The ABC of graphene trilayers

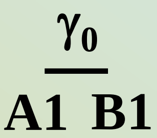
Edward McCann

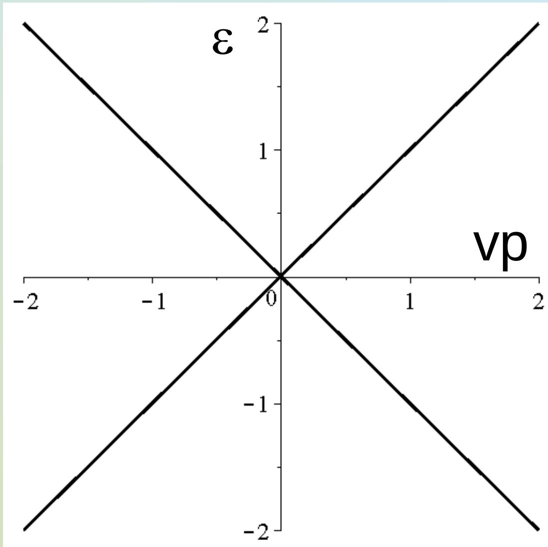
Lancaster University, UK

in collaboration with

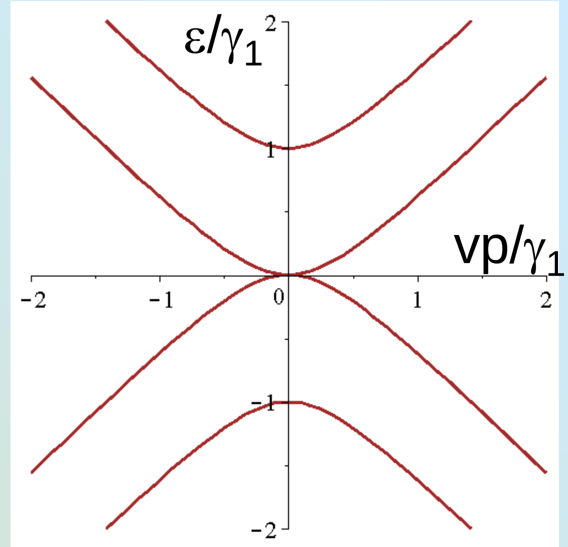
Mikito Koshino

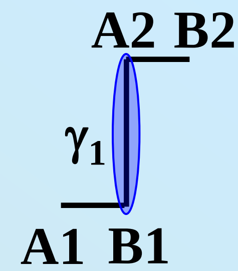
Tokyo Institute of Technology, Japan



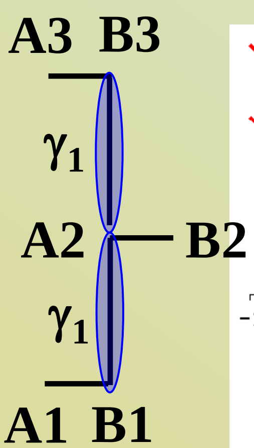


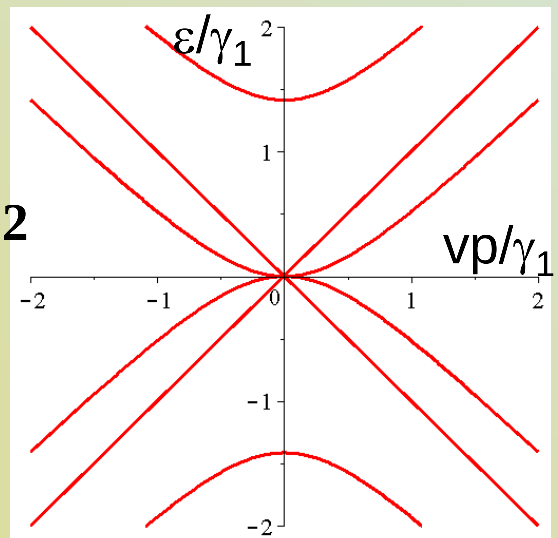
monolayer graphene:
Berry phase π





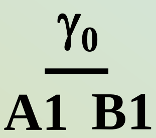
AB-stacked bilayer:
Berry phase 2π

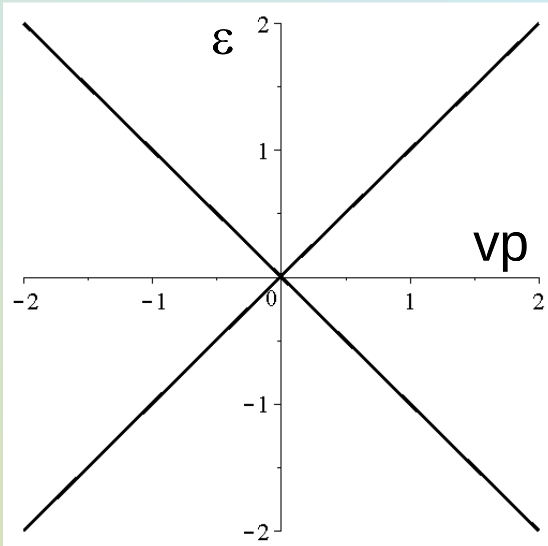




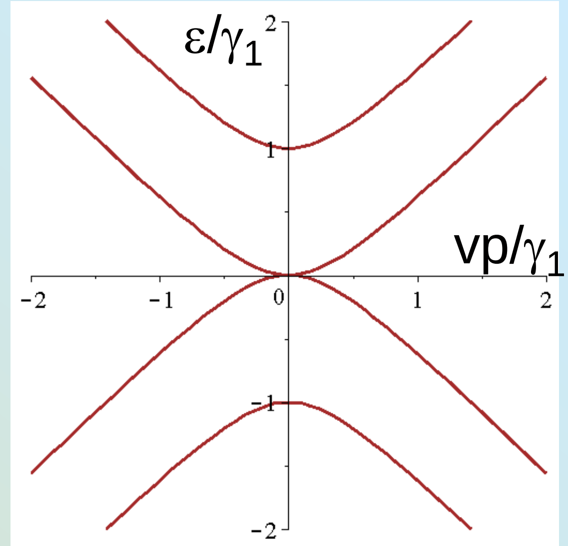
ABA-stacked trilayer:
Berry phase π and 2π

a combination of
monolayer-like and
bilayer-like bands

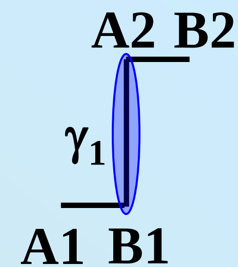


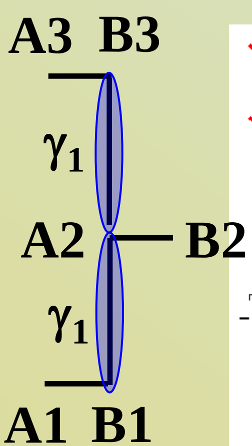


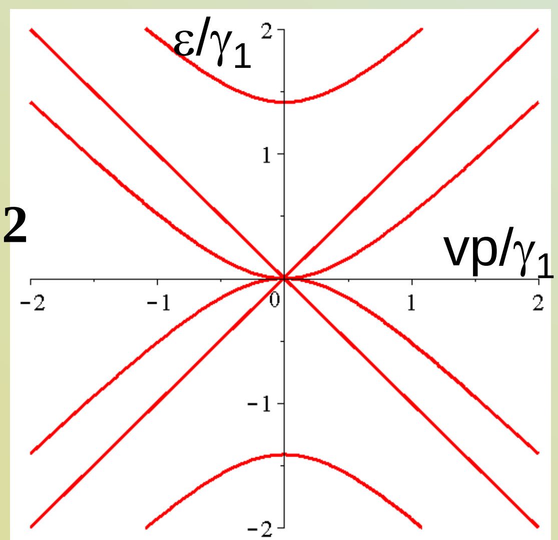
monolayer graphene:
Berry phase π



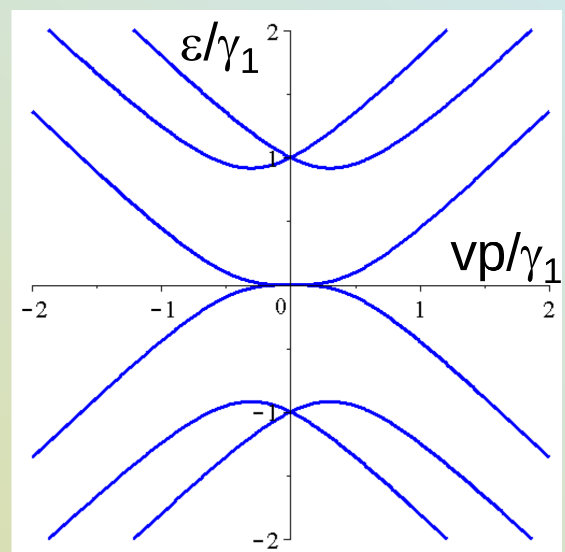
AB-stacked bilayer:
Berry phase 2π



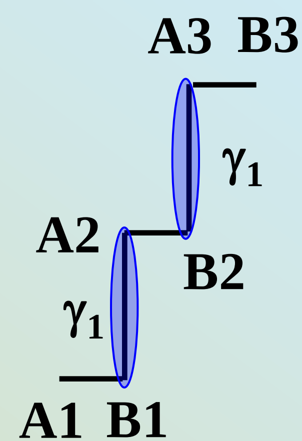




ABA-stacked trilayer:
Berry phase π and 2π



ABC-stacked trilayer:
Berry phase 3π



cubic generalisation of monolayers and bilayers

The ABC of graphene trilayers:

using a simple (tight-binding) model, can we identify any novel features in their low-energy electronic spectrum?

