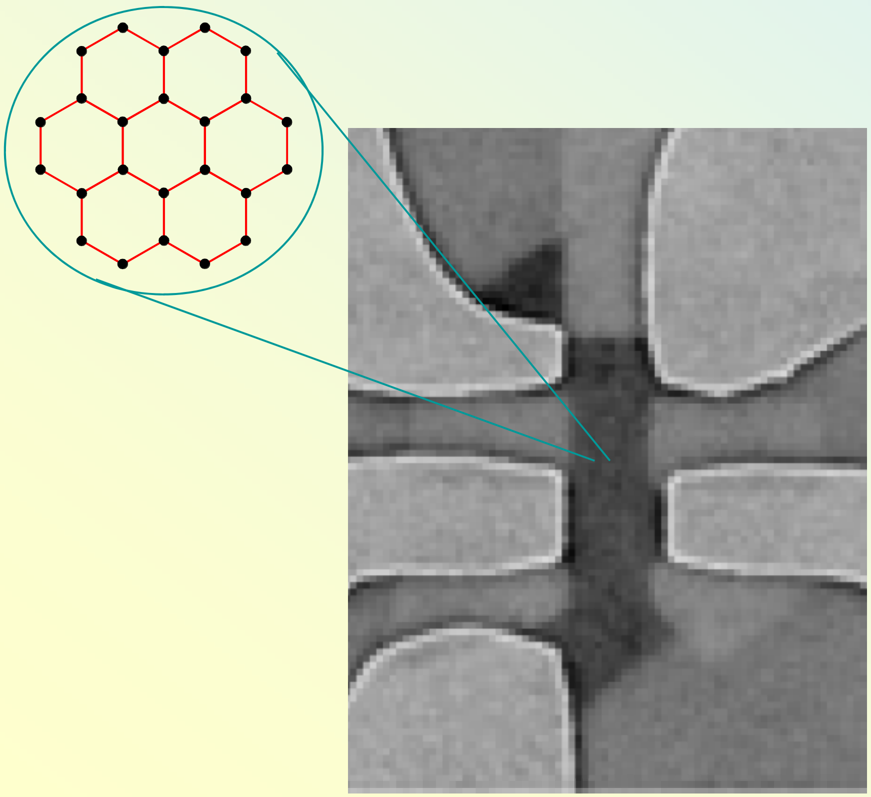
Electronic properties of monolayer and bilayer graphene

Vladimir Falko (Lancaster)

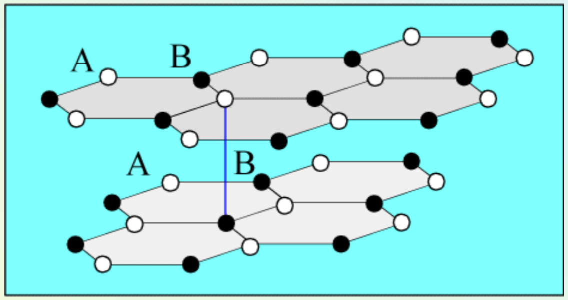


A.Geim and K.Novoselov
Nature Mat. 6, 183 (2007)

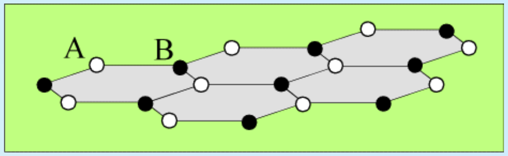
I & II. Electrons
in monolayer graphene.

III. Electrons
in bilayer graphene,
Landau levels and the
quantum Hall effect in
monolayers and bilayers.

Bilayer graphene



Monolayer graphene



Band structure of bilayer graphene and Berry's phase *2π*, effect of trigonal warping and the Lifshitz transition.

Landau levels and the quantum Hall effect in bilayer and monolayer graphene.

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

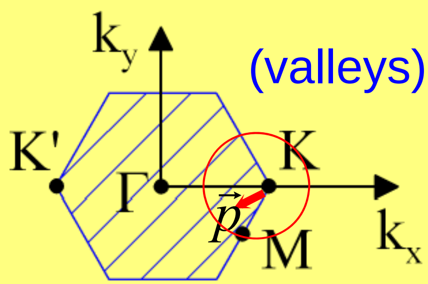
j^{th} atomic orbital: j = A or B

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

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

Brillouin zone

(valleys)

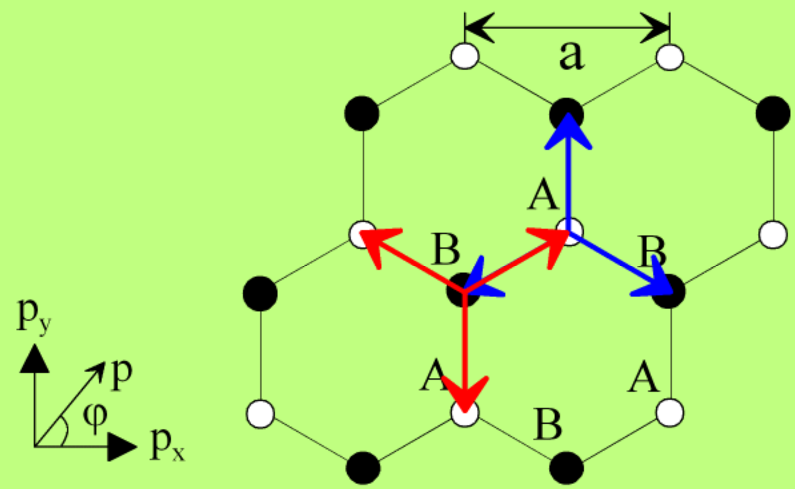


Two non-equivalent K-points

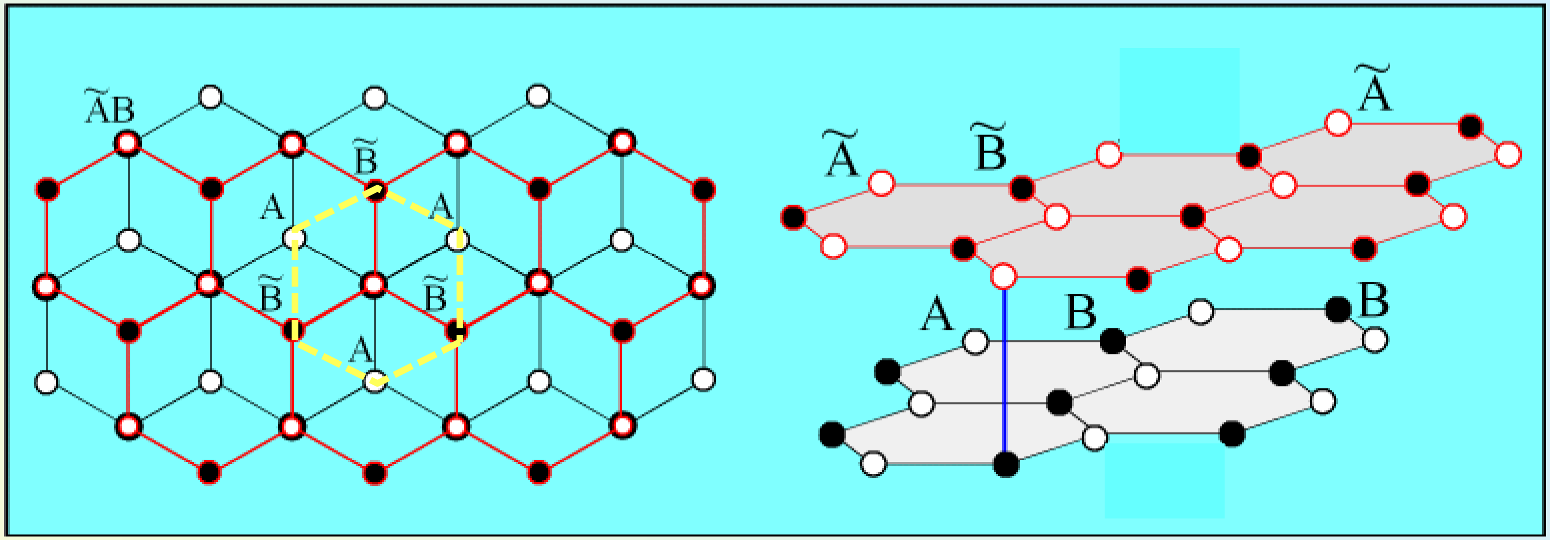
B to A hopping given by $\pi^+ = p_x - ip_y$

