Landau level degeneracy and Quantum Hall effect in a graphite bilayer

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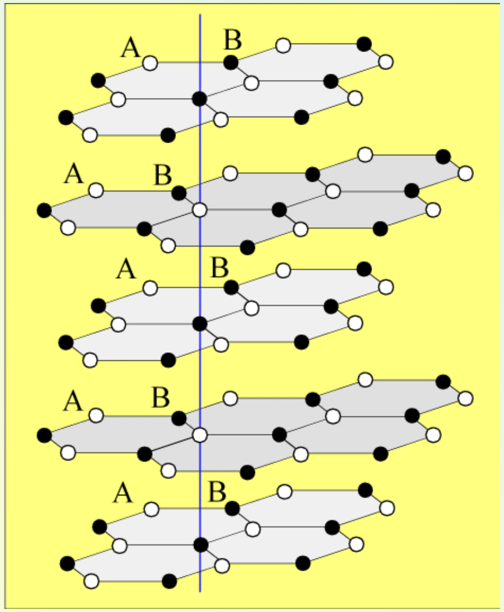
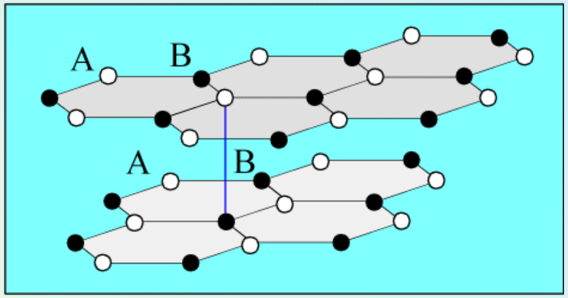
Preprint: E McCann and VI Fal'ko, cond-mat/0510237

Graphite



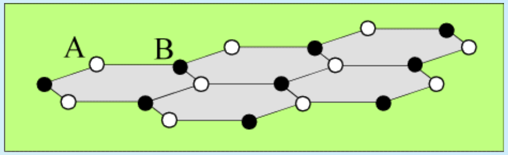
Three dimensional layered material with hexagonal 2D layers [shown here with Bernal (AB) stacking]

Bilayer



Two dimensional material;
Low energy Hamiltonian?

Monolayer



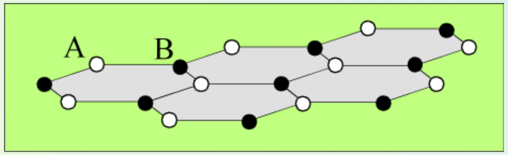
Two dimensional material;
zero gap semiconductor (?);
Dirac spectrum of electrons

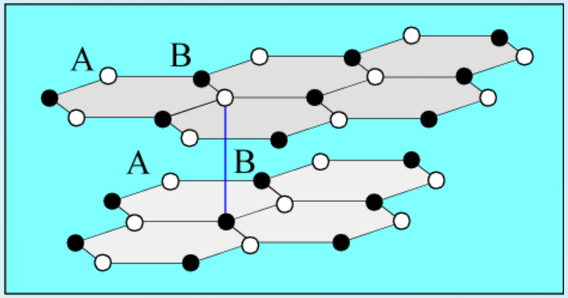
Fabricated two years ago by Manchester group, Novoselov *et al*, Science 306, 666 (2004).

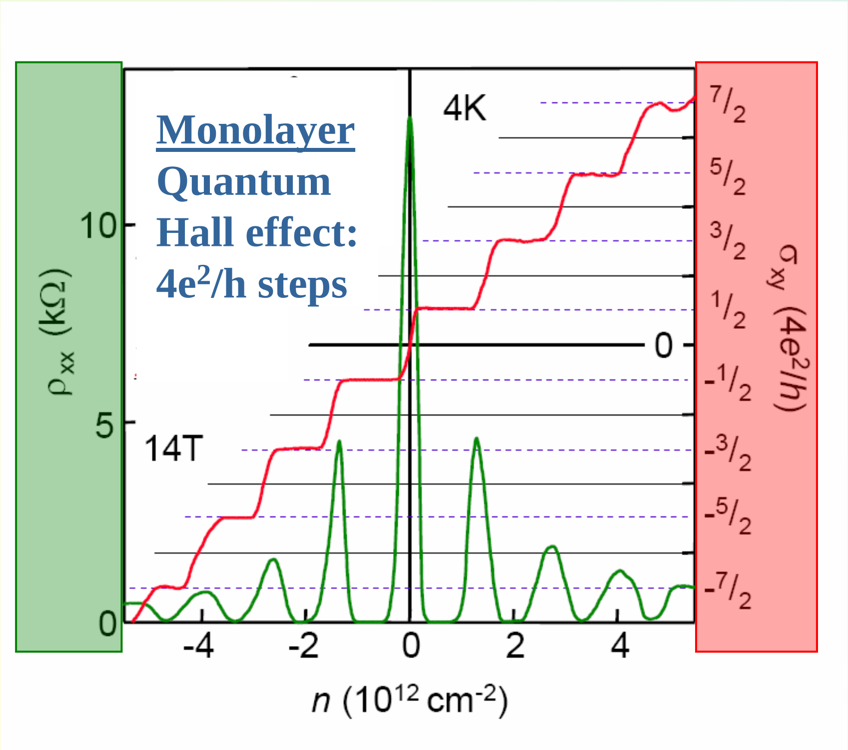
Further reports of quantum Hall effect measurements;
Manchester group: Novoselov *et al*, Nature 438, 197 (2005) [talk of Kostya Novoselov, yesterday];
Columbia group: Zhang *et al*, Nature 438, 201 (2005) [talk of Philip Kim, previous speaker].

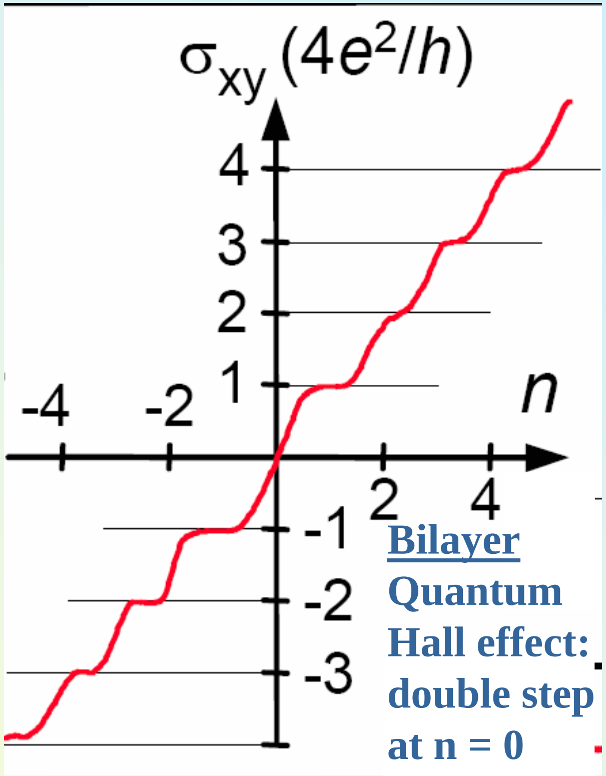
Monolayer

Bilayer









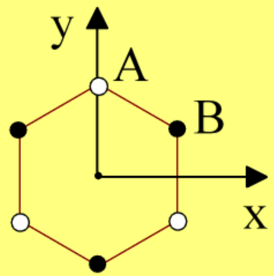
Novoselov *et al*, Nature 438, 197 (2005):

Hall conductivity σ_{xy} for monolayer (left) and bilayer (right).