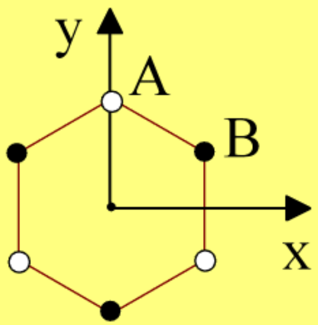
Overview

- Review of tight-binding model of monolayers and bilayers
- ABA-stacked trilayers
- ABC-stacked trilayers

Electronic dispersion of a monolayer

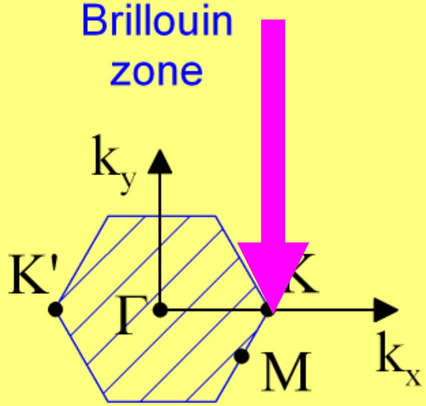
Saito *et al*, "Physical Properties of Carbon Nanotubes" (Imperial College Press, London, 1998)

Symmetrical unit cell

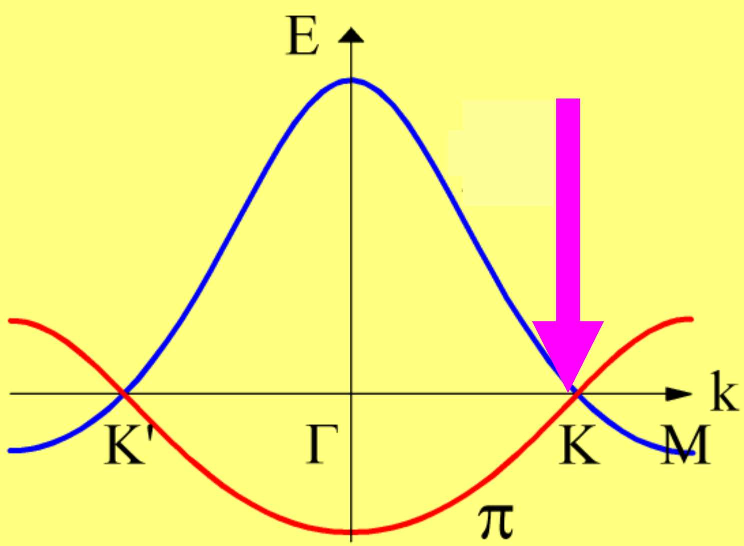


Two non-equivalent carbon positions

Brillouin zone



Two non-equivalent K-points

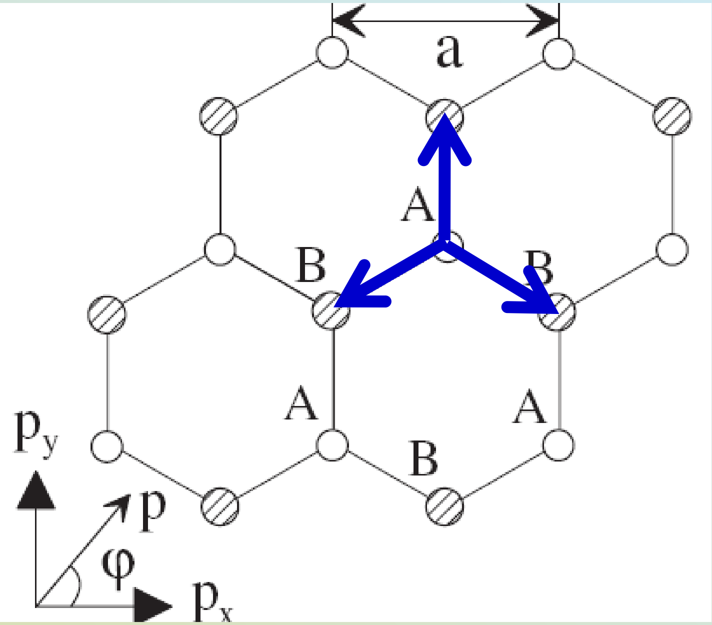


Two bands: no energy gap at the K-points

To calculate the transfer integral for hopping from site A to site B we need to determine factors like

$$e^{i\vec{k}.\left(\vec{R}_B-\vec{R}_A\right)}$$

that depend on the atomic positions $\vec{R}_A, \ \vec{R}_B$



Electronic dispersion of a monolayer

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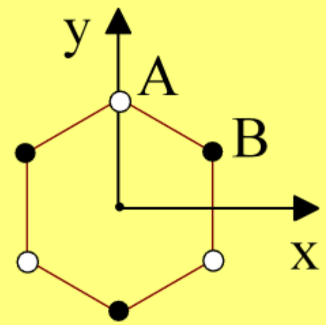
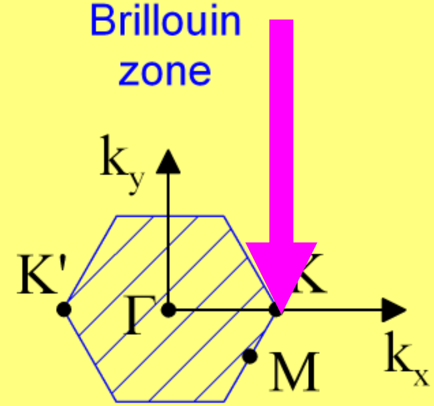
Symmetrical unit cell

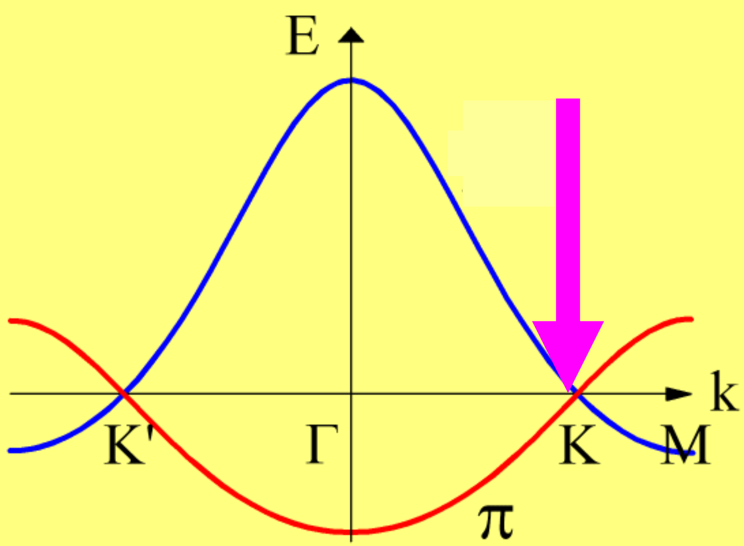


Two non-equivalent carbon positions

Brillouin zone



Two non-equivalent K-points



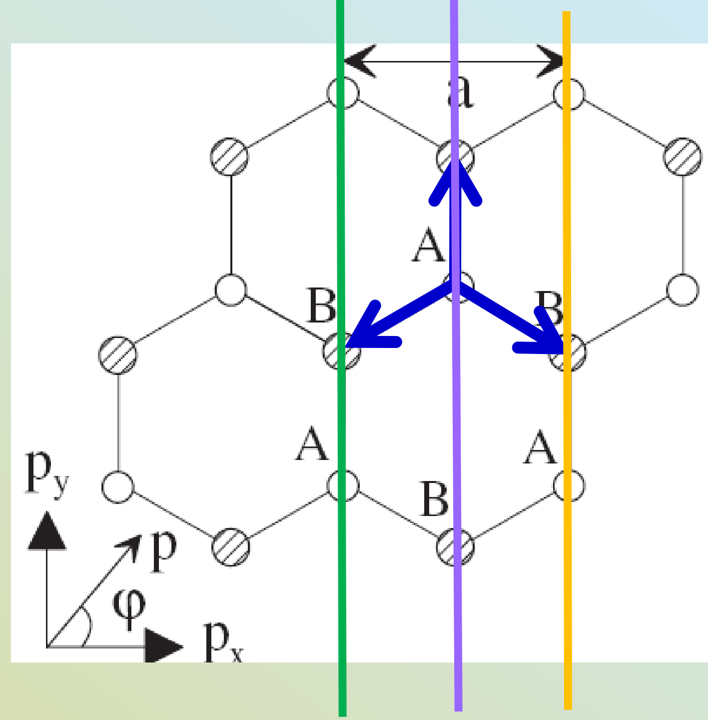
Two bands: no energy gap at the K-points

