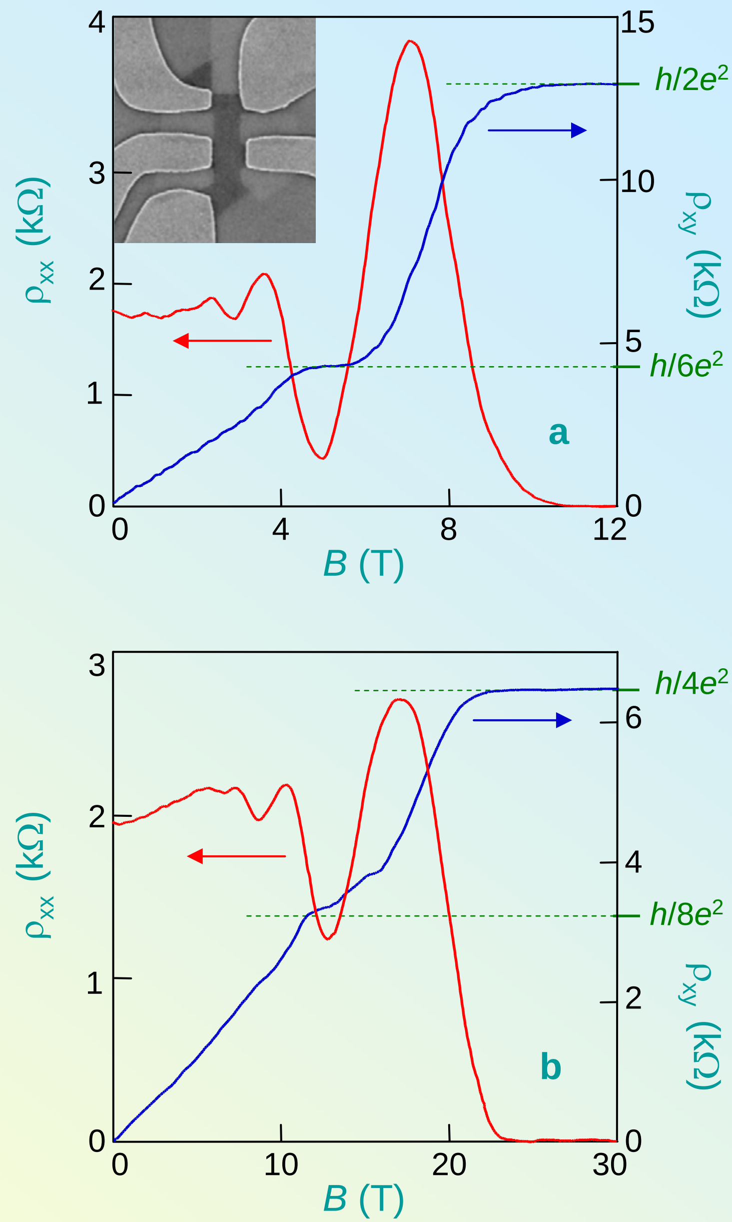
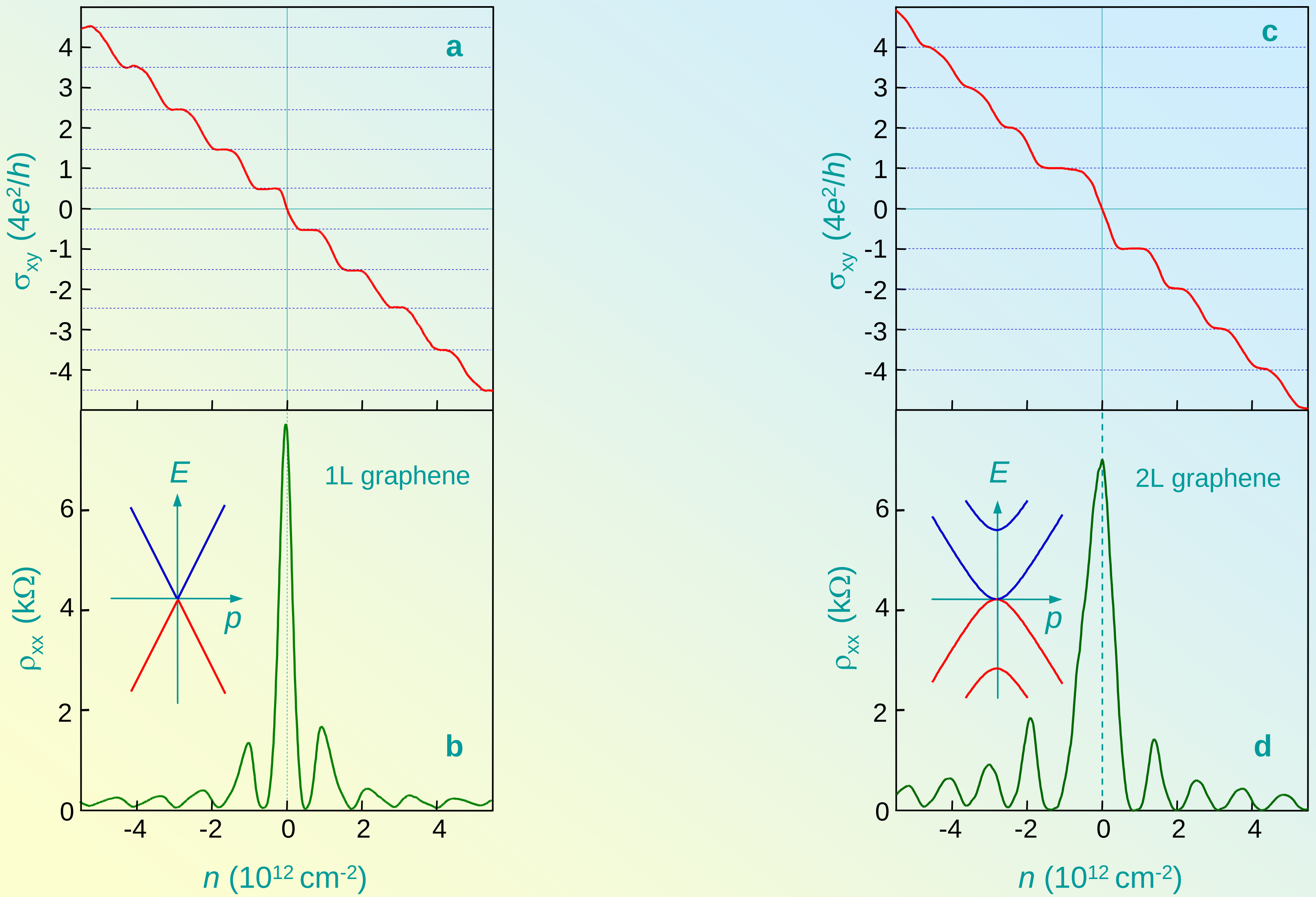


Figure 2



Unconventional Quantum Hall Effect and Berry's Phase of 2π in Bilayer Graphene

K.Novoselov, E.McCann, S.Morozov, V.Fal'ko, M.Katsnelson, U.Zeitler, D.Jiang, F.Schedin, A.Geim

Nature Physics 2, 177-180 (2006)

‘PseudoSpintronics’ summary

Pseudospin chirality of electrons in graphene
Determines a selective transmission in *n-p* junctions.

V.Cheianov, V.F. - to appear in PRB, cond-mat/0603624

Pseudospin leads a rich crossover regime between weak localisation and antilocalisation in graphene (monolayers) and bilayers

E.McCann, K.Kechedzhi, V.F., H.Suzuura, T.Ando, B.Altshuler - cond-mat/0604015

Berry phase $J\pi$ quasiparticles and J times degenerate ‘zero’ energy Landau levels manifested in the quantum Hall effect in graphene and graphitic bilayers.

E.McCann, V.F. - Phys. Rev. Lett. 96, 086805 (2006)
K.Novoselov, E.McCann, S.Morozov, V.F., M.Katsnelson, U.Zeitler, D.Jiang, F.Schedin, A.Geim - Nature Physics 2, 177-180 (2006)