Electronic dispersion of a monolayer

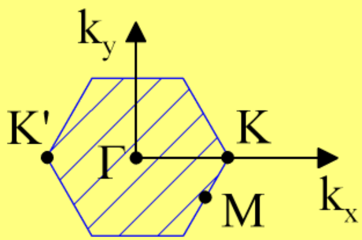
Saito *et al*, "Physical Properties of Carbon Nanotubes" (Imperial College Press, London, 1998)

Symmetrical unit cell

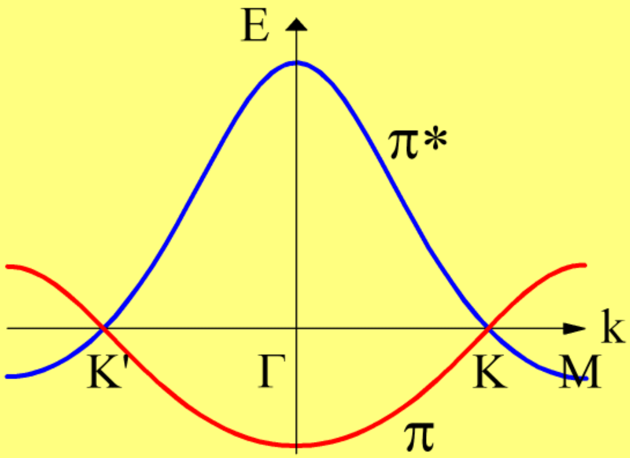


Two non-equivalent carbon positions

Brillouin zone



Two non-equivalent K-points



Two bands: no energy gap at the K-points

Tight binding model of a monolayer

Saito *et al*, "Physical Properties of Carbon Nanotubes" (Imperial College Press, London, 1998): Chapter 2.

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

Eigenfunction

$$\Psi_j(\mathbf{k},\mathbf{r}) = \sum_{i=1}^{2} C_{ji}(\mathbf{k})\,\Phi_i(\mathbf{k},\mathbf{r})$$

Transfer integral matrix $\mathcal{H}_{ij} = <\Phi_i|H|\Phi_j>$

Overlap integral matrix $\mathcal{S}_{ij} = <\Phi_i|\Phi_j>$

Column vector $\mathcal{C}_j = \begin{pmatrix} C_{j1} \\ C_{j2} \end{pmatrix}$

Eigenvalue equation

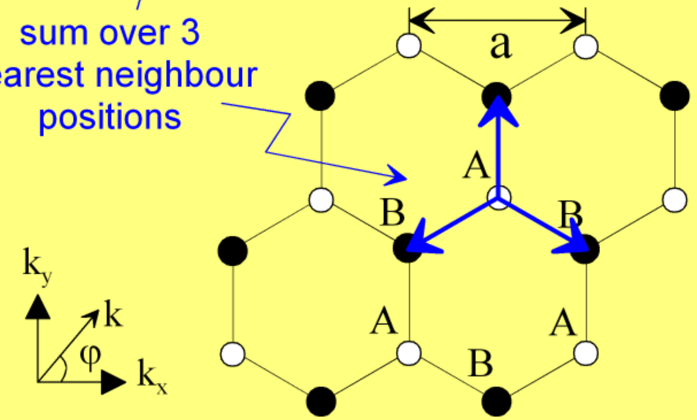
$$\mathcal{H}\mathcal{C}_j = \varepsilon_j \mathcal{S}\mathcal{C}_j$$

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



$$\mathcal{H}_{AB} = -\gamma_0 f(\mathbf{k})\ ; \quad \mathcal{H}_{BA} = -\gamma_0 f^*(\mathbf{k})$$

$$f(\mathbf{k}) = e^{ik_y a/\sqrt{3}} + 2e^{-ik_y a/2\sqrt{3}}\cos(k_x a/2)$$

Tight binding model of a monolayer

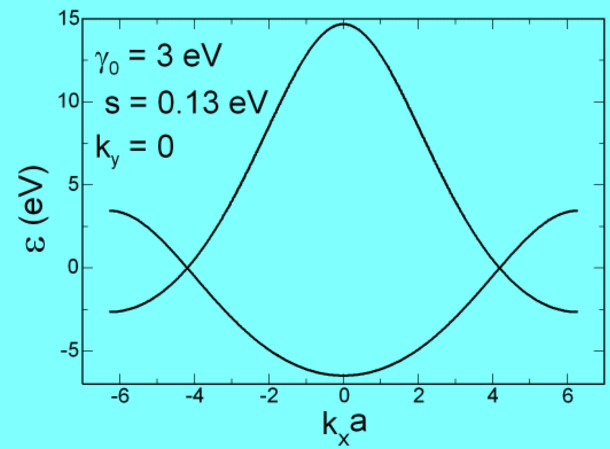
Saito *et al*, "Physical Properties of Carbon Nanotubes" (Imperial College Press, London, 1998): Chapter 2.

Transfer integral matrix $\quad \mathcal{H} = \begin{pmatrix} 0 & -\gamma_0 f(\mathbf{k}) \\ -\gamma_0 f^*(\mathbf{k}) & 0 \end{pmatrix}$

Overlap integral matrix $\quad \mathcal{S} = \begin{pmatrix} 1 & s f(\mathbf{k}) \\ s f^*(\mathbf{k}) & 1 \end{pmatrix}$

Eigenvalue equation $\quad \mathcal{H}C_j = \varepsilon_j \mathcal{S} C_j$

$$\varepsilon = \frac{\pm\gamma_0|f(\mathbf{k})|}{1 \mp s|f(\mathbf{k})|}$$

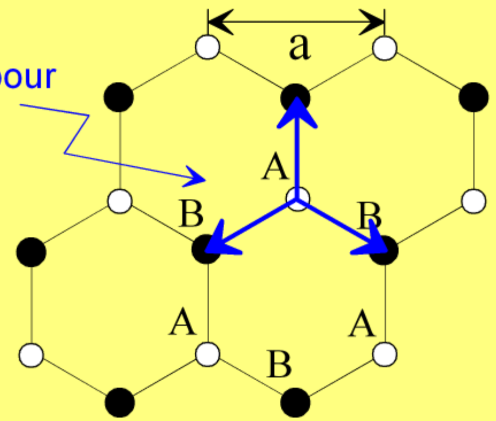


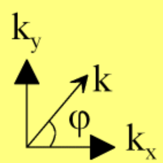
Transfer integral on a hexagonal lattice

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

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

sum over 3 nearest neighbour positions





$$\mathcal{H}_{AB} = -\gamma_0 f(\mathbf{k})\;; \quad \mathcal{H}_{BA} = -\gamma_0 f^*(\mathbf{k})$$

$$f(\mathbf{k}) = e^{ik_y a/\sqrt{3}} + 2e^{-ik_y a/2\sqrt{3}}\cos(k_x a/2)$$

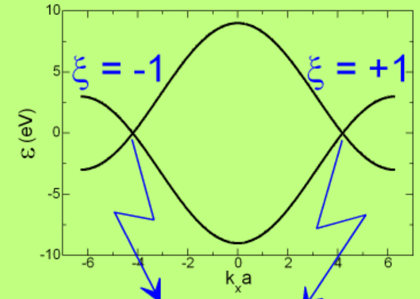
Linear expansion near K point

Transfer integral matrix

$$\mathcal{H} = \begin{pmatrix} 0 & -\gamma_0 f(\mathbf{k}) \\ -\gamma_0 f^*(\mathbf{k}) & 0 \end{pmatrix}$$