Exactly at the K point: $\vec{k} = \left(\frac{4\pi}{3a}, 0 \right)$

$$e^{i\vec{k}.\vec{R}_i} = e^{-2\pi i/3}$$

$$e^{i0}$$

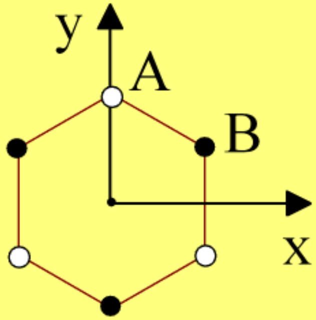
$$e^{+2\pi i/3}$$



Electronic dispersion of a monolayer

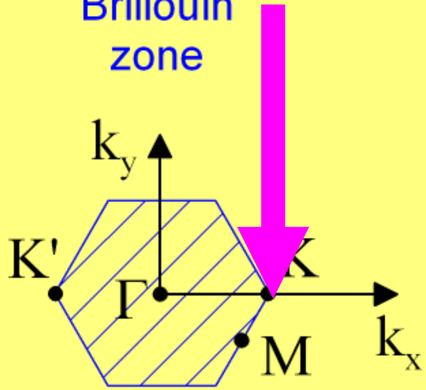
Saito *et al*, "Physical Properties of Carbon Nanotubes" (Imperial College Press, London, 1998)

Symmetrical unit cell

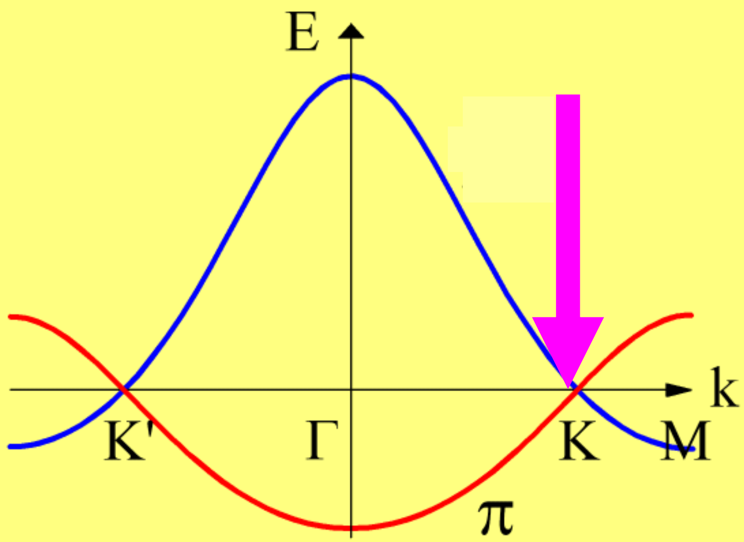


Two non-equivalent carbon positions

Brillouin zone



Two non-equivalent K-points

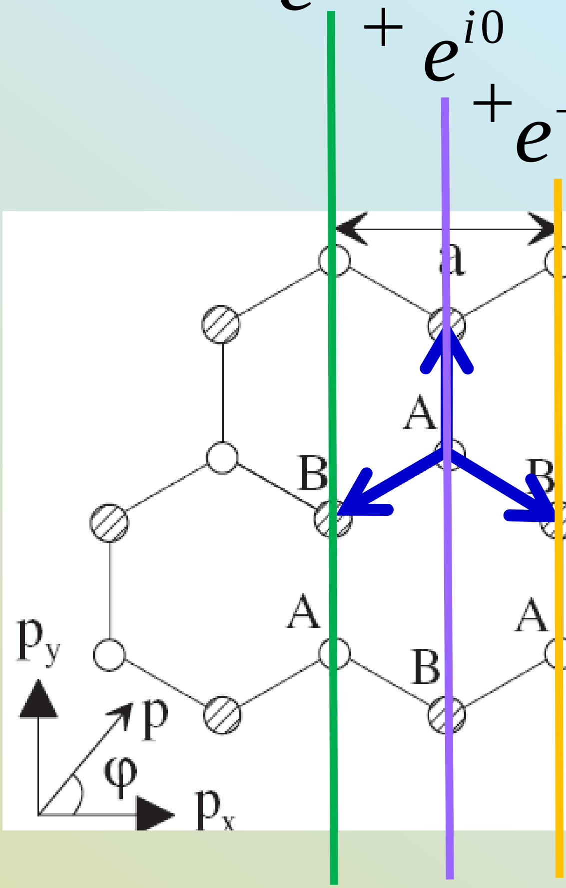


Two bands: no energy gap at the K-points

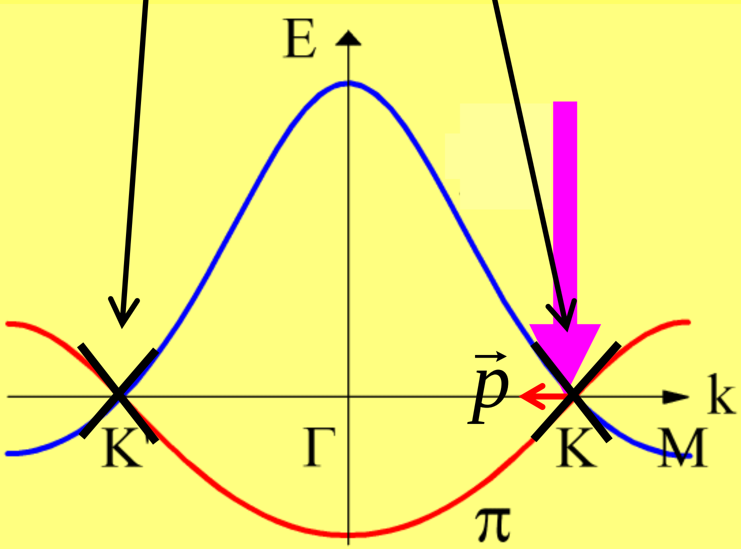
Exactly at the K point: $\vec{k} = \left(\frac{4\pi}{3a}, 0\right)$

Two uncoupled triangular sub-lattices

$$e^{-2\pi i/3} + e^{i0} + e^{+2\pi i/3} = 0$$



The Dirac Hamiltonian gives a linear spectrum E = v|p| around each K point – with no gap between conduction and valence bands.



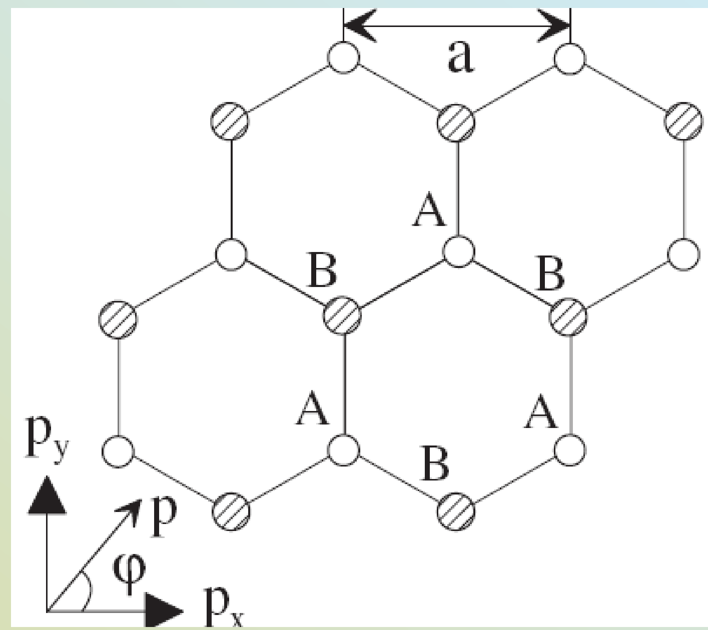
Two bands: no energy gap at the K-points

Near the K point: $\vec{k} = \left(\frac{4\pi}{3a}, 0\right) + \frac{\vec{p}}{\hbar}$

Coupling between triangular sub-lattices occurs in linear-in-momentum terms:

$$\hat{H}_1 = v\begin{pmatrix} 0 & p_x - ip_y \\ p_x + ip_y & 0 \end{pmatrix}$$

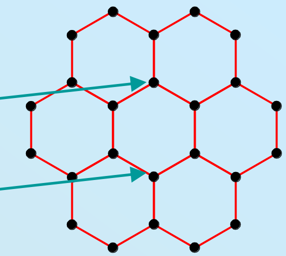
written in a two-component basis of A and B sites.



Bloch function amplitudes (e.g., in the valley K) on the AB sites ('pseudospin') mimic spin components of a relativistic particle.

Pseudospin and chirality: Berry's phase π

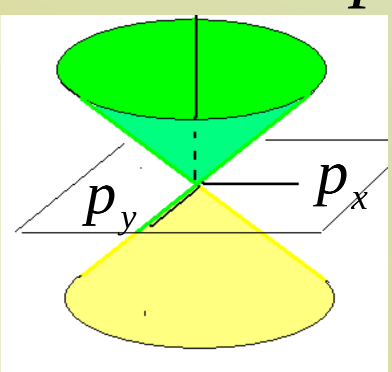
$$\psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

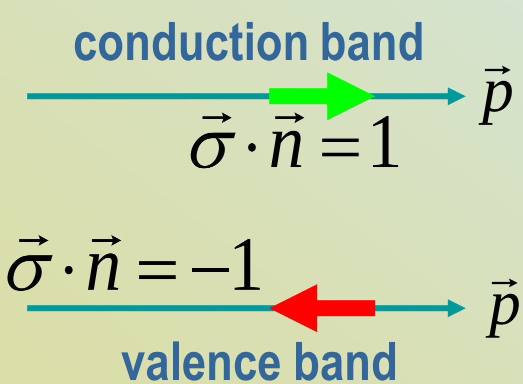


$$\hat{H}_1 = v \begin{pmatrix} 0 & p_x - ip_y \\ p_x + ip_y & 0 \end{pmatrix} = v\vec{\sigma}\cdot\vec{p} = vp\vec{\sigma}\cdot n$$