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

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



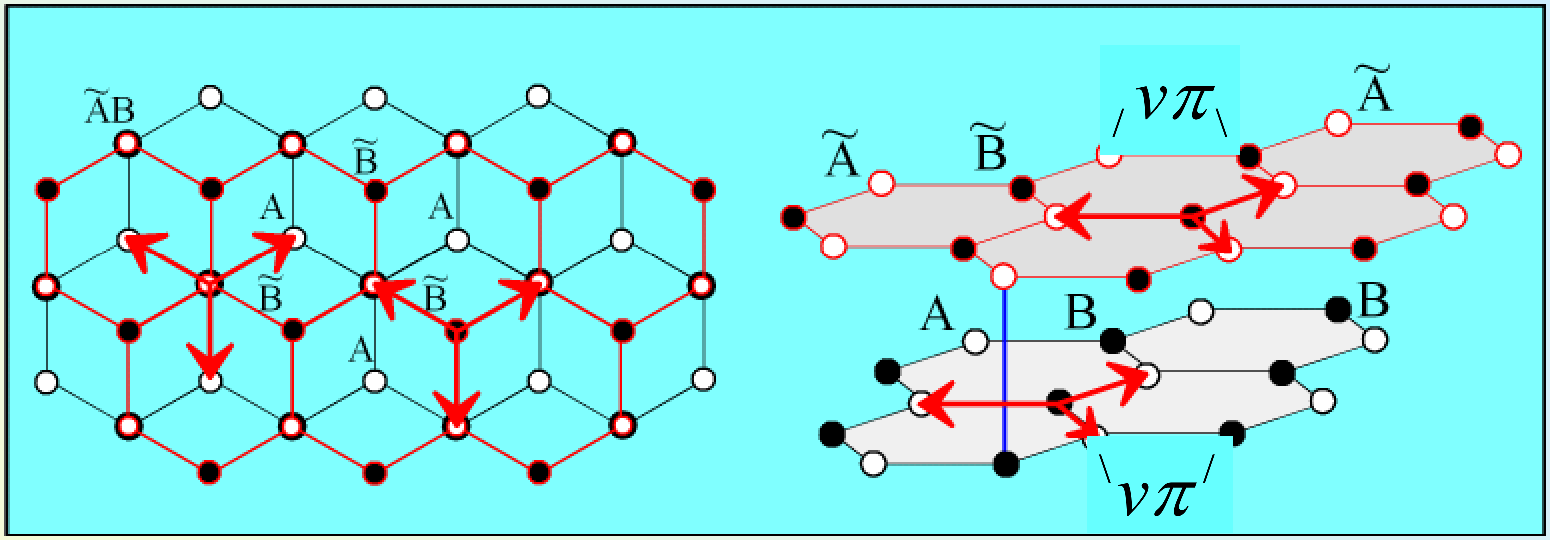
Bilayer [Bernal (AB) stacking]



4 atoms
per unit cell

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

Bilayer [Bernal (AB) stacking]

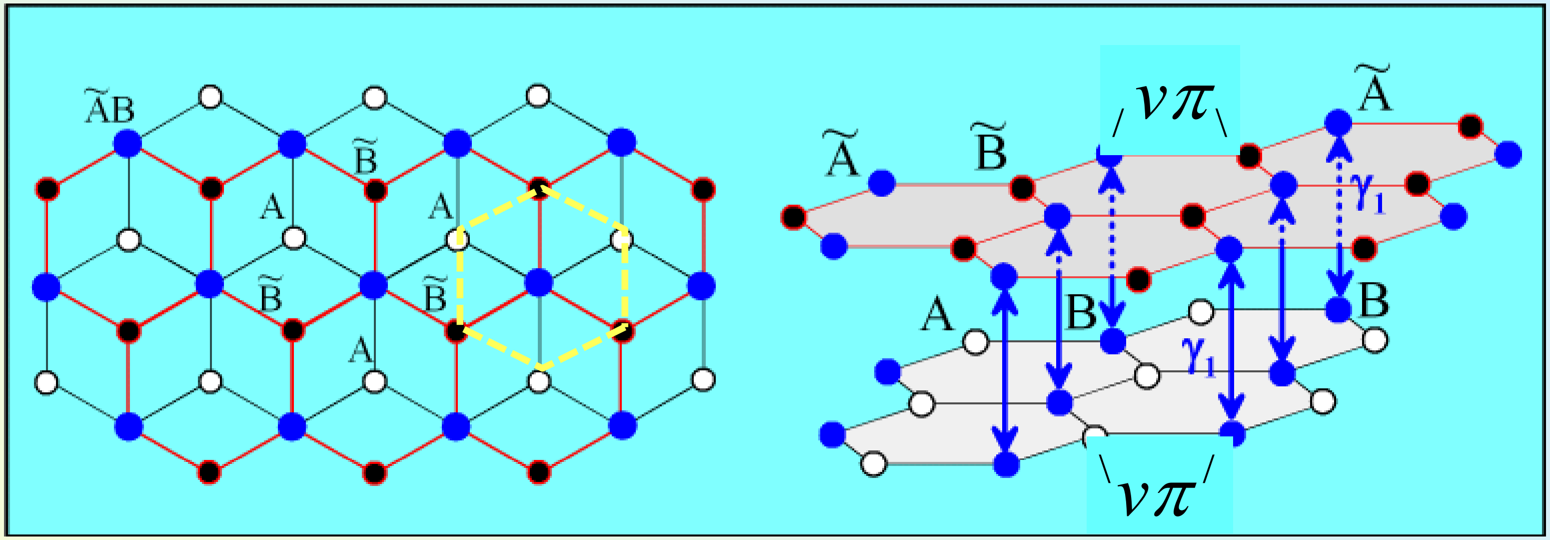


In the vicinity of each of K points

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

$$H = \begin{array}{c} \\ \\ \\ \\ \\ \end{array}\begin{array}{c} \begin{array}{cccc} A & \tilde{B} & \tilde{A} & B \end{array} \\ \begin{pmatrix} & & & v\pi^+ \\ & & v\pi & \\ & v\pi^+ & & \\ v\pi & & & \end{pmatrix} \end{array} \begin{array}{c} \\ A \\ \tilde{B} \\ \tilde{A} \\ B \end{array}$$

Bilayer [Bernal (AB) stacking]



In the vicinity of each of K points

Bilayer Hamiltonian

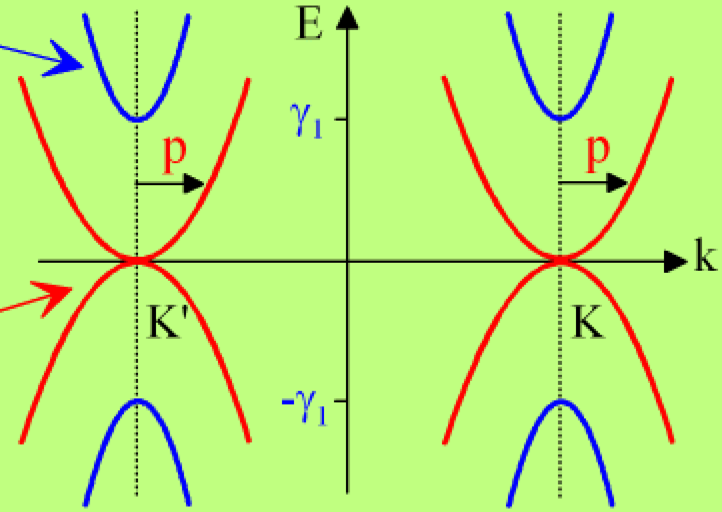
$$
H = \begin{array}{cc}
 & \begin{array}{cccc} A & \tilde{B} & \tilde{A} & B \end{array} \\
 & \left(\begin{array}{cccc}
0 & 0 & 0 & v\pi^{+} \\
0 & 0 & v\pi & 0 \\
0 & v\pi^{+} & 0 & \gamma_1 \\
v\pi & 0 & \gamma_1 & 0
\end{array} \right)
\begin{array}{c} A \\ \tilde{B} \\ \tilde{A} \\ B \end{array}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

McCann, VF
PRL 96, 086805
(2006)

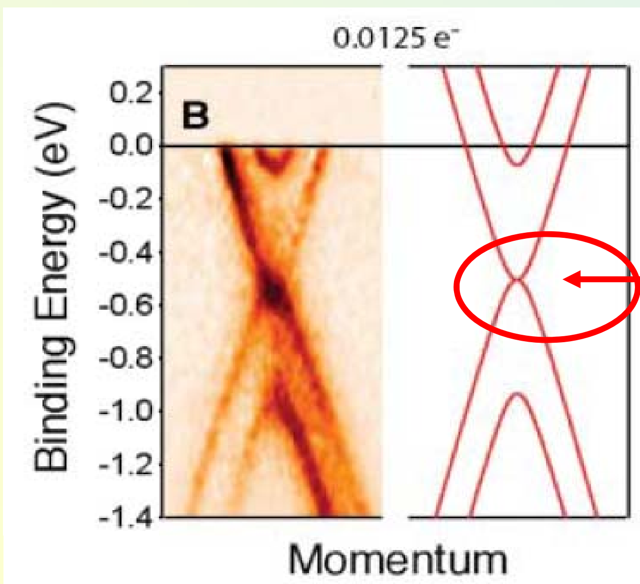
$\tilde{A}B$ orbitals form dimers
with energy $|E| \gtrsim \gamma_1$

Quadratic dispersion at low energy:

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



$$\gamma_1 \approx 0.4eV$$

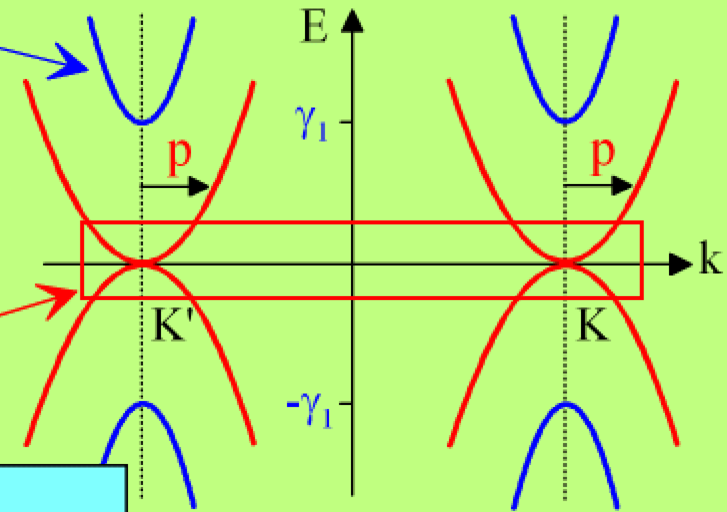


ARPES: heavily doped bilayer graphene synthesized on silicon carbide

T. Ohta *et al* – Science 313, 951 (2006)
(Rotenberg's group at Berkeley NL)

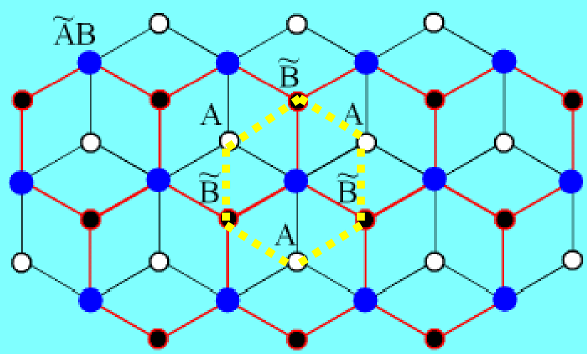
Fermi level in undoped bilayer graphene

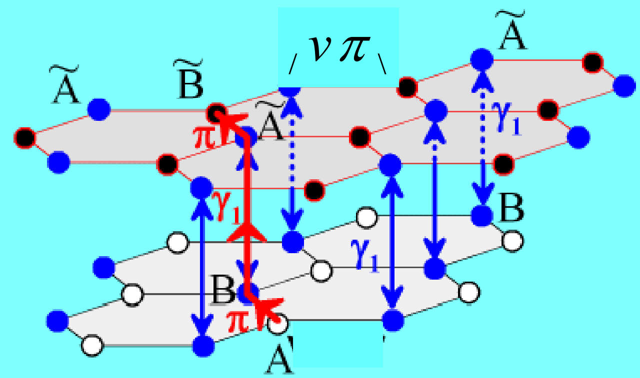
$\tilde{A}B$ orbitals form dimers with energy $|E| \gtrsim \gamma_1$



Quadratic dispersion at low energy:

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





$$m \sim 0.035 m_e$$

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

$m = \gamma_1 / v^2$

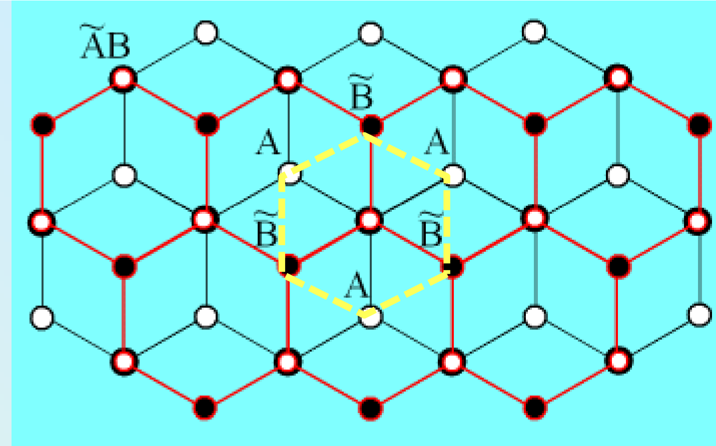
A to $\tilde{B}$ hopping

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

$$\pi = p_x + i p_y$$

McCann, VF
PRL 96, 086805
(2006)

$$\hat{H}_2 = \frac{-1}{2m}\begin{pmatrix} 0 & (\pi^+)^2 \\ \pi^2 & 0 \end{pmatrix} = \frac{-p^2}{2m}\vec{n}\cdot\vec{\sigma}$$



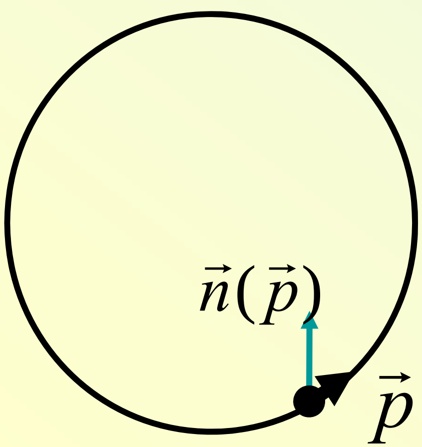
$$\vec{p} = (p\cos\vartheta, p\sin\vartheta)$$

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

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

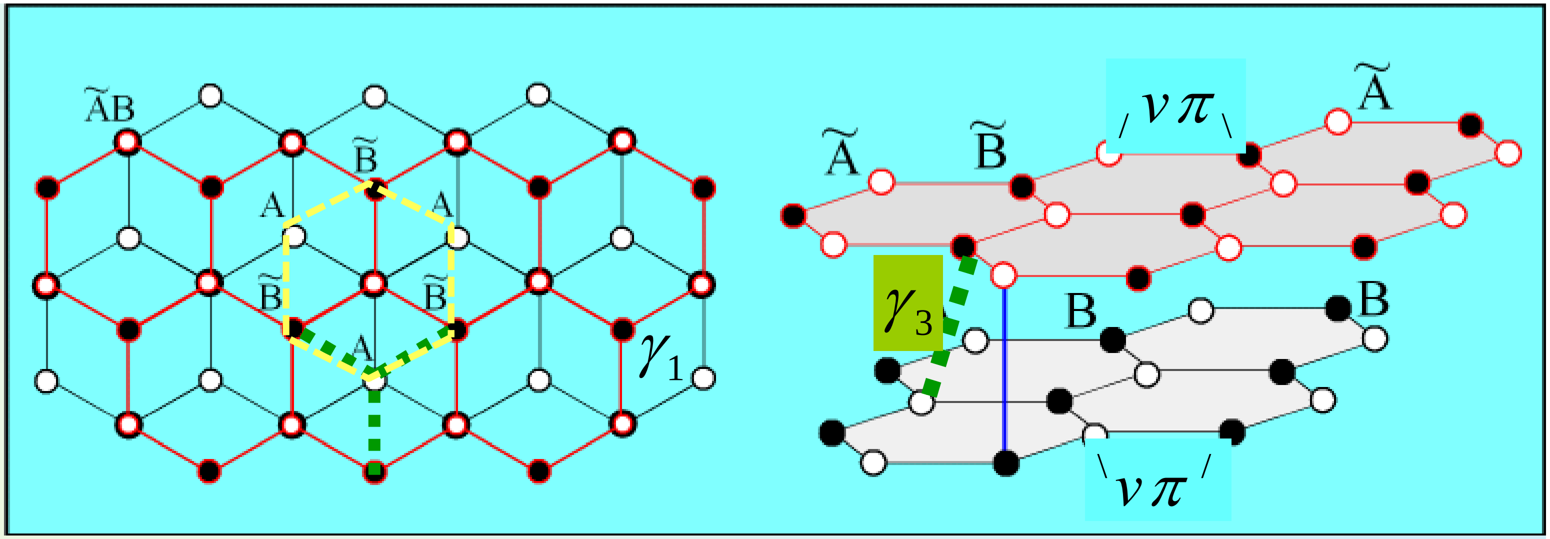
$$\vec{n}(\vec{p}) = (\cos 2\vartheta, \sin 2\vartheta)$$

$$\psi_{\vec{p}} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm e^{-i2\vartheta} \end{pmatrix} = \begin{pmatrix} \varphi_A \\ \varphi_{\tilde{B}} \end{pmatrix}$$



$$\psi \to e^{2\times 2\pi \frac{i}{2}\sigma_3}\psi = e^{i2\pi}\psi$$

Berry phase 2π



Hops between A and $\tilde{B}$ via $\tilde{A}B$

$$\hat{H}_2 = -\frac{v^2}{\gamma_1}\begin{pmatrix} 0 & (\pi^\dagger)^2 \\ \pi^2 & 0 \end{pmatrix} + \xi v_3 \begin{pmatrix} 0 & \pi \\ \pi^\dagger & 0 \end{pmatrix}$$

$$\pi = p_x + ip_y$$

Direct inter-layer hops between A and $\tilde{B}$, $\frac{v_3}{v} \sim 0.1$

$$\hat{H}_2 = -\frac{v^2}{\gamma_1}\begin{pmatrix} 0 & \left(\pi^\dagger\right)^2 \\ \pi^2 & 0 \end{pmatrix} + \xi v_3 \begin{pmatrix} 0 & \pi \\ \pi^\dagger & 0 \end{pmatrix}$$