Neglect off-diagonal overlap

$$\langle \phi_A | \phi_B \rangle = 0$$



$$\mathcal{H}_{AB} = -\gamma_0 f(\mathbf{k}) \approx v(\xi p_x - ip_y)$$

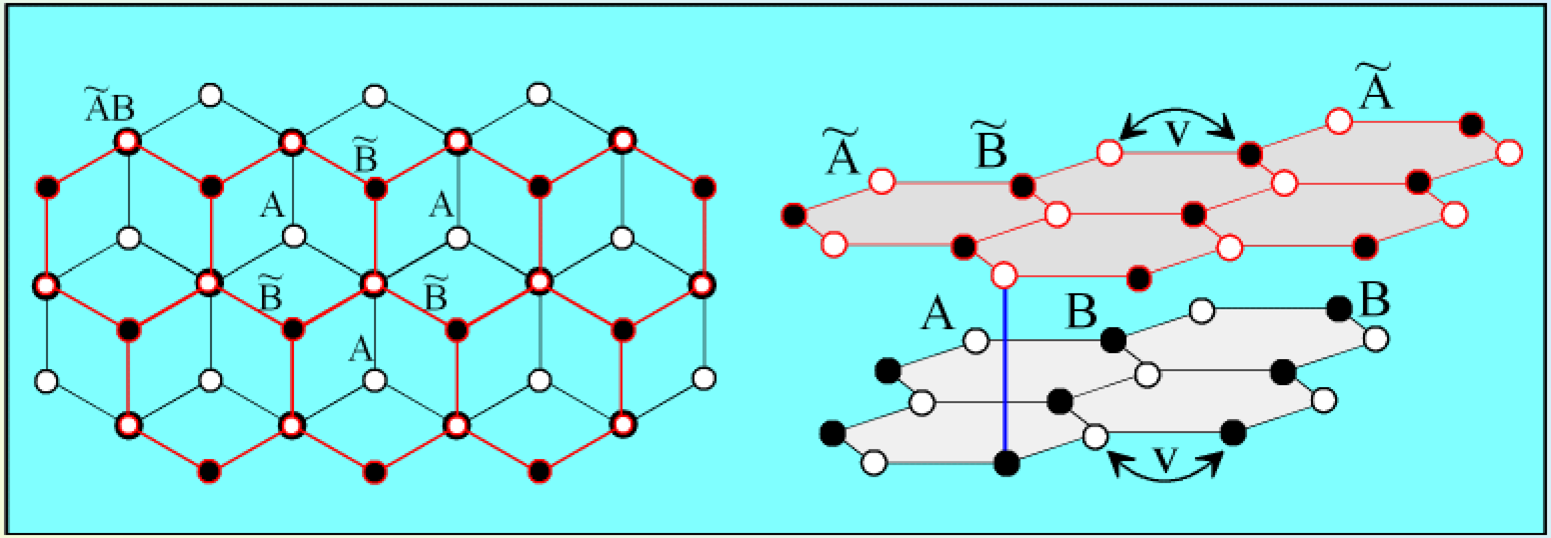
ξ = +1 or -1 labels K point

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

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

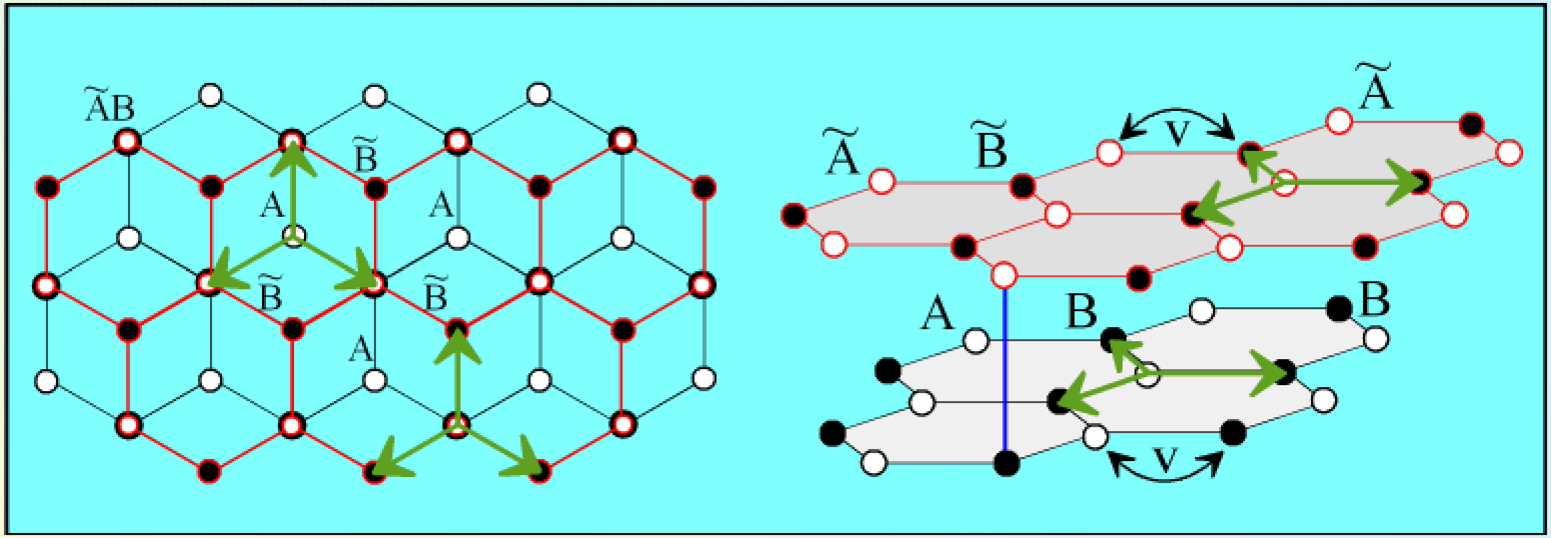
hopping strength proportional to velocity