Chiral Dirac-type (relativistic) electrons: pseudospin of plane waves is linked to the momentum direction, which determines unusual transport properties of graphene.

$$\varepsilon = \pm vp$$



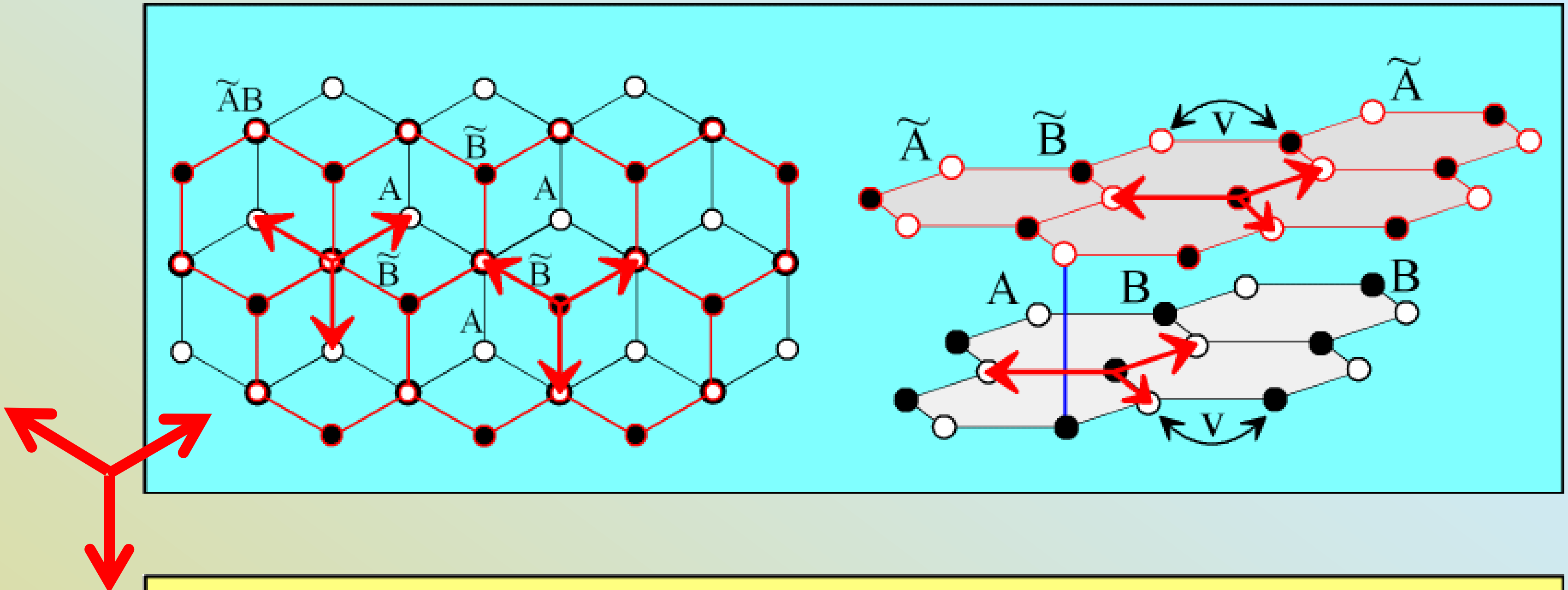


$$\vec{p} = (p\cos\varphi, p\sin\varphi)$$

$$\psi_{\pm} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\varphi/2} \\ \pm e^{-i\varphi/2} \end{pmatrix}$$

chiral plane wave states

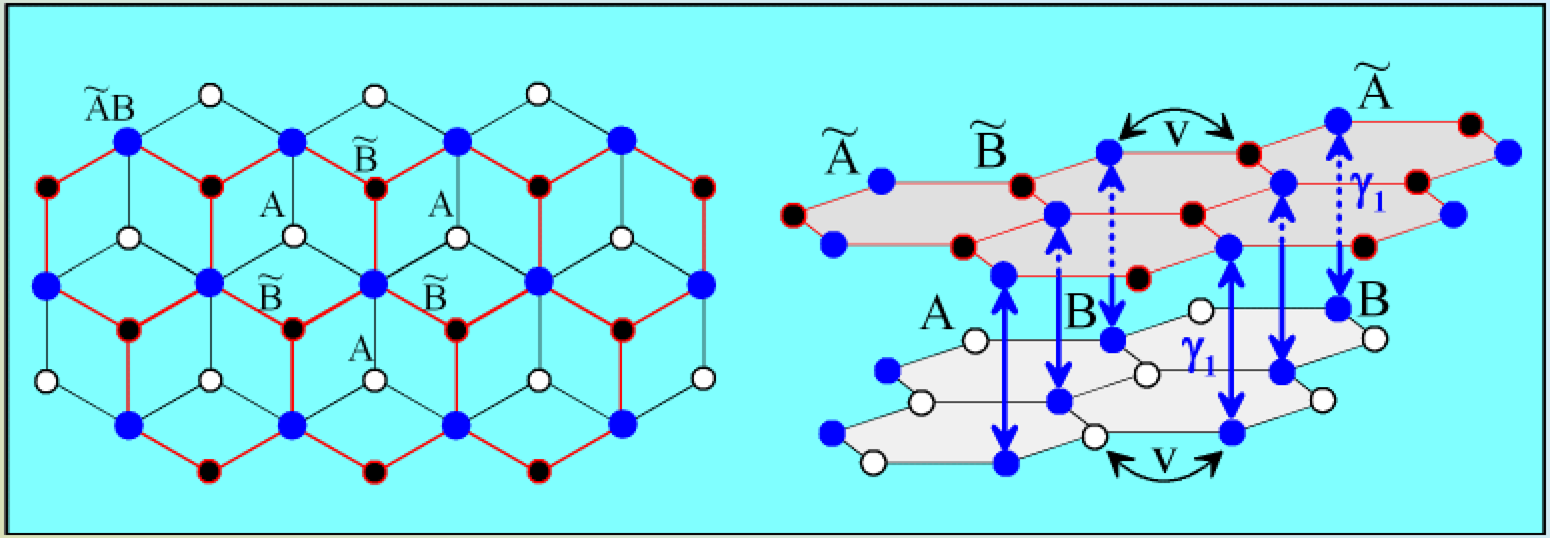
Bilayer [Bernal (AB) stacking]



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

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

Bilayer [Bernal (AB) stacking]



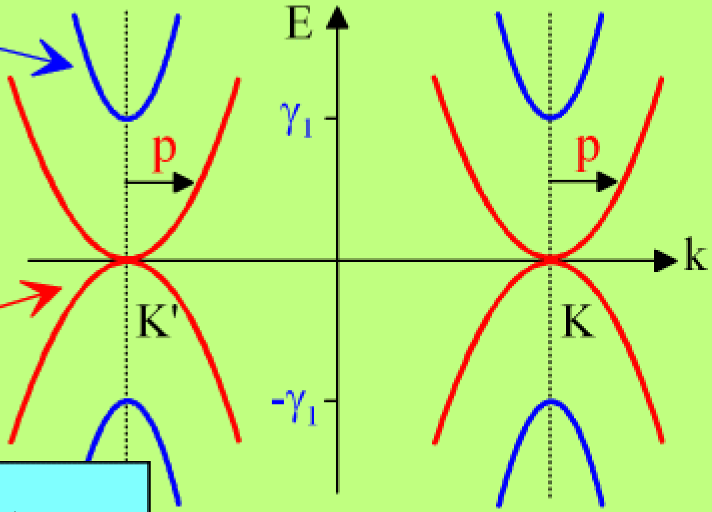
Bilayer Hamiltonian

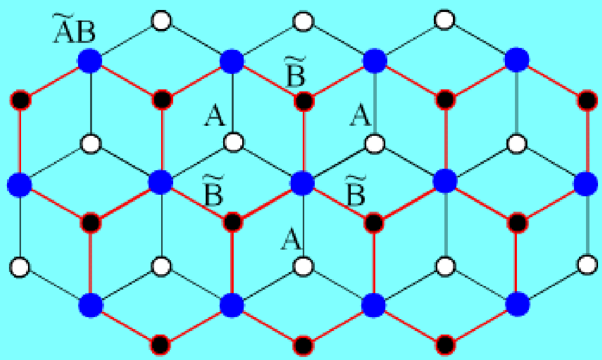
$$H = \begin{array}{c} \\ \\ \\ \\ \\ \end{array}\begin{array}{cc} \begin{array}{cccc} A & \tilde{B} & \tilde{A} & B \end{array} & \\ \begin{pmatrix} 0 & 0 & 0 & v\pi^{+} \\ 0 & 0 & v\pi & 0 \\ 0 & v\pi^{+} & 0 & \gamma_1 \\ v\pi & 0 & \gamma_1 & 0 \end{pmatrix} & \begin{array}{c} A \\ \tilde{B} \\ \tilde{A}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

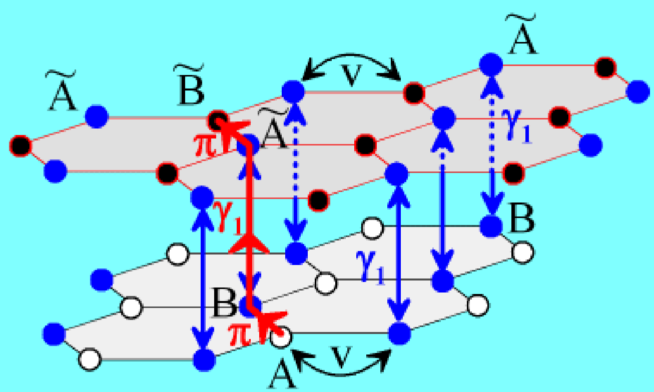
$\tilde{A}B$ orbitals form dimers with energy $|E| \gtrsim \gamma_1$