Berry phase:

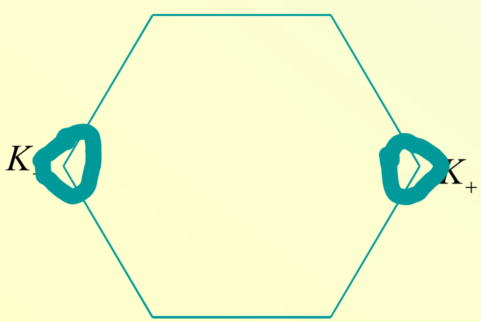
$2\pi = 3\pi - \pi$

weak magnetic field

$$\lambda_B^{-1} \sim p < m v_3$$

strong magnetic field

$$\lambda_B^{-1} \sim p >> m v_3$$



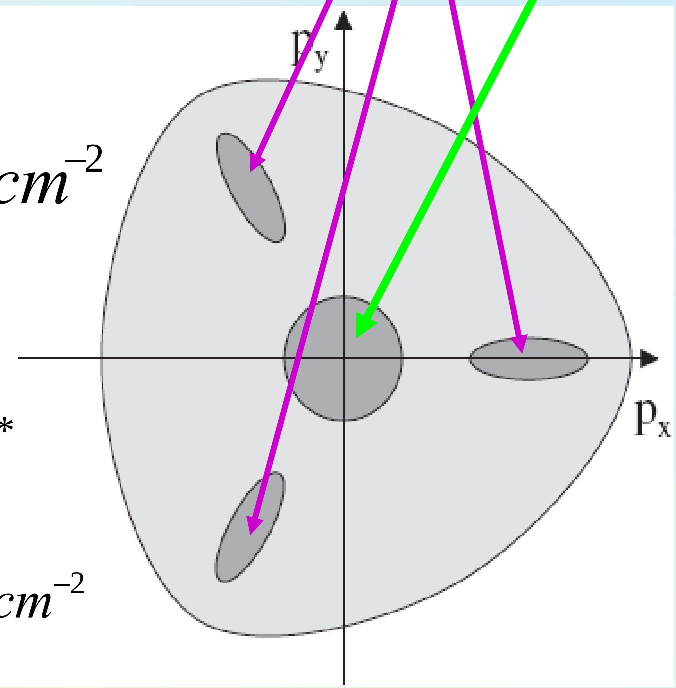
$0 < \varepsilon < \frac{\gamma_1}{2}\left(\frac{v_3}{v}\right)^2$

$N < N_L \sim 10^{11} cm^{-2}$

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

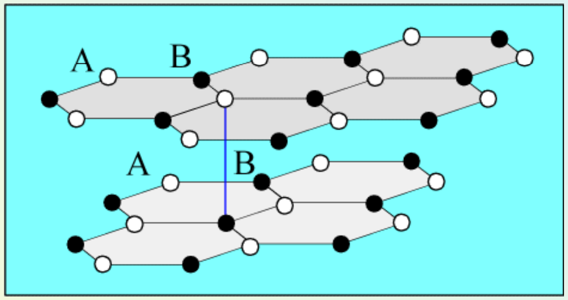
$N_L < N < 8N^*$

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

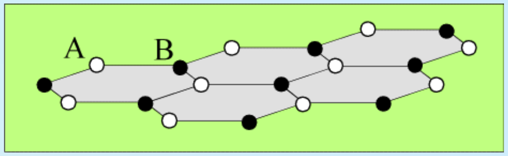


$$N_L = 2\left(\frac{v_3}{v}\right)^2 \frac{\gamma_1}{4\pi\hbar^2 v^2} \sim 10^{11} cm^{-2}$$ **Lifshitz transition**

Bilayer graphene



Monolayer graphene



Band structure of bilayer graphene and Berry's phase 2π, effect of trigonal warping and the Lifshitz transition.

Landau levels and the quantum Hall effect in bilayer and monolayer graphene.

2D Landau levels

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

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

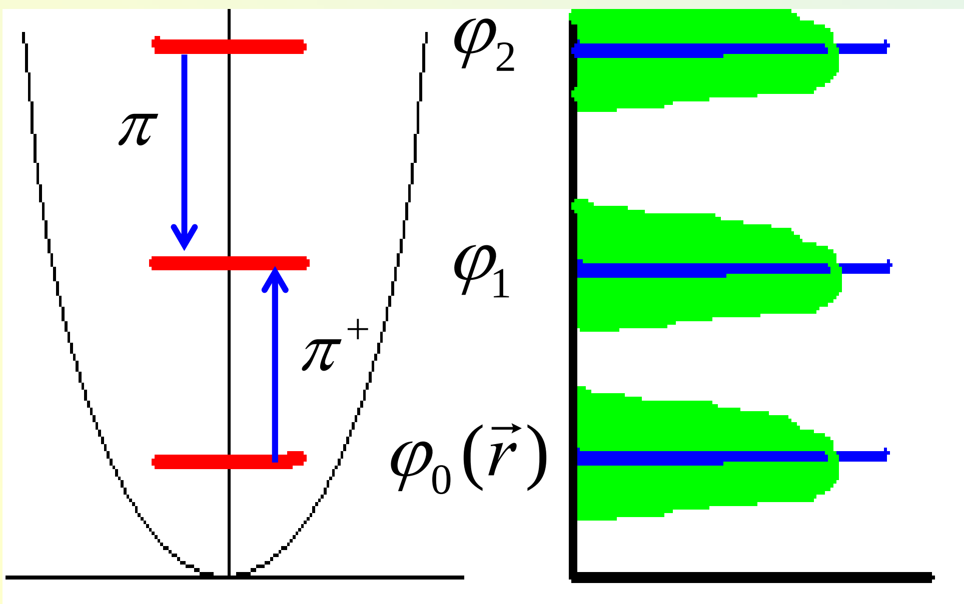
semiconductor
QW / heterostructure
(GaAs/AlGaAs)

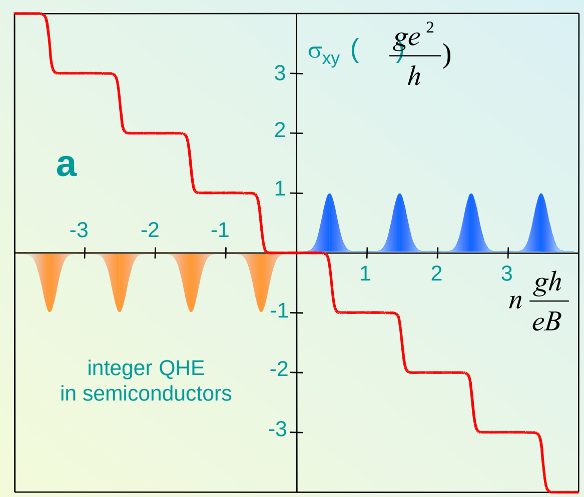
$$\pi\varphi_0 = 0$$

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

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

energies / wave functions





Landau levels and the QHE

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:

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

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

$\pi \rightarrow$ lowering operator
$\pi^+ \rightarrow$ raising operator
} of magnetic oscillator eigenstates ϕ_n

We are able to determine the spectrum of discrete Landau levels

States at zero energy are determined by

monolayer: $\pi\phi_0 = 0$

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

$$H_1\psi = v\begin{pmatrix} 0 & \pi^+ \\ \pi & 0 \end{pmatrix}\begin{pmatrix} \varphi_0 \\ 0 \end{pmatrix} = 0 \qquad\qquad H_2\psi = \frac{-1}{2m}\begin{pmatrix} 0 & \pi^{+2} \\ \pi^2 & 0 \end{pmatrix}\begin{pmatrix} \varphi_{0,1} \\ 0 \end{pmatrix} = 0$$

$$\begin{pmatrix} \varphi_0 \\ 0 \end{pmatrix} \qquad\qquad \begin{pmatrix} \varphi_0 \\ 0 \end{pmatrix}, \begin{pmatrix} \varphi_1 \\ 0 \end{pmatrix}$$

$$\boxed{\varepsilon = 0}$$

***4J*-degenerate**
zero-energy Landau level
J=1 - monolayer, J=2 - bilayer

$$\begin{pmatrix} 0 & \left(-\pi^+\right)^J & & \\ (-\pi)^J & 0 & & \\ & & 0 & \left(\pi^+\right)^J \\ & & \pi^J & 0 \end{pmatrix} \begin{array}{c} \begin{array}{cc} & \text{valley index} \end{array} \\ \begin{pmatrix} A & + \\ \tilde{B} & + \\ \tilde{B} & - \\ A & - \end{pmatrix} \end{array}$$