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



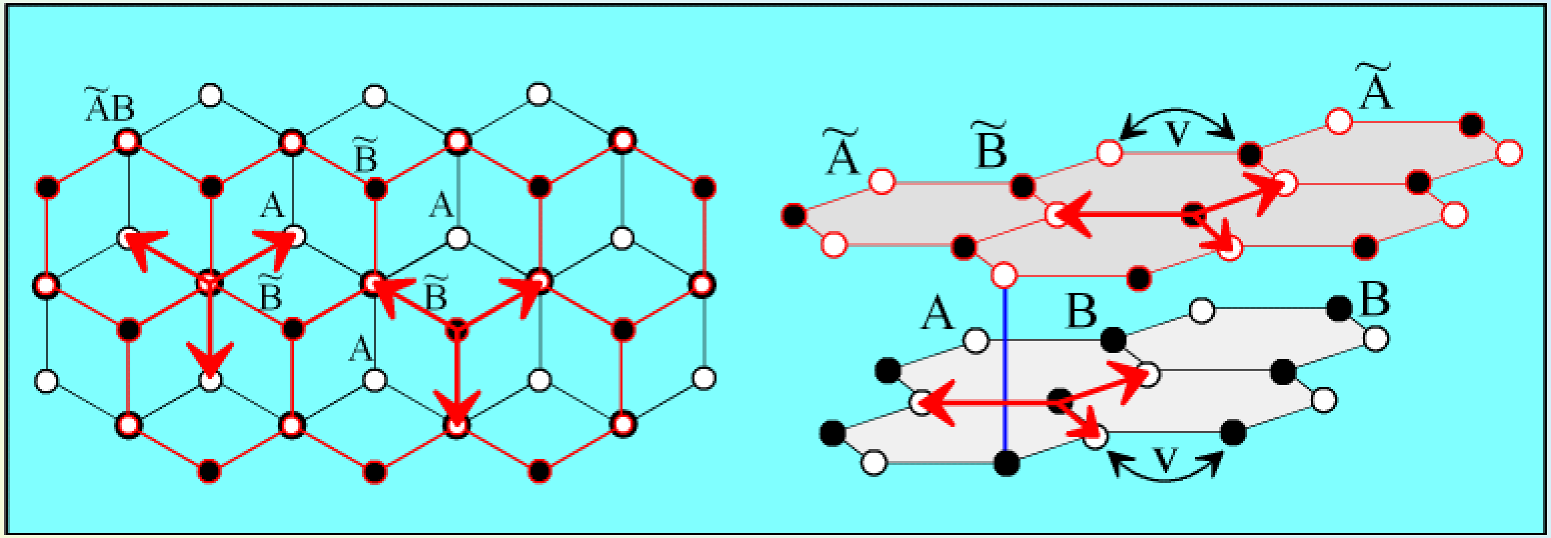
4 atoms
per unit cell

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



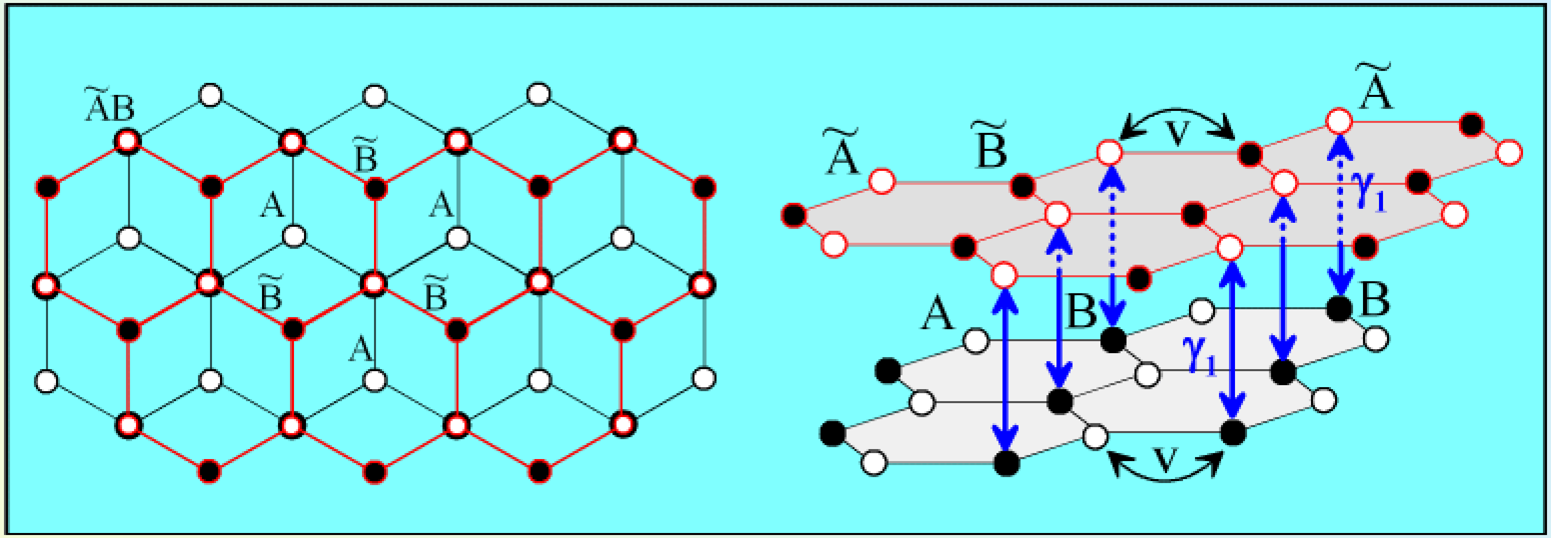
(A to B) and ($\tilde{A}$ to $\tilde{B}$) hopping given by $-\gamma_0 f^*$

$$\begin{array}{cc} & \begin{array}{cccc} A & \tilde{B} & \tilde{A} & B \end{array} \\ \mathcal{H} = & \left(\begin{array}{cccc} & & & \\ & & -\gamma_0 f^* & \\ & & & \\ -\gamma_0 f^* & & & \end{array}\right) \begin{array}{c} A \\ \tilde{B} \\ \tilde{A} \\ B \end{array} \end{array}$$



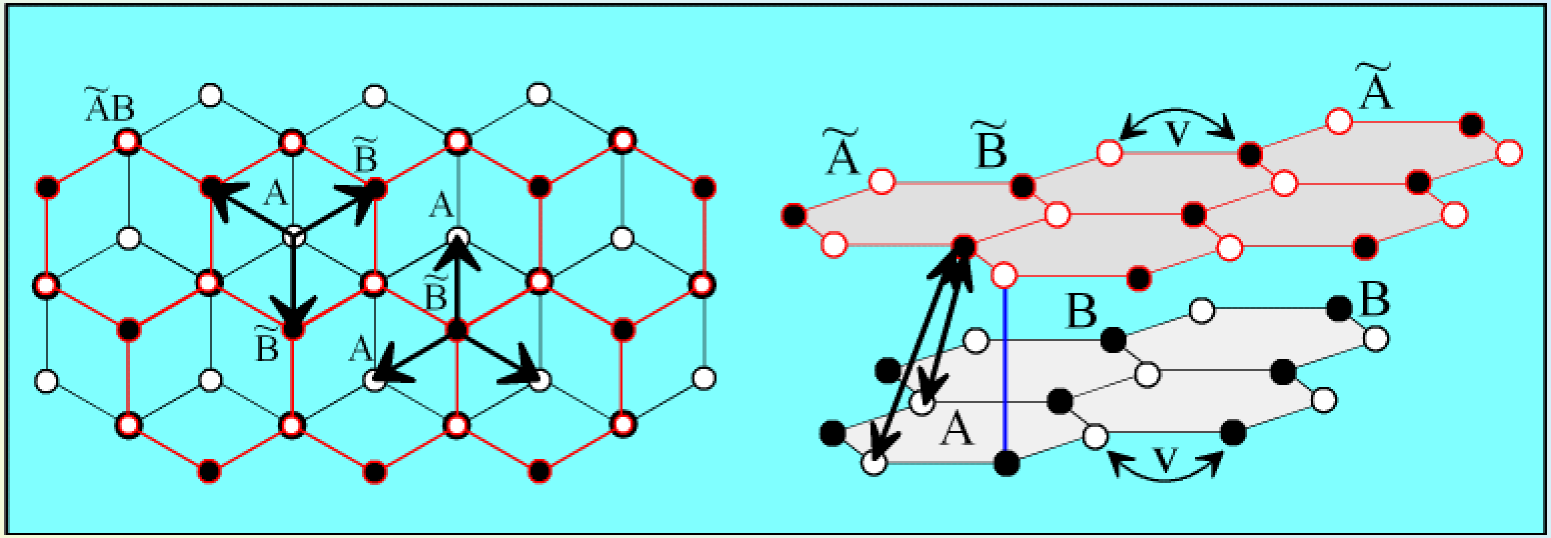
(B to A) and ($\tilde{B}$ to $\tilde{A}$) hopping given by $-\gamma_0 f$

$$\begin{array}{c} \\ \mathcal{H} = \end{array} \begin{array}{c} \begin{array}{cccc} A & \tilde{B} & \tilde{A} & B \end{array} \\ \begin{pmatrix} & & & -\gamma_0 f \\ & & -\gamma_0 f^* & \\ & -\gamma_0 f & & \\ -\gamma_0 f^* & & & \end{pmatrix} \end{array} \begin{array}{c} \\ A \\ \tilde{B} \\ \tilde{A} \\ B \end{array}$$