Quadratic dispersion at low energy:

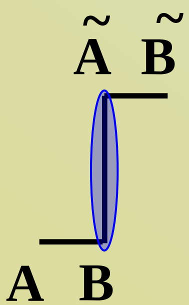
$$E = \pm \frac{p^2}{2m}$$







E. McCann and V.I. Fal'ko
PRL 96, 086805 (2006)



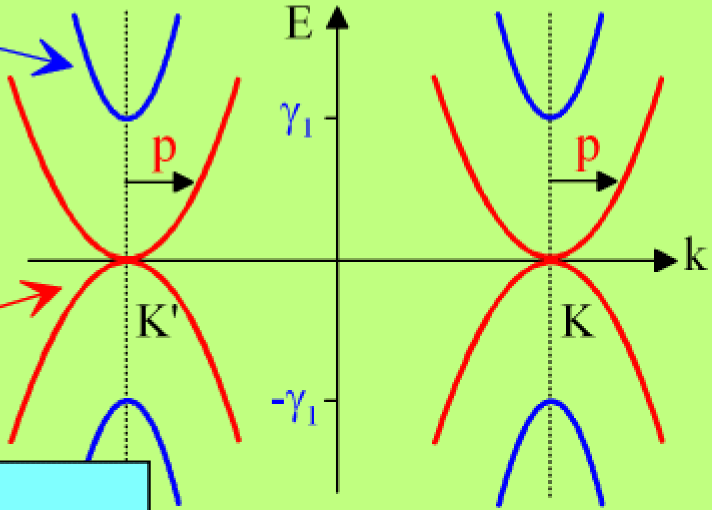
Bilayer Hamiltonian

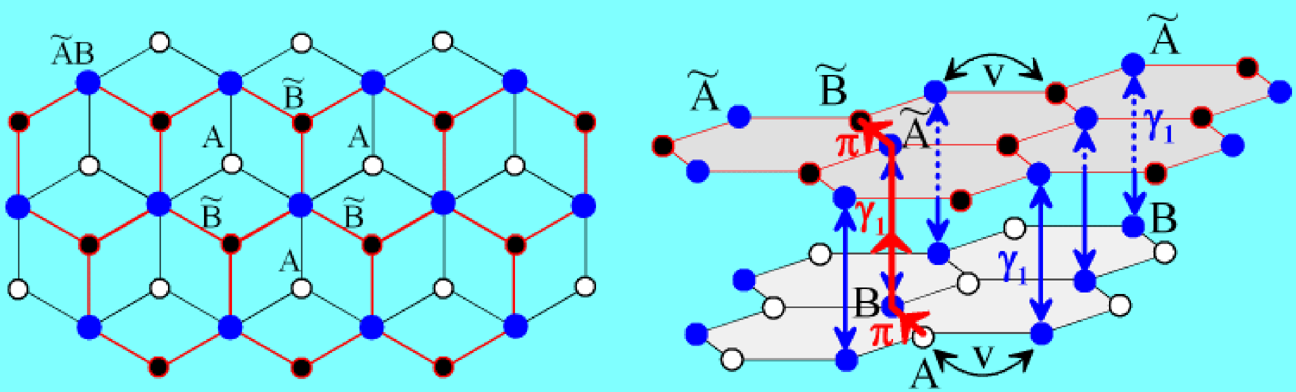
$$H = \begin{array}{c} \\ \end{array}\begin{array}{cc} \begin{array}{cccc} A & \tilde{B} & \tilde{A} & B \end{array} & \\ \begin{pmatrix} 0 & 0 & 0 & v\pi^+ \\ 0 & 0 & v\pi & 0 \\ 0 & v\pi^+ & 0 & \gamma_1 \\ v\pi & 0 & \gamma_1 & 0 \end{pmatrix} & \begin{array}{c} A \\ \tilde{B} \\ \tilde{A} \\ B \end{array}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

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

Quadratic dispersion at low energy:

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





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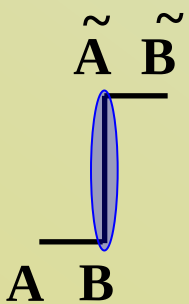


Bilayer Hamiltonian written in a 2 component basis of A and $\tilde{B}$ sites

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

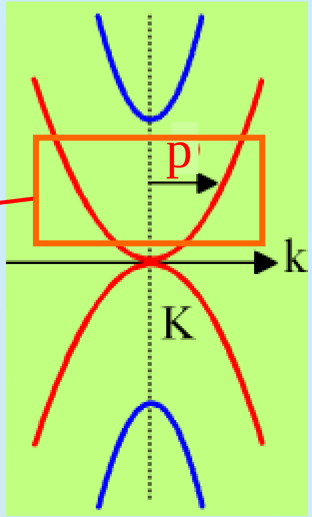
mass
$m = \gamma_1 / v^2$

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)

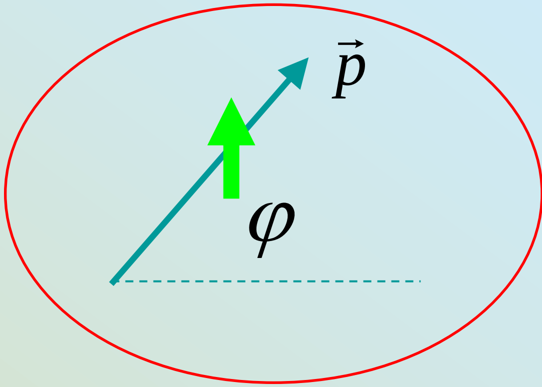
$$\pi = p_x + ip_y$$

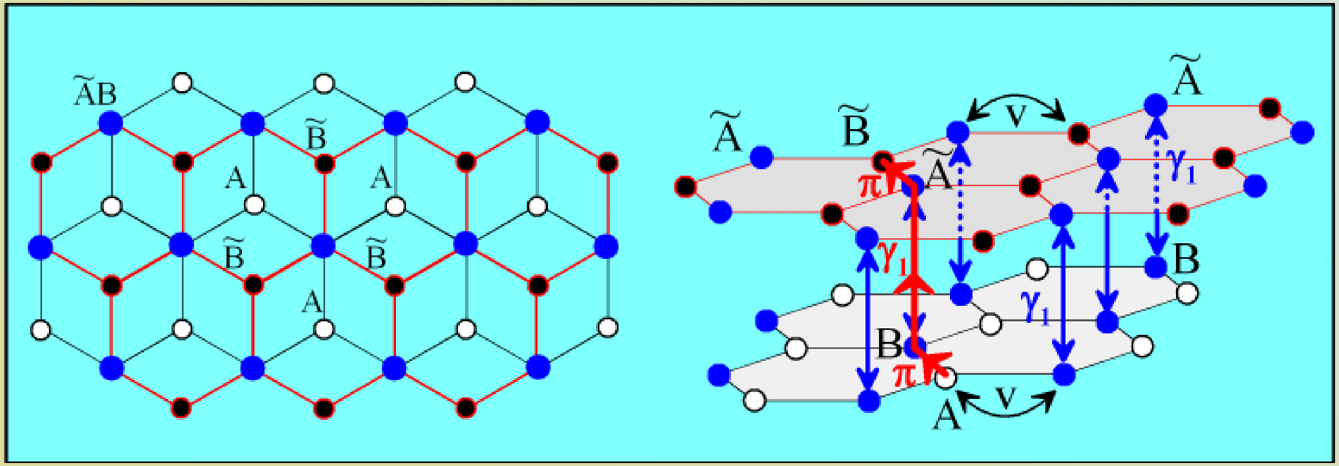
Chiral electrons in bilayer graphene: Berry's phase 2π



$$H \approx -\frac{1}{2m}\begin{pmatrix} 0 & \left(\pi^{+}\right)^{2} \\ \pi^{2} & 0 \end{pmatrix} = -\frac{p^{2}}{2m}\begin{pmatrix} 0 & e^{-2i\varphi} \\ e^{2i\varphi} & 0 \end{pmatrix}$$

$$\varepsilon \approx \pm\frac{p^{2}}{2m} \quad \Leftrightarrow \quad \psi_{\pm} = \begin{pmatrix} \psi_{A} \\ \psi_{\tilde{B}} \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{-i\varphi} \\ -e^{i\varphi} \end{pmatrix}$$

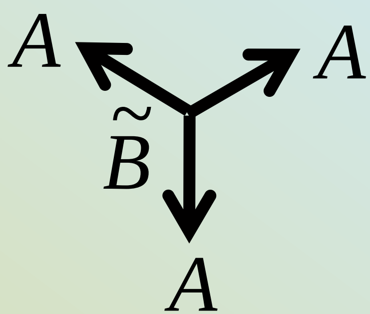




E. McCann and V.I. Fal'ko, PRL 96, 086805 (2006)

Trigonal warping in bilayer graphene

EM and V.I. Fal'ko, PRL **96**, 086805 (2006)