also, two-fold real spin degeneracy

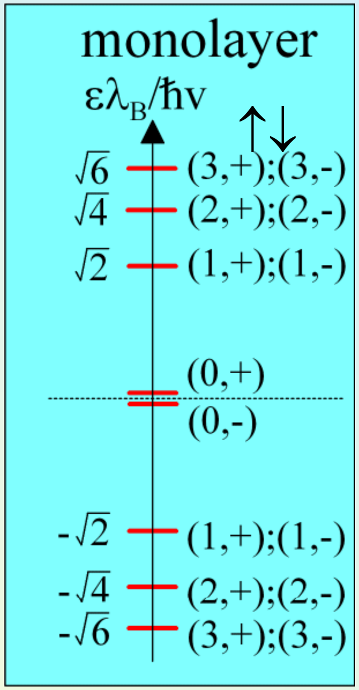
monolayer:

energy scale $\hbar v/\lambda_B$

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

state at zero energy:

$$\pi\phi_0 = 0$$



Monolayer, Berry's phase π

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

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

4-fold degenerate Landau levels

$$\varepsilon^{\pm} = \pm\sqrt{2n}\,\frac{v}{\lambda_B}$$

bilayer:

energy scale $\hbar\omega_c$

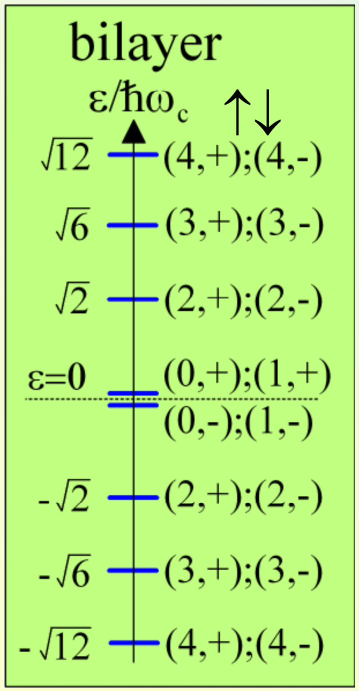
where $\omega_c = \dfrac{eB}{m}$

$m \sim 0.05 m_e$

states at zero energy:

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

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



Bilayer, Berry's phase 2π

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

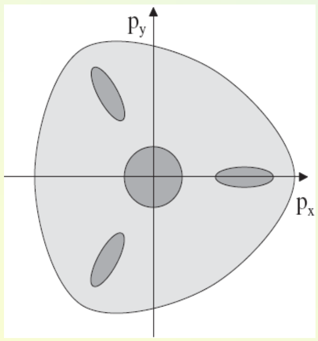
$$\varepsilon^{\pm} = \pm\hbar\omega_c\sqrt{n(n-1)}$$

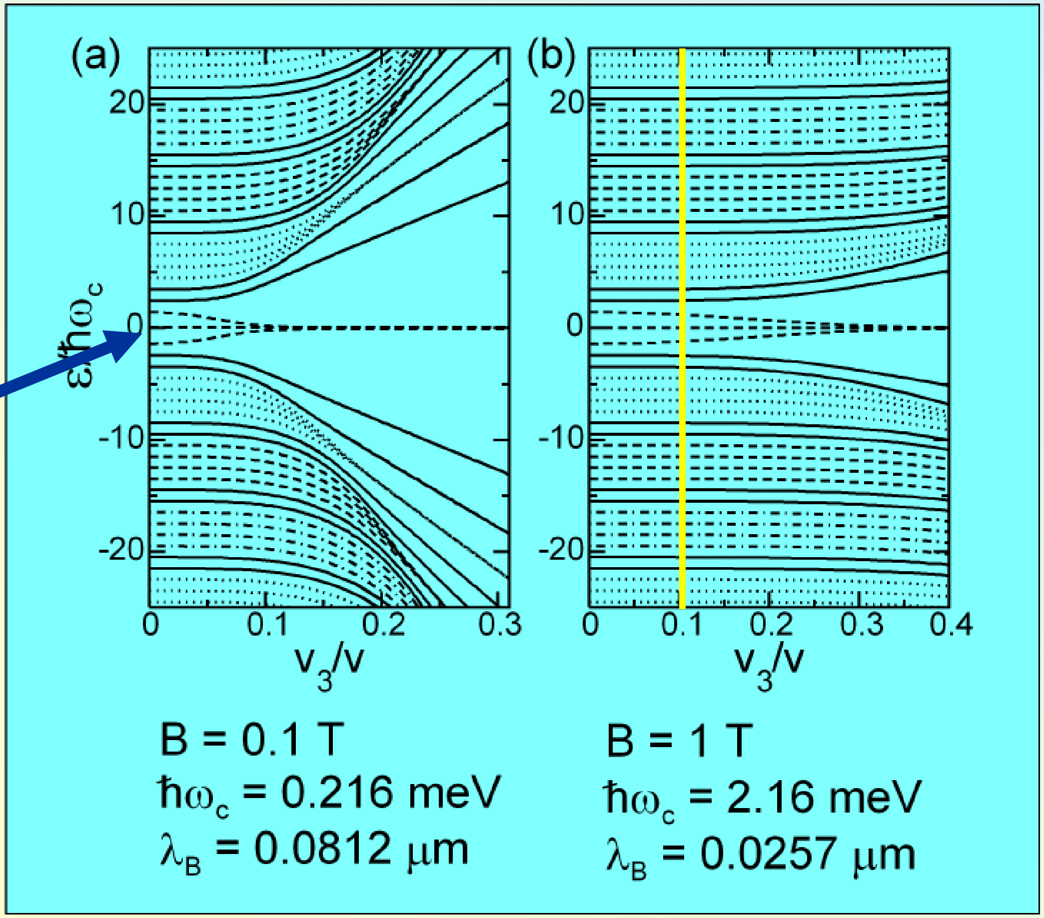
***8*-fold degenerate $\varepsilon=0$ Landau level**

McCann, VF - Phys. Rev. Lett. 96, 086805 (2006)

$$\hat{H}_2 = -\frac{v^2}{\gamma_1}\begin{pmatrix} 0 & (\pi^\dagger)^2 \\ \pi^2 & 0 \end{pmatrix} + \xi v_3 \begin{pmatrix} 0 & \pi \\ \pi^\dagger & 0 \end{pmatrix}$$

$$\frac{v_3}{v} \sim 0.1$$





***8*-fold degenerate zero-energy Landau level**

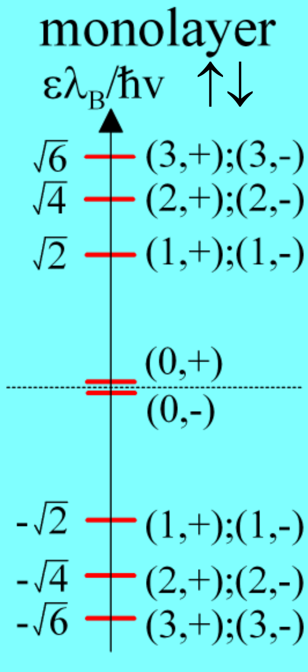
Effect of the trigonal warping term

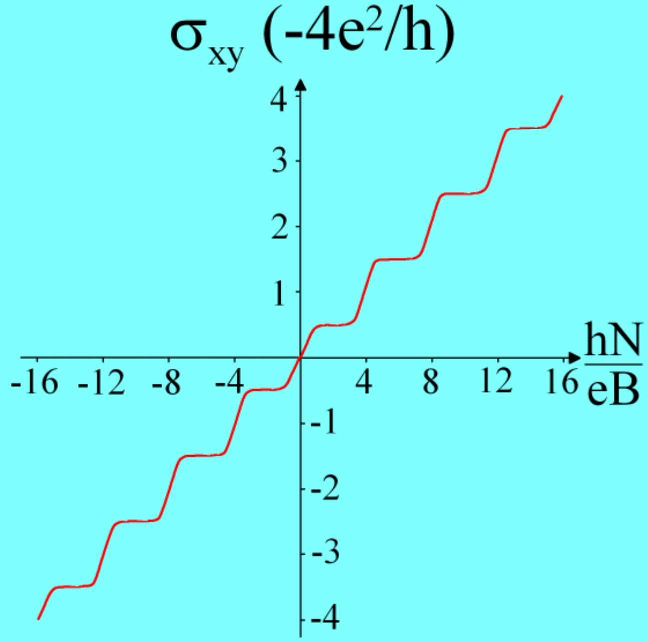
monolayer:

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

state at zero energy:

$$\pi\phi_0 = 0$$





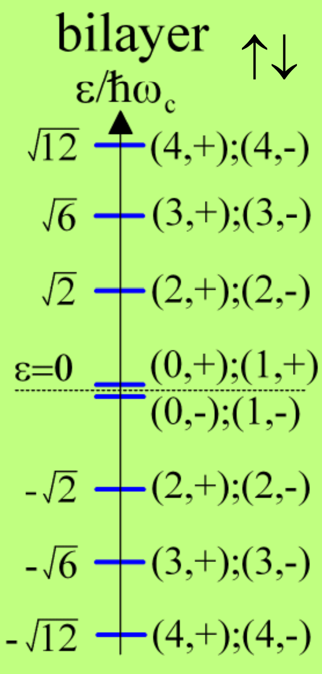
bilayer:

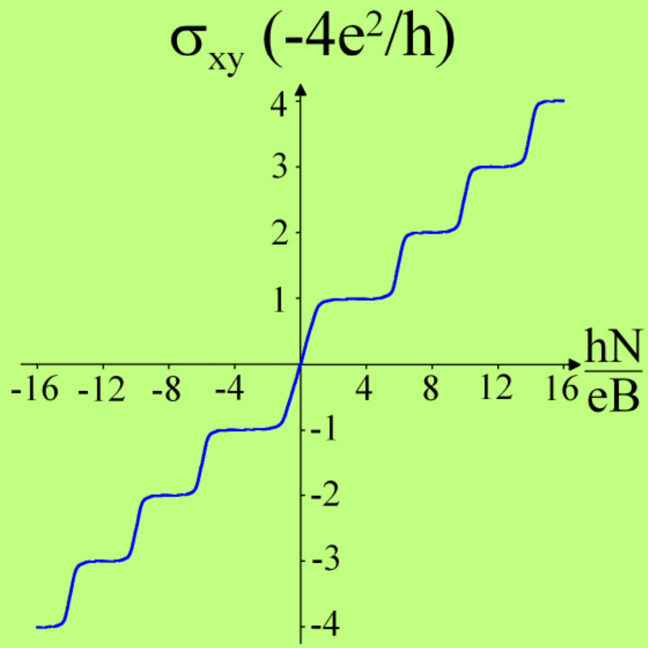
$$H = \frac{-1}{2m} \begin{pmatrix} 0 & (\pi^{+})^2 \\ \pi^2 & 0 \end{pmatrix}$$

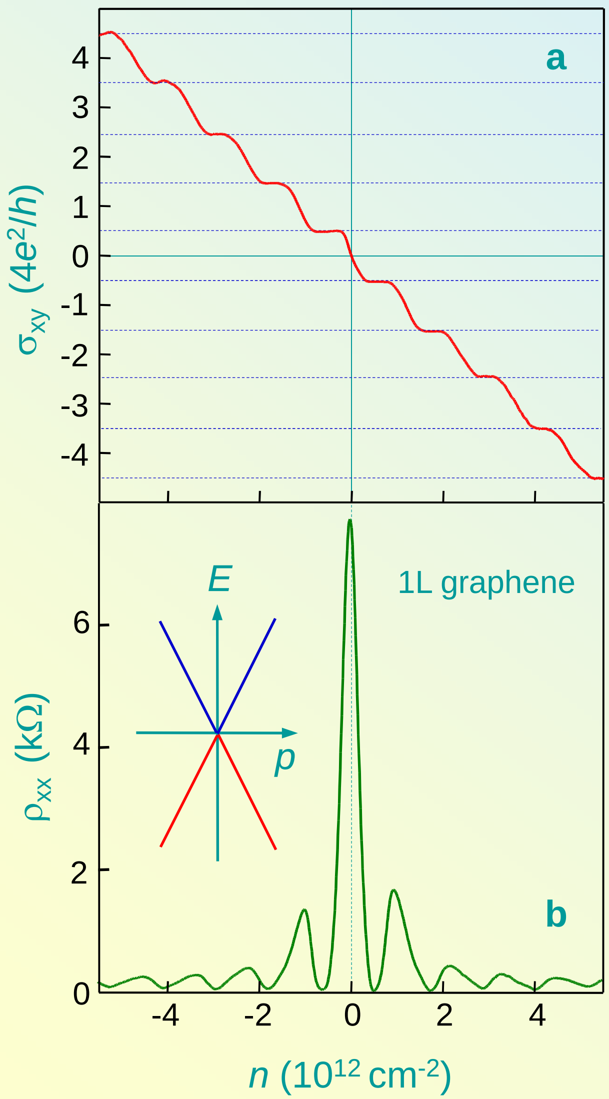
states at zero energy:

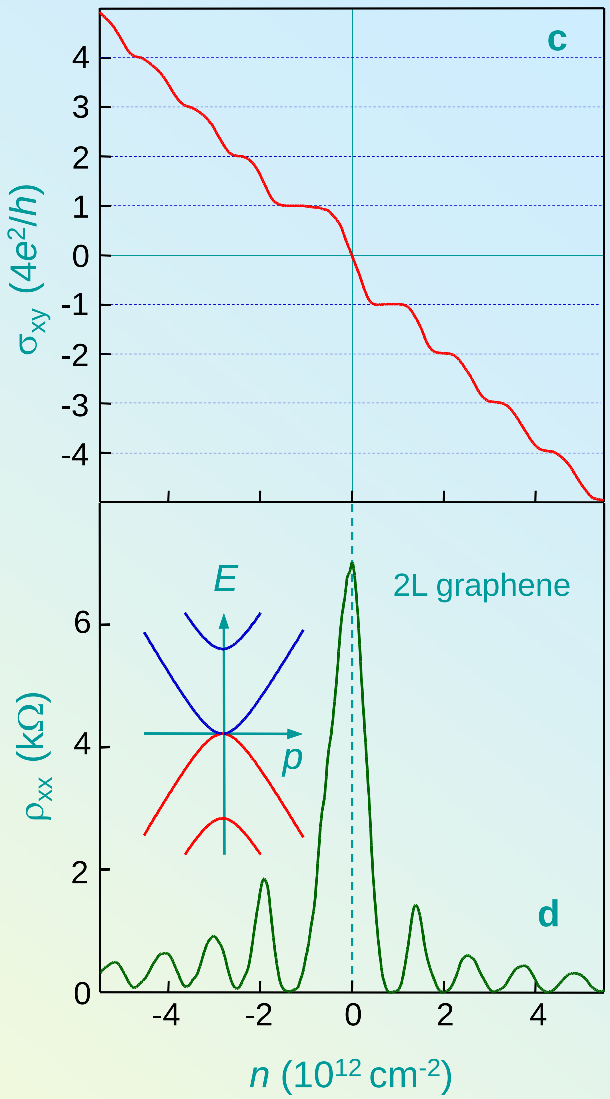
$$\pi^2\phi_0 = 0$$

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







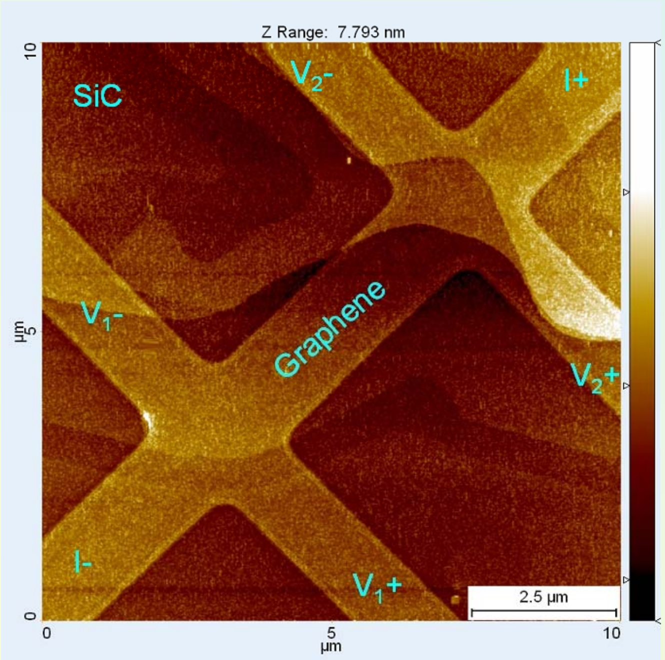


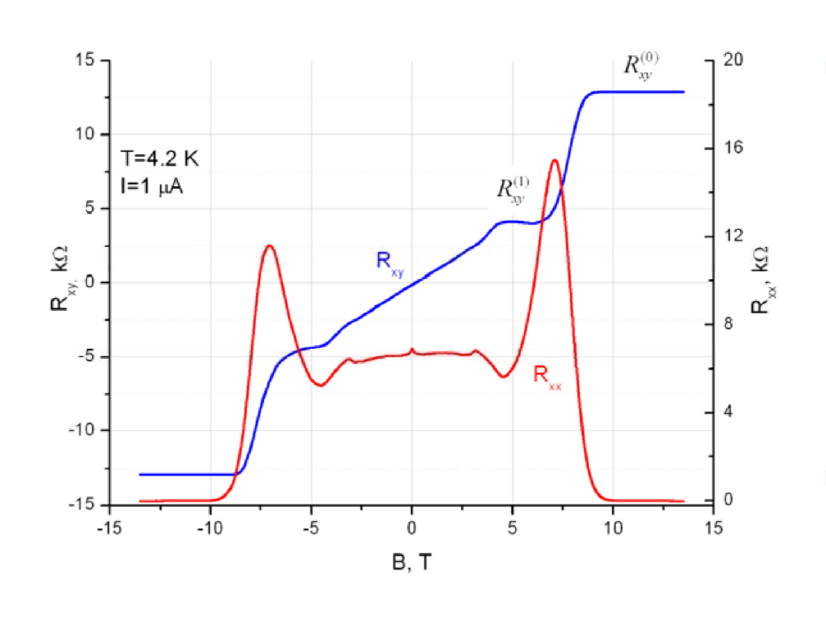
Unconventional quantum Hall effect and Berry's phase of *2π* in bilayer graphene