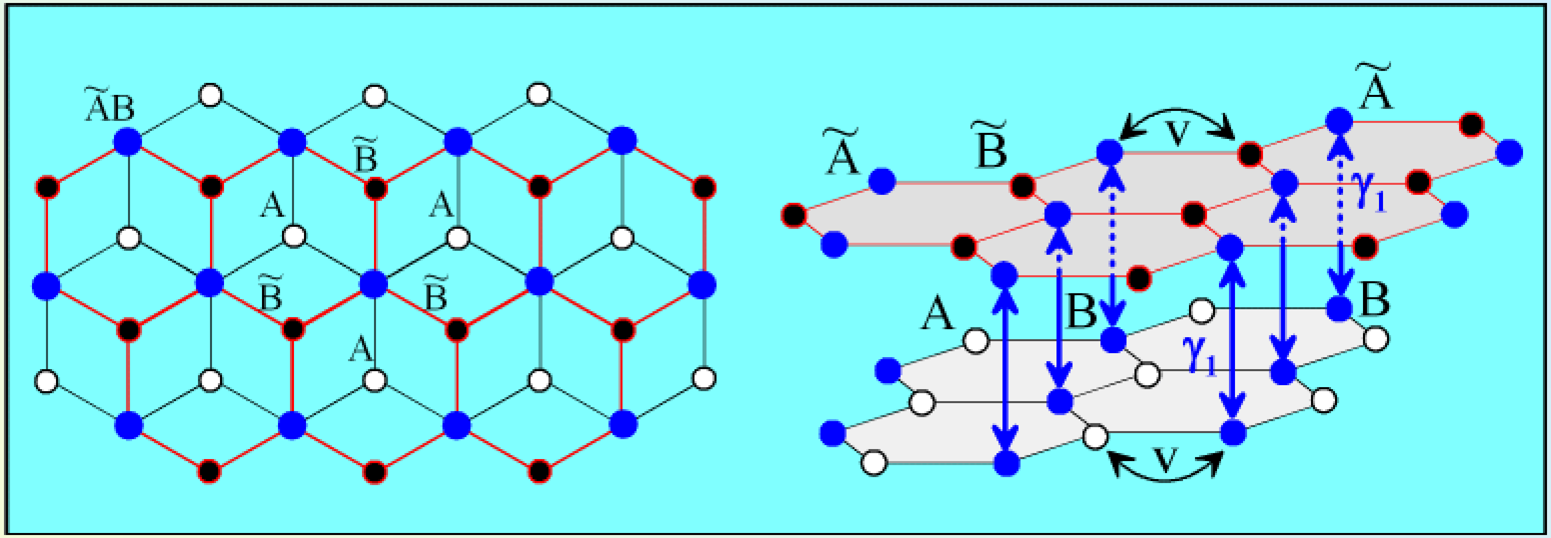
(B to Ã) interlayer hopping parameterised by γ_1

$$
\mathcal{H} = \begin{array}{c} \\ \\ \end{array}
\begin{array}{cc}
\begin{array}{cccc} A & \tilde{B} & \tilde{A} & B \end{array} & \\
\begin{pmatrix} & & & -\gamma_0 f \\ & & -\gamma_0 f^* & \\ & -\gamma_0 f & & \gamma_1 \\ -\gamma_0 f^* & & \gamma_1 & \end{pmatrix} & \begin{array}{c} A \\ \tilde{B} \\ \tilde{A} \\ B \end{array}
\end{array}
$$



($\tilde{B}$ to A) by $-\gamma_3 f^*$
and
(A to $\tilde{B}$) by $-\gamma_3 f$

$$\mathcal{H} = \begin{array}{cc} \begin{array}{cccc} A & \tilde{B} & \tilde{A} & B \end{array} & \\ \begin{pmatrix} & -\gamma_3 f^* & & -\gamma_0 f \\ -\gamma_3 f & & -\gamma_0 f^* & \\ & -\gamma_0 f & & \gamma_1 \\ -\gamma_0 f^* & & \gamma_1 & \end{pmatrix} & \begin{array}{c} A \\ \tilde{B} \\ \tilde{A} \\ B \end{array} \end{array}$$

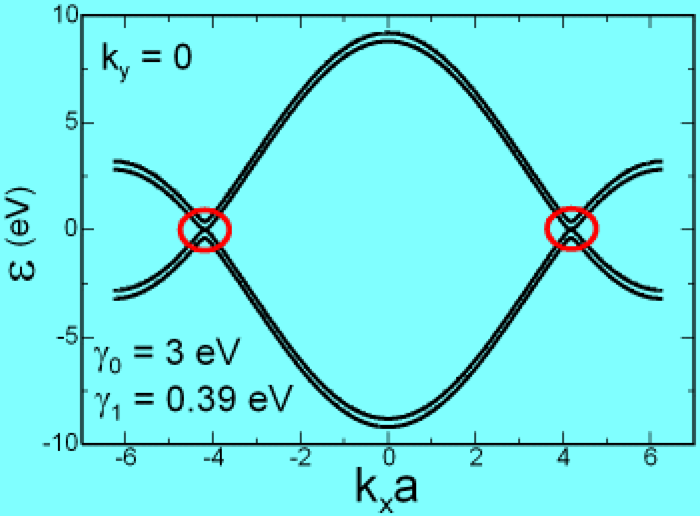


Bilayer transfer integral matrix

$$
\mathcal{H} = \begin{array}{cc}
\begin{array}{cccc} A & \tilde{B} & \tilde{A} & B \end{array} & \\
\begin{pmatrix} 0 & 0 & 0 & -\gamma_0 f \\ 0 & 0 & -\gamma_0 f^* & 0 \\ 0 & -\gamma_0 f & 0 & \gamma_1 \\ -\gamma_0 f^* & 0 & \gamma_1 & 0 \end{pmatrix} & \begin{array}{c} A \\ \tilde{B} \\ \tilde{A} \\ B \end{array}
\end{array}
$$

For $S = \mathrm{I}$:

$$\varepsilon^2 = \frac{\gamma_1^2}{4}\left[\sqrt{1 + \frac{4\gamma_0^2|f(\mathbf{k})|^2}{\gamma_1^2}} \pm 1\right]^2$$



Linear approximation near K point:

$- \gamma_0 f(\mathbf{k}) \approx v(p_x - ip_y)$

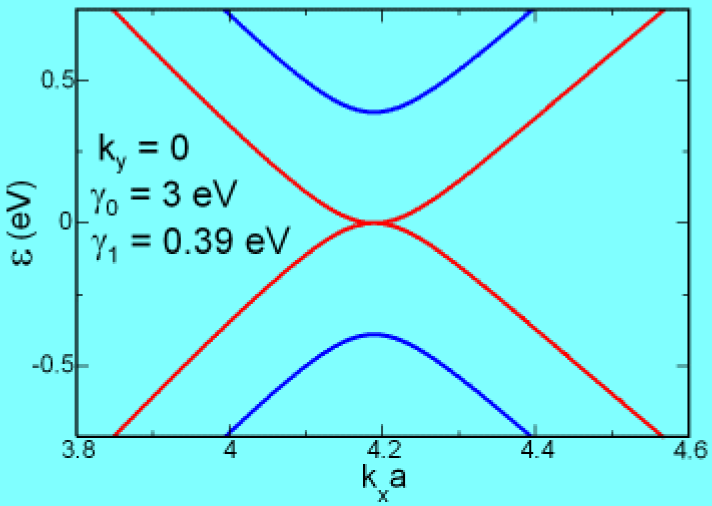
Bilayer Hamiltonian

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

$$\mathcal{H} = \begin{array}{cc} \begin{array}{cccc} A & \tilde{B} & \tilde{A} & B \end{array} & \\ \begin{pmatrix} 0 & 0 & 0 & v\pi^+ \\ 0 & 0 & v\pi & 0 \\ 0 & v\pi^+ & 0 & \gamma_1 \\ v\pi & 0 & \gamma_1 & 0 \end{pmatrix} & \begin{array}{c} A \\ \tilde{B} \\ \tilde{A} \\ B \end{array} \end{array}$$

Linear approximation:

$$\varepsilon^2 = \frac{\gamma_1^{\,2}}{4}\left[\sqrt{1 + \frac{4\hbar v^2|\mathbf{k}|^2}{\gamma_1^{\,2}}} \pm 1\right]^2$$



Linear approximation near K point:

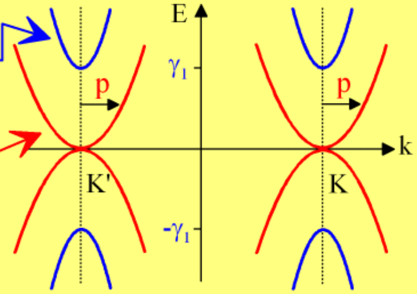
$$-\gamma_0 f(\mathbf{k}) \approx v(p_x - ip_y)$$

Bilayer Hamiltonian

$$\begin{array}{cc} & \begin{array}{cccc} A & \tilde{B} & \tilde{A} & B \end{array} \\ \mathcal{H} = & \begin{pmatrix} 0 & 0 & 0 & v\pi^{+} \\ 0 & 0 & v\pi & 0 \\ 0 & v\pi^{+} & 0 & \gamma_1 \\ v\pi & 0 & \gamma_1 & 0 \end{pmatrix} \begin{array}{c} A \\ \tilde{B} \\ \tilde{A} \\ B \end{array} \end{array}$$

Low energy behaviour

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



Low energy bands:

$$E \approx \pm \frac{\gamma_1}{2}\left[\sqrt{1+\frac{4v^2|p|^2}{\gamma_1^{\,2}}} - 1\right]$$

Crossover from linear spectrum $E = vp$ at higher momenta to quadratic $E = p^2/2m$ at low momenta.