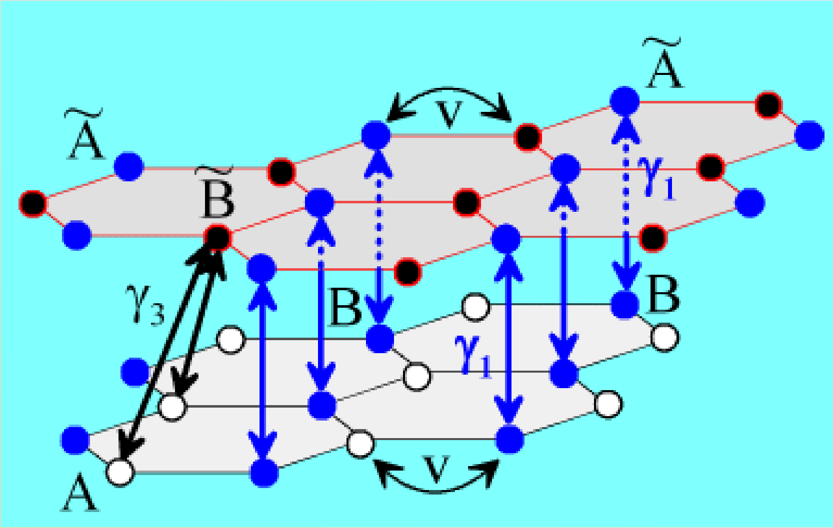


$$v_3 = \tfrac{\sqrt{3}}{2} a\gamma_3/\hbar$$

$$\pi = p_x + ip_y$$

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

$$H = \begin{pmatrix} 0 & v_3\pi & 0 & v\pi^{+} \\ v_3\pi^{+} & 0 & v\pi & 0 \\ 0 & v\pi^{+} & 0 & \gamma_1 \\ v\pi & 0 & \gamma_1 & 0 \end{pmatrix} \begin{array}{c} A \\ \tilde{B} \\ \tilde{A} \\ B \end{array}$$



Trigonal warping in bilayer graphene

EM and V.I. Fal'ko, PRL **96**, 086805 (2006)

$$H_2 = \frac{-1}{2m}\begin{pmatrix} 0 & (\pi^+)^2 \\ \pi^2 & 0 \end{pmatrix} + v_3 \begin{pmatrix} 0 & \pi \\ \pi^+ & 0 \end{pmatrix} + \ldots$$

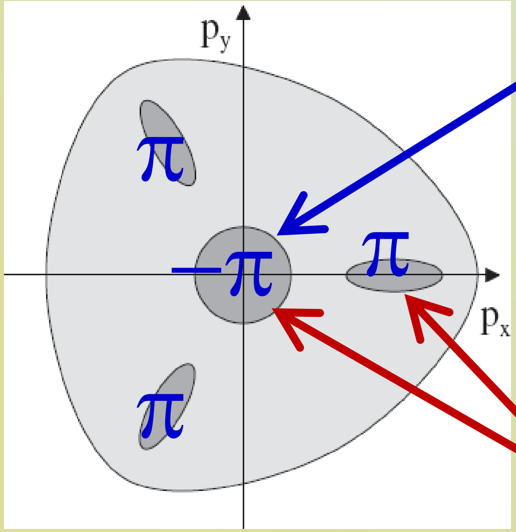
Perturbation arising from "skew" interlayer coupling

$$v_3 = \tfrac{\sqrt{3}}{2} a\gamma_3/\hbar$$

$$\pi = p_x + ip_y$$

Trigonal warping

$$\varepsilon^2 = \left(\frac{p^2}{2m}\right)^2 - \frac{\xi v_3 p^3}{m}\cos 3\phi + v_3^2 p^2$$



Dispersion is linear inside each pocket, with chirality corresponding to that of a monolayer

J.L. Manes, F. Guinea, and M.A. Vozmediano, PRB **75**, 155424 (2007);
G.P. Mikitik and Y. Sharlai, PRB **77**, 113407 (2008).

Lifshitz transition:
Fermi surface separation $\varepsilon_L \approx \frac{\gamma_1}{4}\left(\frac{v_3}{v}\right)^2 \sim 1meV$

Low-energy Hamiltonian of bilayer graphene

EM and V.I. Fal'ko, PRL **96**, 086805 (2006)

$$H_2 = \frac{-1}{2m}\begin{pmatrix} 0 & (\pi^+)^2 \\ \pi^2 & 0 \end{pmatrix} + v_3 \begin{pmatrix} 0 & \pi \\ \pi^+ & 0 \end{pmatrix} + \ldots$$

Perturbation arising from "skew" interlayer coupling

$$v_3 = \tfrac{\sqrt{3}}{2} a\gamma_3 / \hbar$$

$$\pi = p_x + ip_y$$

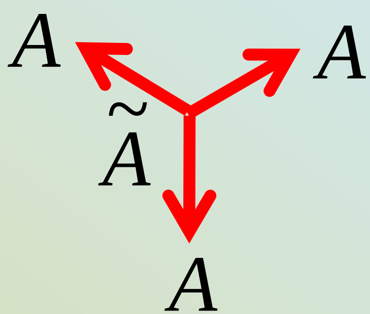
Low-energy Hamiltonian of monolayer graphene

Ajiki and Ando, JPSJ **62**, 2470 (1993)
Ando, Nakanishi, and Saito, JPSJ **67**, 2857 (1998)

$$H_1 = v\begin{pmatrix} 0 & \pi^+ \\ \pi & 0 \end{pmatrix} - \mu \begin{pmatrix} 0 & \pi^2 \\ (\pi^+)^2 & 0 \end{pmatrix} + \ldots$$

Perturbation arising from higher-order in momentum expansion

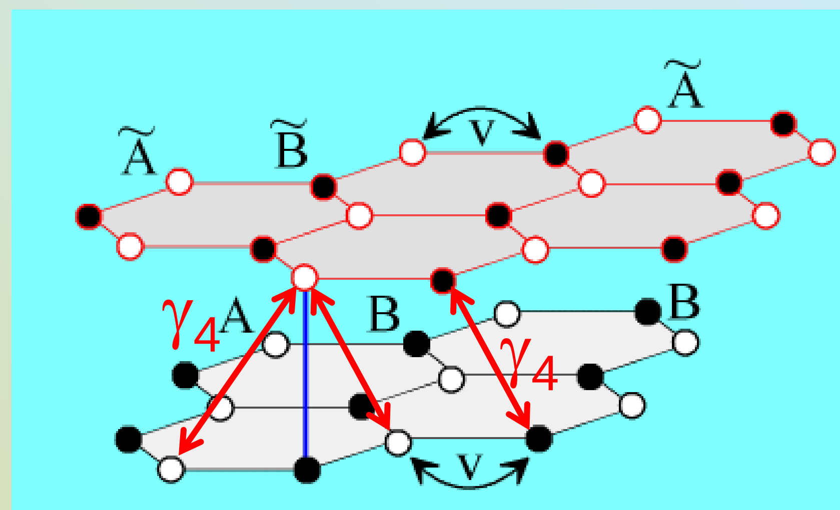
Role of γ_4 in bilayer graphene



$$v_4 = \frac{\sqrt{3}}{2} a\gamma_4 / \hbar$$

$$\pi = p_x + ip_y$$

$$H = \begin{array}{cc} \begin{array}{cccc} A & \tilde{B} & \tilde{A} & B \end{array} & \\ \begin{pmatrix} 0 & v_3\pi & v_4\pi^+ & v\pi^+ \\ v_3\pi^+ & 0 & v\pi & v_4\pi \\ v_4\pi & v\pi^+ & 0 & \gamma_1 \\ v\pi & v_4\pi^+ & \gamma_1 & 0 \end{pmatrix} & \begin{array}{c} A \\ \tilde{B} \\ \tilde{A} \\ B \end{array} \end{array}$$



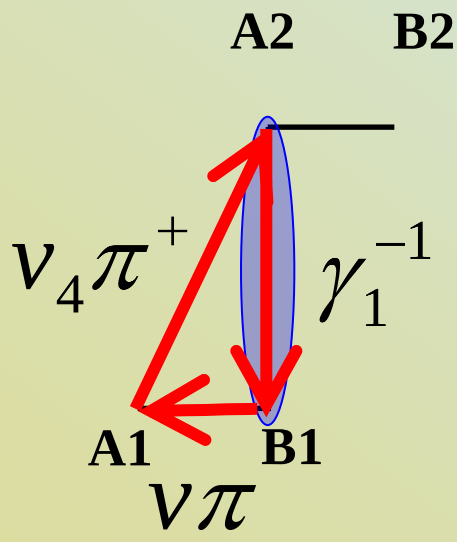
Role of γ_4 in bilayer graphene

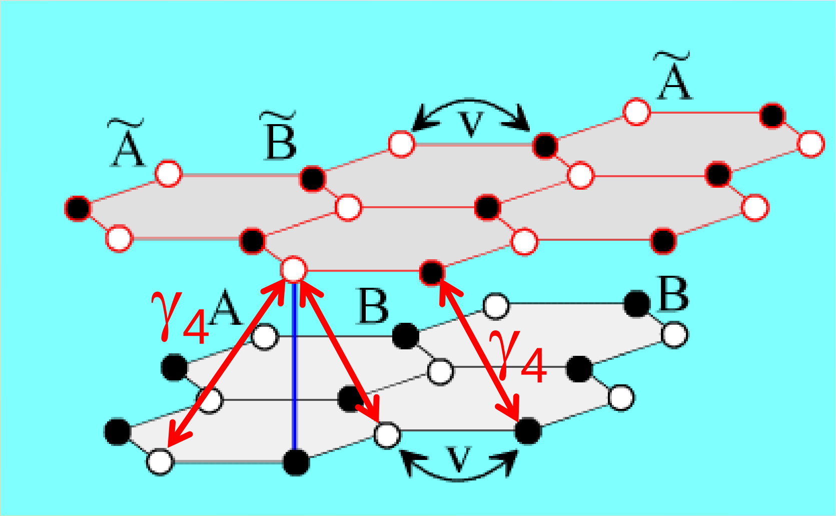
$$H_2 = \frac{-1}{2m}\begin{pmatrix} 0 & (\pi^+)^2 \\ \pi^2 & 0 \end{pmatrix} + \frac{2vv_4 p^2}{\gamma_1}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \ldots$$