K.Novoselov, E.McCann, S.Morozov, VF, M.Katsnelson, U.Zeitler, D.Jiang, F.Schedin, A.Geim

Nature Physics 2, 177 (2006)

QHE in graphene synthesised on SiC

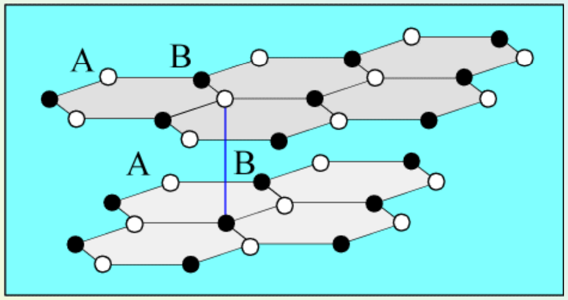




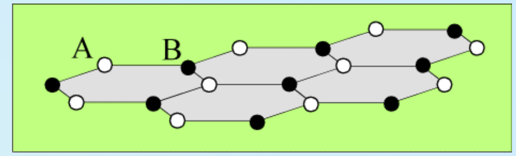
QHE resistance quantisation with accuracy of 3 parts per billion.

A. Tzalenchuk, S. Lara-Avila, A. Kalaboukhov, S. Paolillo, M. Syväjärvi, R. Yakimova, O. Kazakova, T.J.B.M. Janssen, V. Fal’ko, S. Kubatkin, *Towards Towards Quantum Resistance Standard Based on Epitaxial Graphene*, arXiv:0909.1220 – to appear in Nature Nanotechnology

Bilayer graphene



Monolayer graphene



Band structure of bilayer graphene, Berry's phase *2π*, effect of trigonal warping and the Lifshitz transition.

Landau levels and the quantum Hall effect in bilayer and monolayer graphene.

Interlayer asymmetry gap in bilayers.

Interlayer asymmetry gap in bilayer graphene

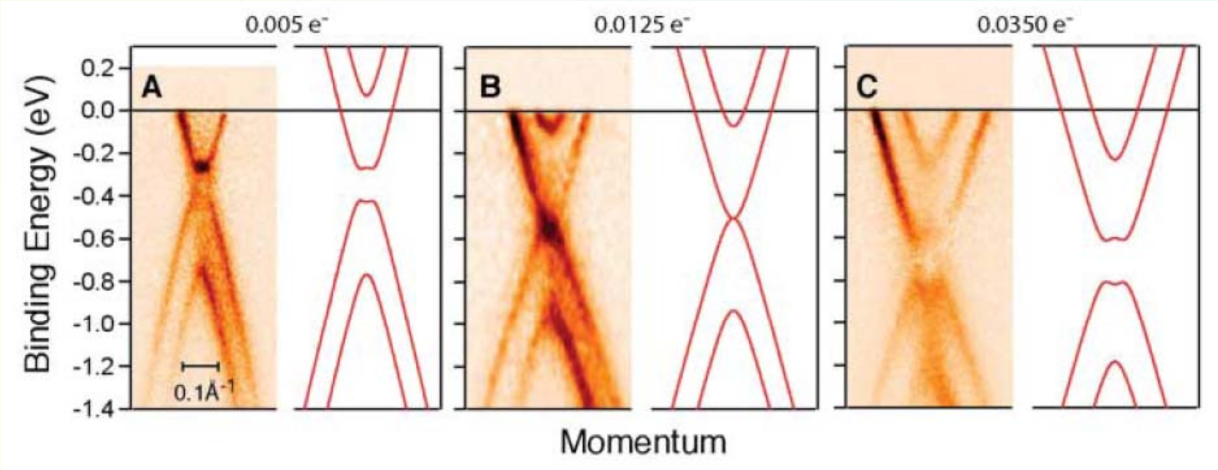
$$\hat{H}_2 = -\frac{v^2}{\gamma_1}\begin{pmatrix} 0 & (\pi^\dagger)^2 \\ \pi^2 & 0 \end{pmatrix} + \xi v_3 \begin{pmatrix} 0 & \pi \\ \pi^\dagger & 0 \end{pmatrix}$$

$$+ \begin{pmatrix} \xi\Delta & 0 \\ 0 & -\xi\Delta \end{pmatrix}$$

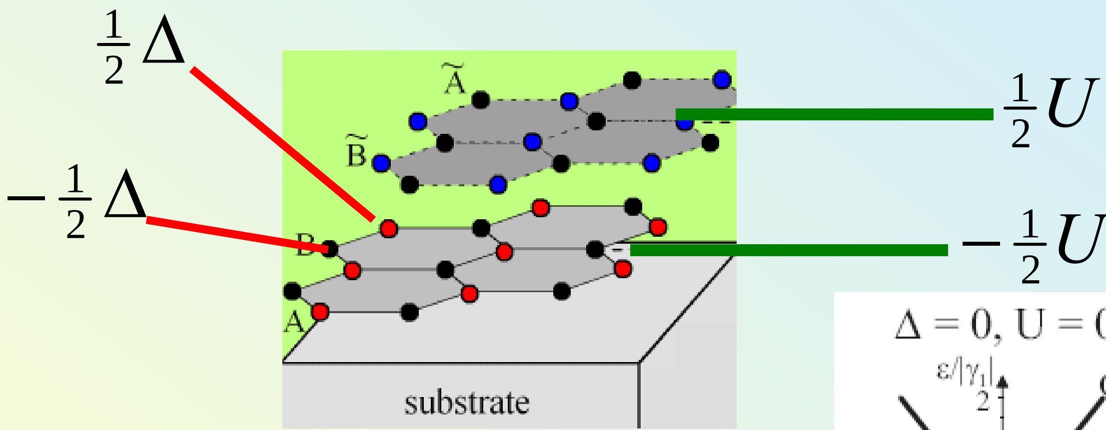
inter-layer asymmetry gap
(can be controlled using electrostatic gate)

McCann, VF - PRL 96, 086805 (2006)
McCann - PRB 74, 161403 (2006)

T. Ohta *et al* – Science 313, 951 (‘06)
(Rotenberg’s group at Berkeley NL)

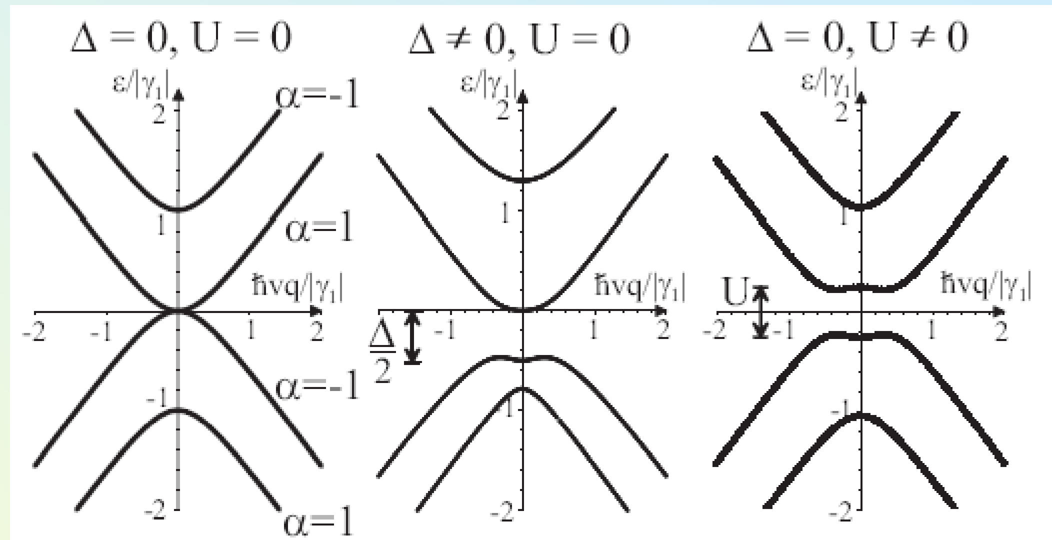


Interlayer asymmetry gap

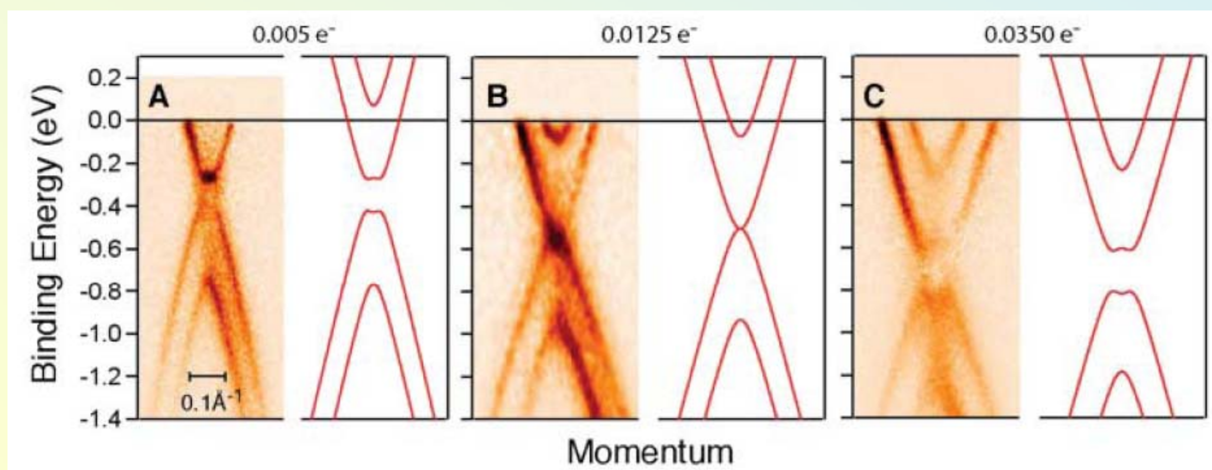


Mucha-Kruczynski, Tsyplyatyev, Grishin, McCann, VF, Boswick, Rotenberg Phys. Rev. B 77, 195403 (2008)