Crossover occurs at $p \approx \gamma_1/2v$.
This corresponds to carrier density $N^* \approx \frac{\gamma_1^{\,2}}{4\pi\hbar^2 v^2}$

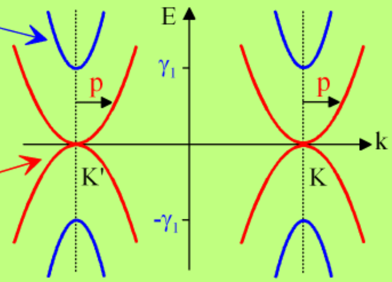
Rough estimate: $N^* \sim 4.4\times10^{12}\,\mathrm{cm}^{-2}$

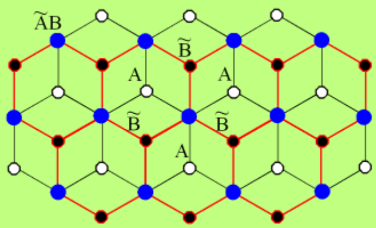
The higher "dimer" band becomes occupied for $N \approx 8N^* \sim 3.5\times10^{13}\,\mathrm{cm}^{-2}$

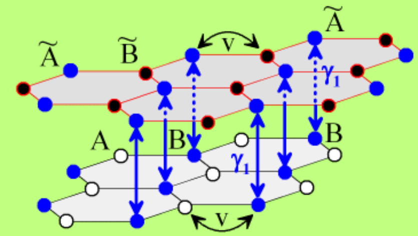
Two component Hamiltonian in basis of A and $\tilde{B}$ orbitals

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

Quadratic dispersion at low energy:
$E = \pm \frac{p^2}{2m}$

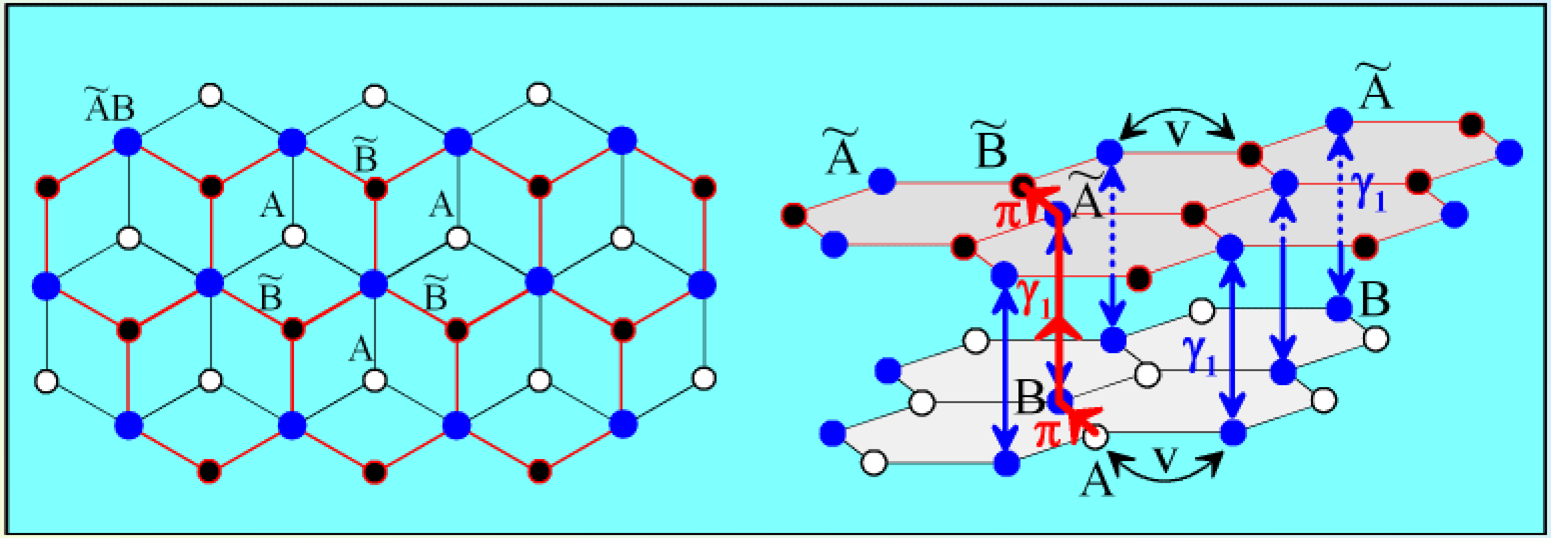






$$\begin{array}{c c}
 & \begin{array}{cccc} A & \tilde{B} & \tilde{A} & B \end{array} \\
\mathcal{H} = & \begin{pmatrix} 0 & 0 & 0 & v\pi^+ \\ 0 & 0 & v\pi & 0 \\ 0 & v\pi^+ & 0 & \gamma_1 \\ v\pi & 0 & \gamma_1 & 0 \end{pmatrix} \begin{array}{c} A \\ \tilde{B} \\ \tilde{A} \\ B \end{array}
\end{array}$$

We eliminate $\tilde{A}$ and B components (dimers) to get a Hamiltonian describing effect hopping between A and $\tilde{B}$ sites



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)

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

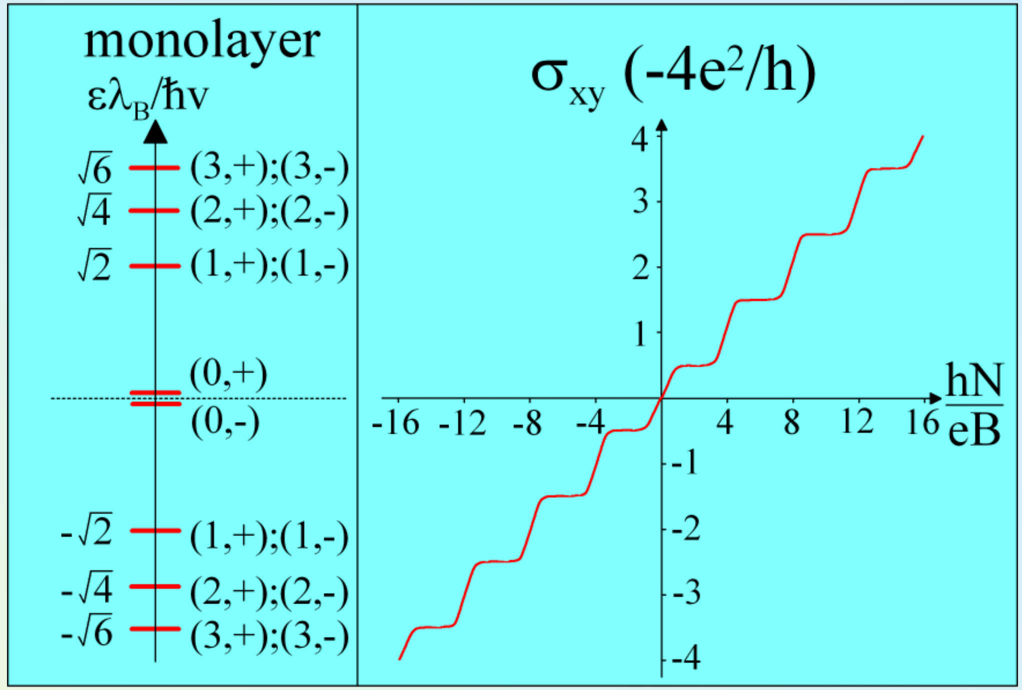
monolayer:

energy scale $\hbar v/\lambda_B$

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

state at zero energy:

$$\pi\phi_0 = 0$$



bilayer:

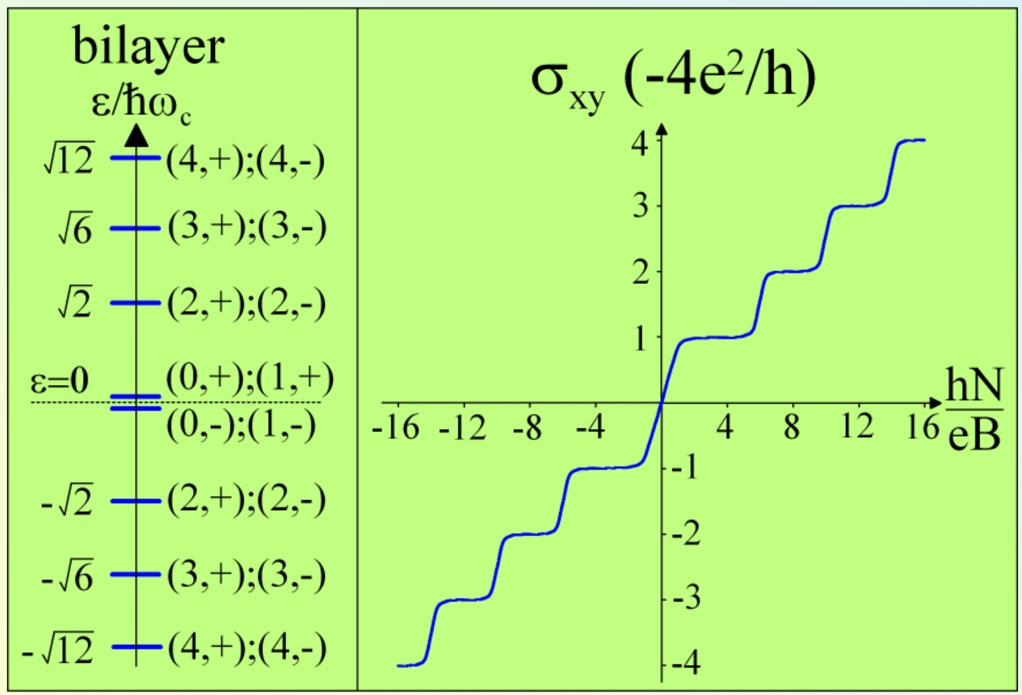
energy scale $\hbar\omega_c$

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

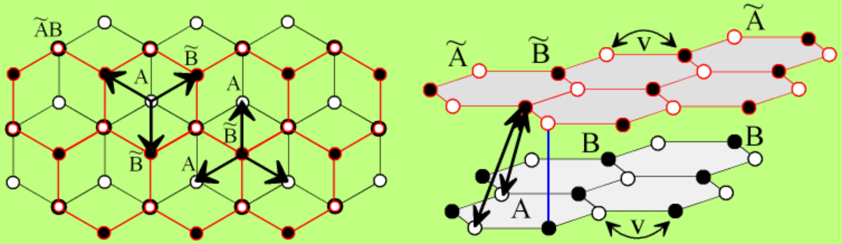
states at zero energy:

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

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



Trigonal warping - role of v_3



($\tilde{B}$ to A) by $-\gamma_3 f^*$
and
(A to $\tilde{B}$) by $-\gamma_3 f$

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

$$\begin{array}{cc} & \begin{array}{cccc} A & \tilde{B} & \tilde{A} & B \end{array} \\ \mathcal{H} = & \begin{pmatrix} & -\gamma_3 f^* & & -\gamma_0 f \\ -\gamma_3 f & & -\gamma_0 f^* & \\ & -\gamma_0 f & & \gamma_1 \\ -\gamma_0 f^* & & \gamma_1 & \end{pmatrix} \begin{array}{c} A \\ \tilde{B} \\ \tilde{A} \\ B \end{array} \end{array}$$

Two component model:

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

Trigonal warping - role of v_3

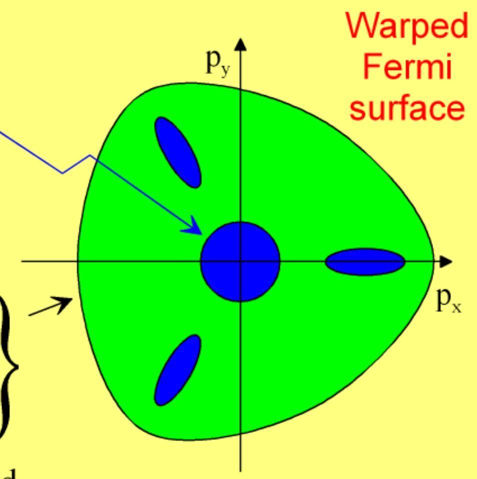
Two component model:

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

weak magnetic field

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

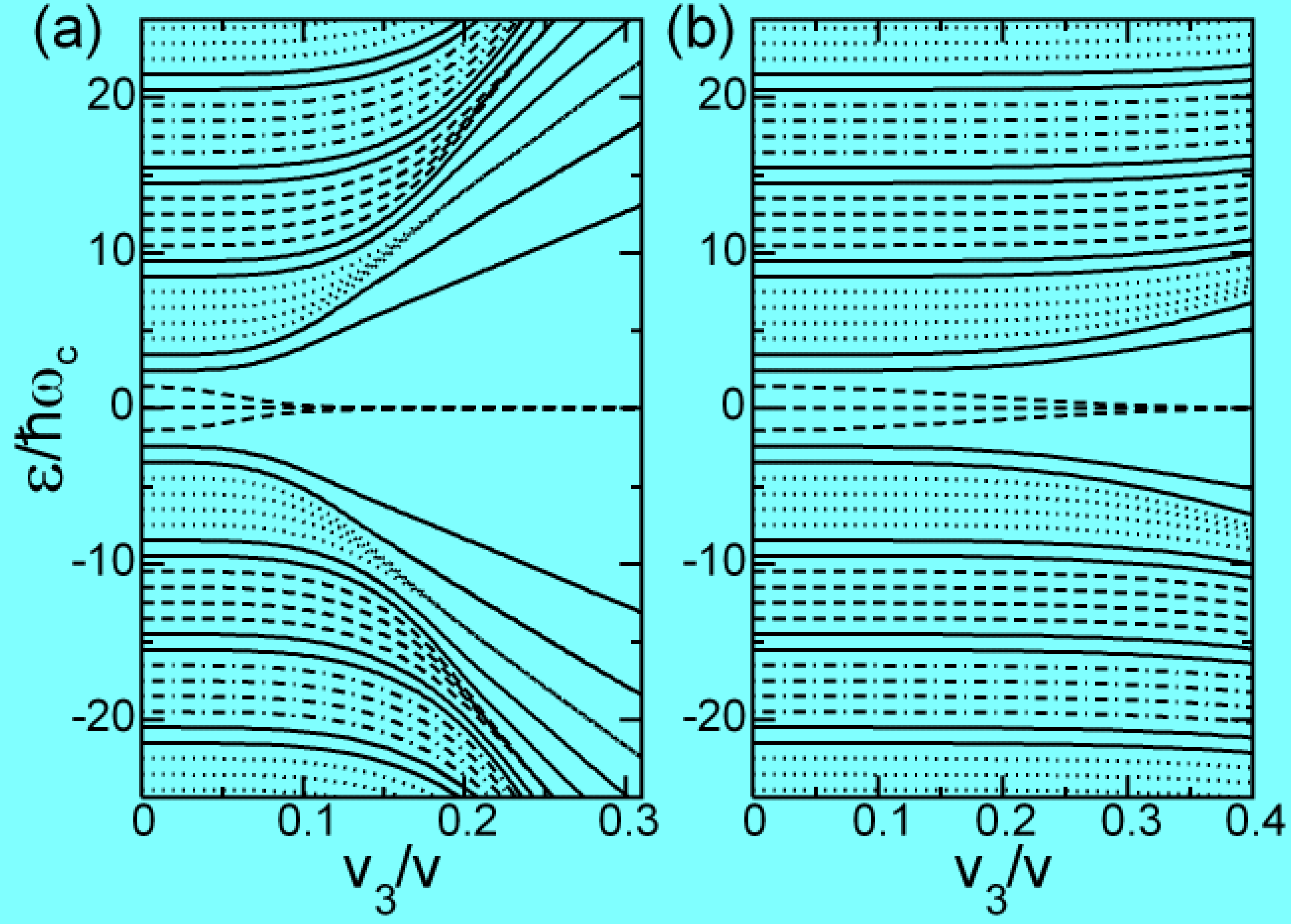
$$\left.\begin{array}{l} 0 < \varepsilon < \frac{\gamma_1}{2}\left(\frac{v_3}{v}\right)^2 \\ 0 < N < 2\left(\frac{v_3}{v}\right)^2 N^* \end{array}\right\}$$