electron-hole asymmetry arising from "skew" interlayer coupling

$$v_4 = \tfrac{\sqrt{3}}{2} a\gamma_4 / \hbar$$

$$\pi = p_x + ip_y$$

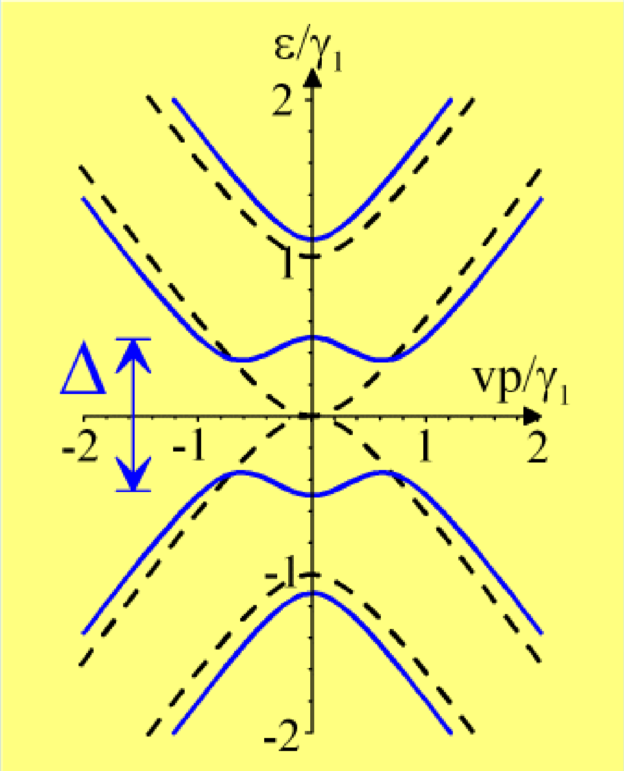




Interlayer asymmetry gap in bilayer graphene

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

$$H = \begin{array}{cc} & \begin{array}{cccc} A & \tilde{B} & \tilde{A} & B \end{array} \\ & \begin{pmatrix} -\Delta/2 & 0 & 0 & v\pi^{+} \\ 0 & \Delta/2 & v\pi & 0 \\ 0 & v\pi^{+} & \Delta/2 & \gamma_1 \\ v\pi & 0 & \gamma_1 & -\Delta/2 \end{pmatrix} \begin{array}{c} A \\ \tilde{B} \\ \tilde{A} \\ B \end{array} \end{array}$$



Interlayer asymmetry gap in bilayer graphene

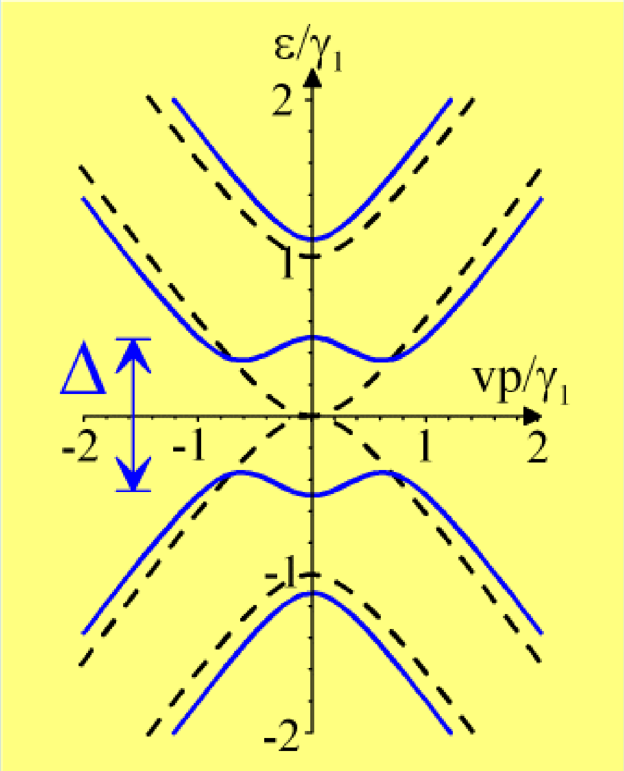
Bilayer

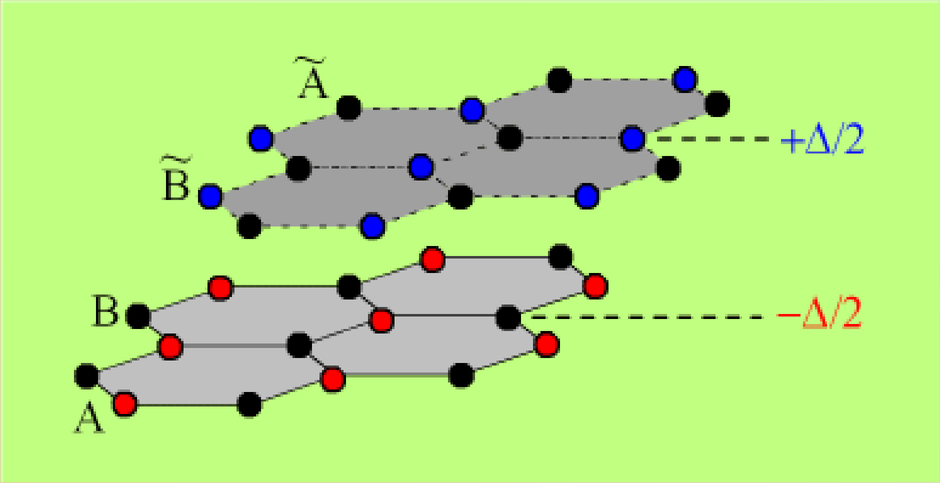
A site; lower layer

$$H = \begin{pmatrix} -\Delta/2 & -p^2 e^{-2i\varphi}/2m \\ -p^2 e^{2i\varphi}/2m & \Delta/2 \end{pmatrix}$$

$$\Rightarrow \quad E = \pm\sqrt{\frac{\Delta^2}{4} + \left(\frac{p^2}{2m}\right)^2}$$

$\tilde{B}$ site; upper layer





EMcC and VI Fal'ko, PRL **96**, 086805 (2006);
EMcC, PRB **74**, 161403(R) (2006);
H Min, BR Sahu, SK Banerjee, and AH MacDonald, PRB **75**, 155115 (2007);
EV Castro *et al*, PRL **99**, 216802 (2007)

AB-stacked bilayer

$$\hat{H}^{(eff)}_{bilayer} =$$

$$-\frac{v^2}{\gamma_1}\begin{pmatrix} 0 & (p_x - ip_y)^2 \\ (p_x + ip_y)^2 & 0 \end{pmatrix}$$ chirality

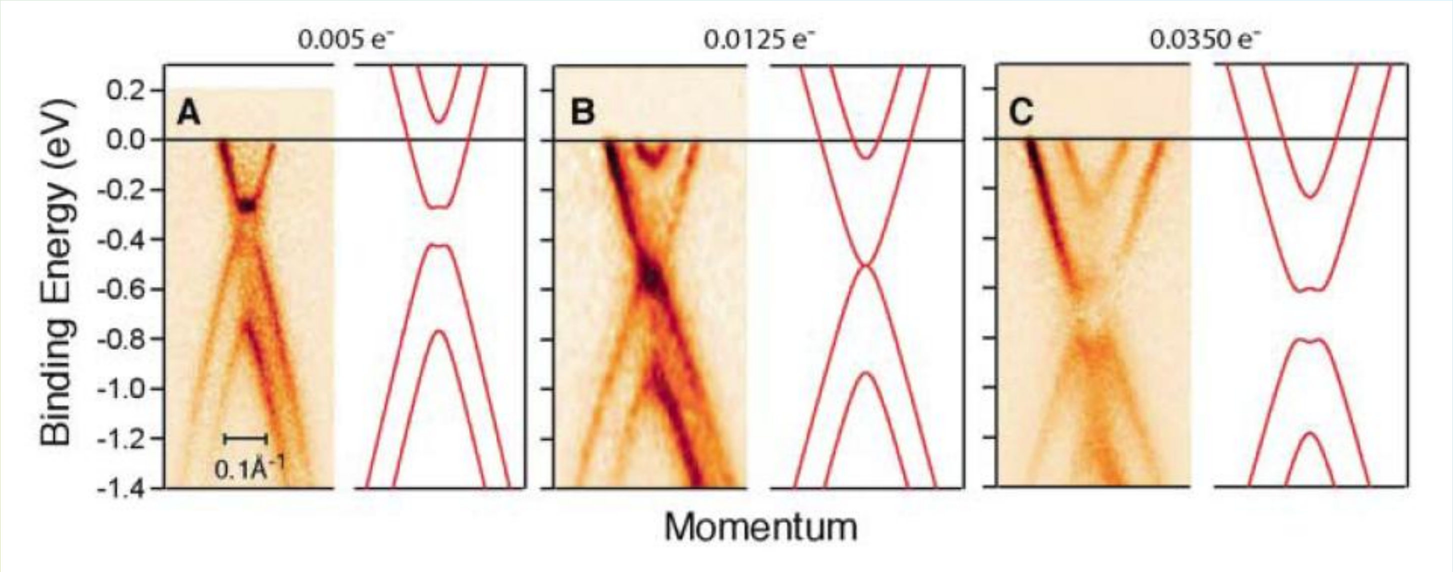
$$+v_3\begin{pmatrix} 0 & p_x + ip_y \\ p_x - ip_y & 0 \end{pmatrix}$$ γ_3: trigonal warping

$$+\frac{2vv_4p^2}{\gamma_1}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$ γ_4: e-h asymmetry

$$+\Delta\left[1-\frac{2v^2p^2}{\gamma_1^2}\right]\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$ asymmetry gap

This isn't an exhaustive list: e.g. next-nearest neighbours, non-orthogonality, other on-site asymmetry terms, ...