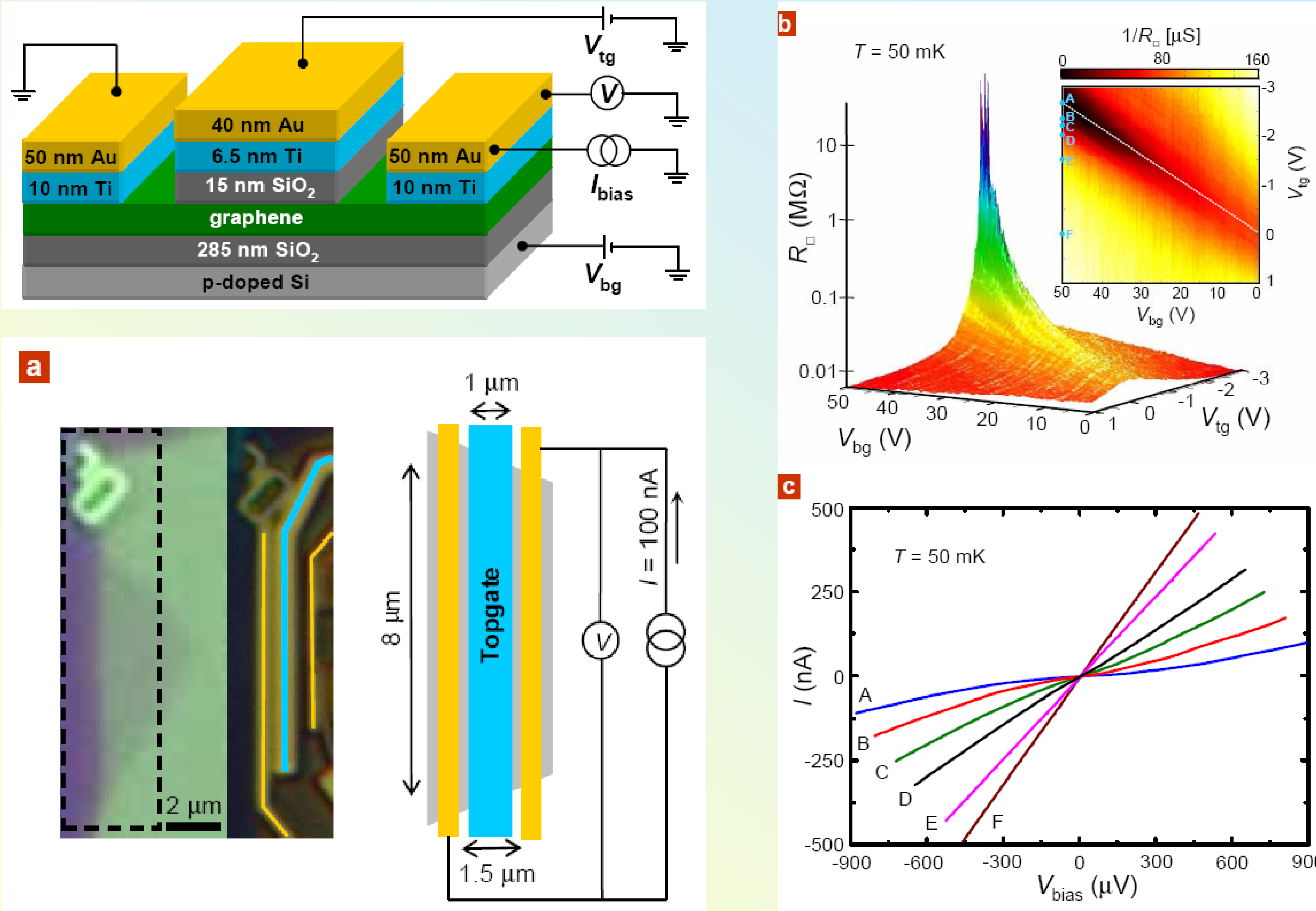
McCann, VF - PRL 96, 086805 (2006)
McCann - PRB 74, 161403 (2006)



T. Ohta *et al* – Science 313, 951 (‘06)
(Rotenberg’s group at Berkeley NL)
SiC-based highly doped
bilayer graphene

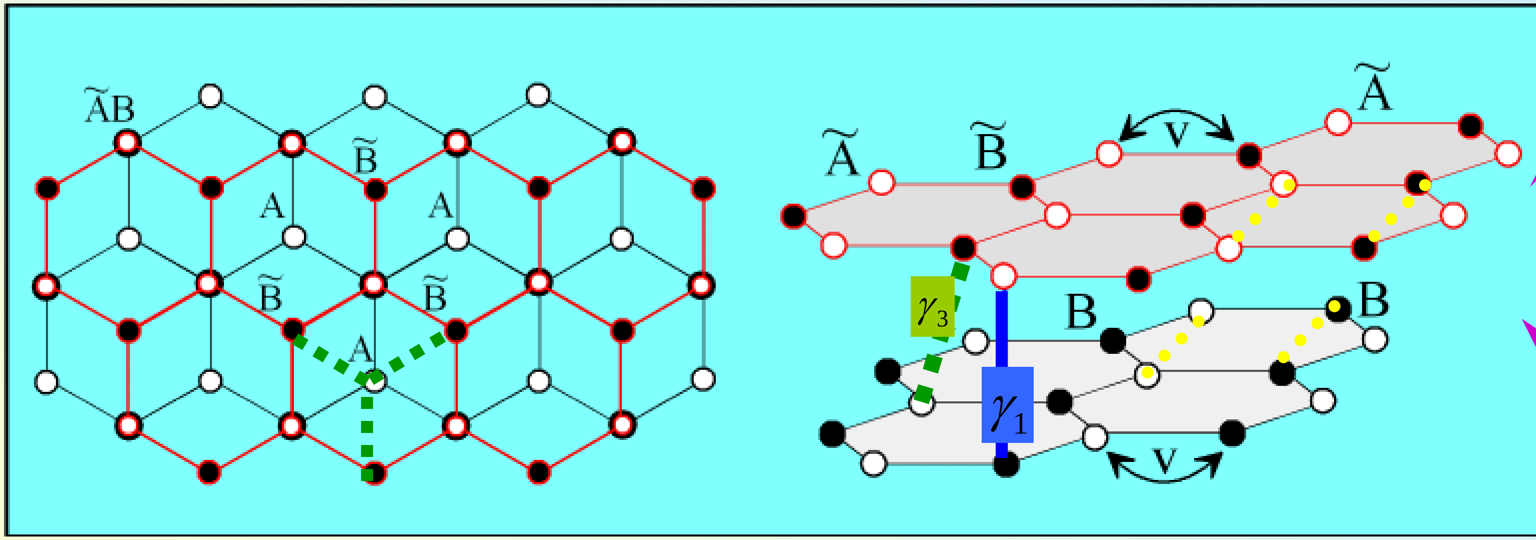


Gate-controlled interlayer asymmetry gap (transport measurements)



Oostinga, Heersche, Liu, Morpurgo, and Vandersypen, Nature Physics (2007)

How robust is the degeneracy of $\varepsilon_0 = \varepsilon_1 = 0$ Landau level in bilayer graphene?



$$\Delta = E_z d$$

Direct inter-layer $A\tilde{B}$ hops
(warping term, Lifshitz trans.)

$$\varepsilon_0 = \varepsilon_1$$

McCann, VF - PRL 96, 086805 (2006)

Distant intra-layer
AA,*BB* hops

$$|\,\varepsilon_1 - \varepsilon_0\,| = \delta\hbar\omega_c$$

$$\delta \sim \frac{\gamma_1\gamma_4}{\gamma_0^2} \sim 10^{-2(3)}$$

Inter-layer asymmetry
(substrate, gate)

$$|\,\varepsilon_1 - \varepsilon_0\,| = \Delta$$