$$\left.\begin{array}{l} \frac{\gamma_1}{2}\left(\frac{v_3}{v}\right)^2 < \varepsilon < \gamma_1 \\ 2\left(\frac{v_3}{v}\right)^2 N^* < N < 8N^* \end{array}\right\}$$

strong magnetic field

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



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:

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

Bilayer:

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

General case: $H = g \begin{pmatrix} 0 & (\pi^+)^J \\ \pi^J & 0 \end{pmatrix}$; $\begin{cases} J=1 \text{ monolayer} \\ J=2 \text{ bilayer} \end{cases}$

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

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

$$H = g\,|p|^J\,(\boldsymbol{\sigma}.\mathbf{n})$$

$$\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$$

$$\mathbf{n} = (\cos J\varphi, \sin J\varphi)$$

Monolayer

$H = v\xi|p|\,(\boldsymbol{\sigma}.\mathbf{n})$

$\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$

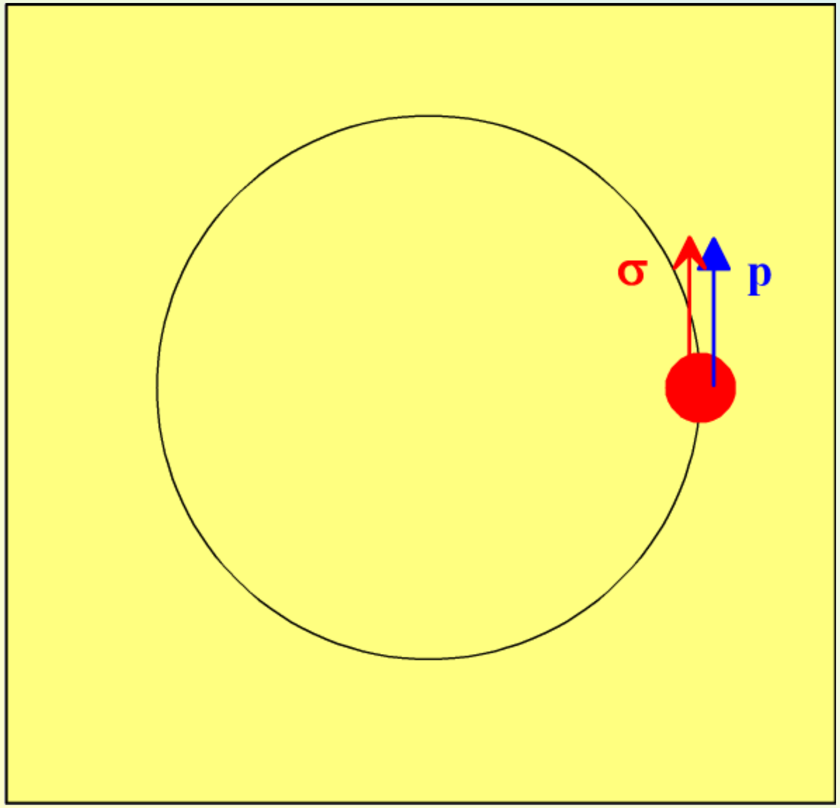
$\mathbf{n} = (\cos\varphi, \sin\varphi)$

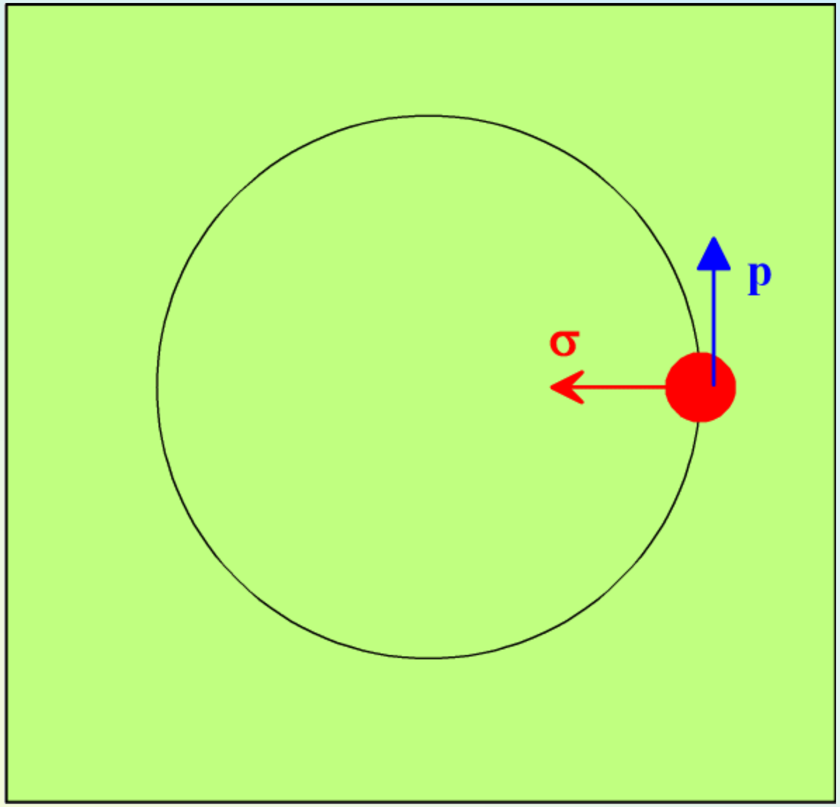
Bilayer

$H = -\frac{|p|^2}{2m}\,(\boldsymbol{\sigma}.\mathbf{n})$

$\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$

$\mathbf{n} = (\cos 2\varphi, \sin 2\varphi)$





Berry's phase of π

Berry's phase of 2π

General case:

$$H = g\begin{pmatrix} 0 & (\pi^+)^J \\ \pi^J & 0 \end{pmatrix} \Rightarrow g\begin{pmatrix} 0 & (\pi^+)^J \\ \pi^J & 0 \end{pmatrix}\begin{pmatrix} \phi_{n\leqslant J} \\ 0 \end{pmatrix} = 0$$

$$\begin{pmatrix} \phi_0 \\ 0 \end{pmatrix}, \begin{pmatrix} \phi_1 \\ 0 \end{pmatrix}, \cdots \begin{pmatrix} \phi_J \\ 0 \end{pmatrix} \Rightarrow \varepsilon = 0$$

chiral quasiparticles with Berry phase $J\pi$ and $4J$ - fold degenerate Landau levels at zero energy

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

valley index

The End