Interlayer asymmetry gap in bilayer graphene



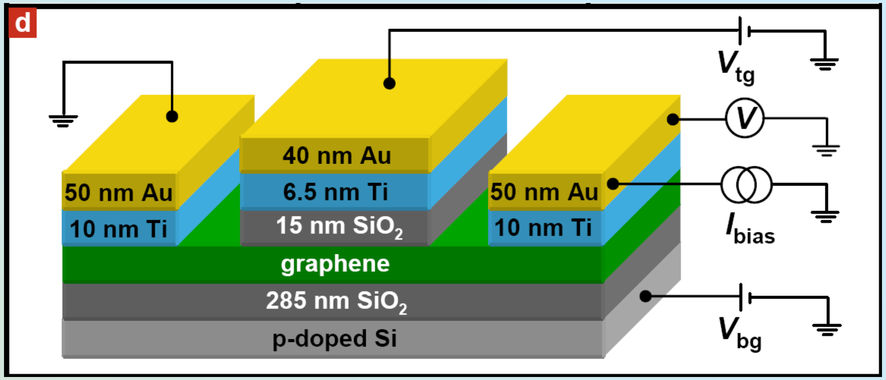
T Ohta, A Bostwick, T Seyller, K Horn, E Rotenberg, Science 313, 951 (2006)

Lawrence Berkeley National Lab. (US), Fritz-Haber-Institut and University of Erlangen-Nuremburg (Germany).

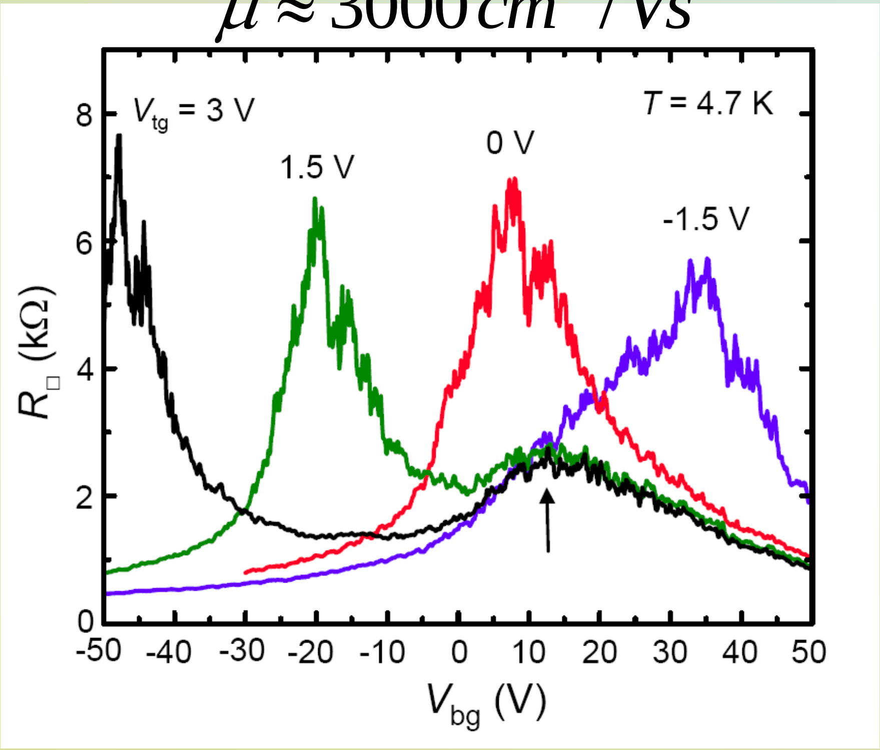
ARPES measurements of heavily doped bilayer graphene synthesized on a silicon carbide substrate

Gate-tunable band-gap in bilayer graphene

JB Oostinga, HB Heersche, X Liu, AF Morpurgo, LMK Vandersypen, Nature Materials **7**, 151 (2007)

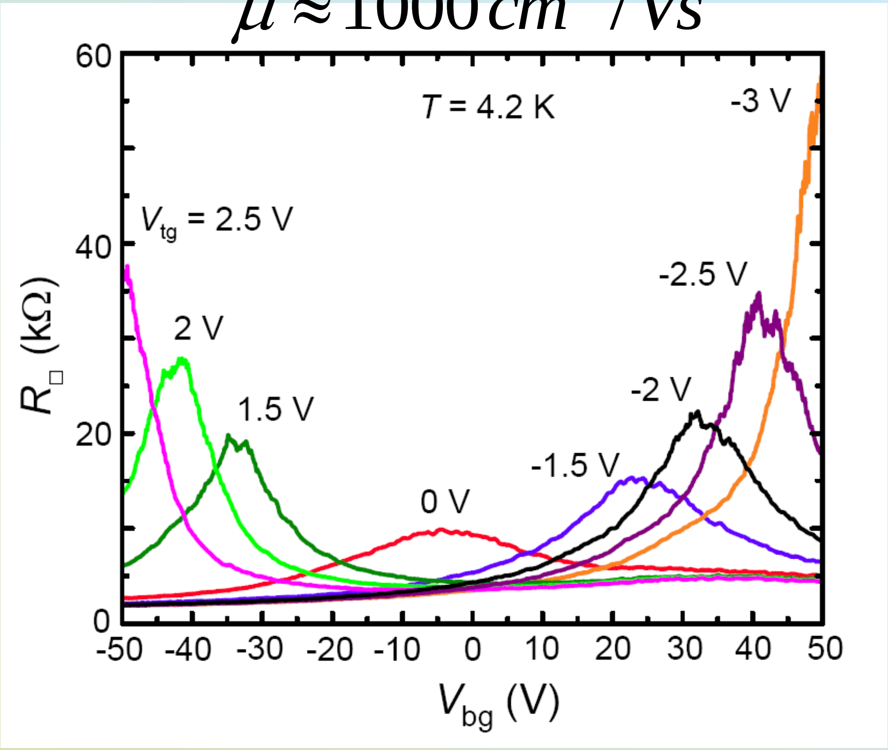


$\mu \approx 3000\, cm^2/Vs$



monolayer

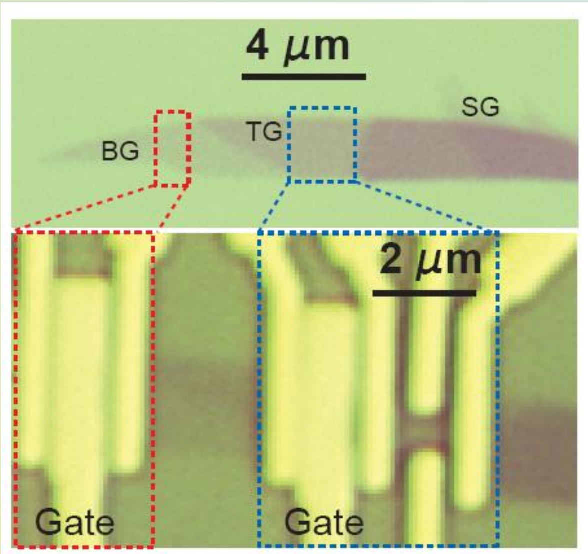
$\mu \approx 1000\, cm^2/Vs$

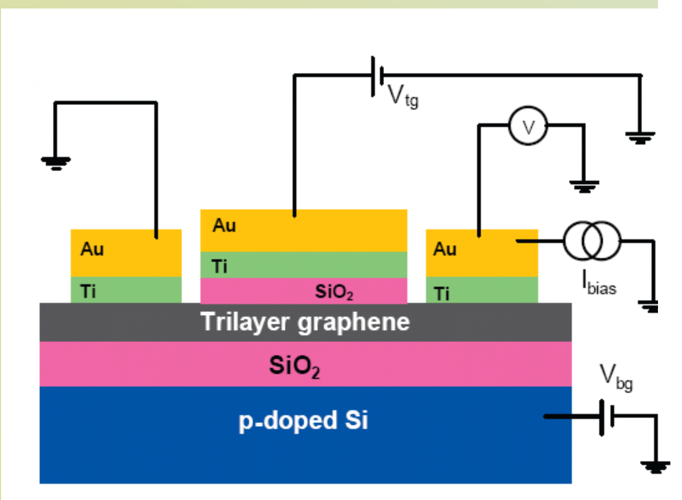


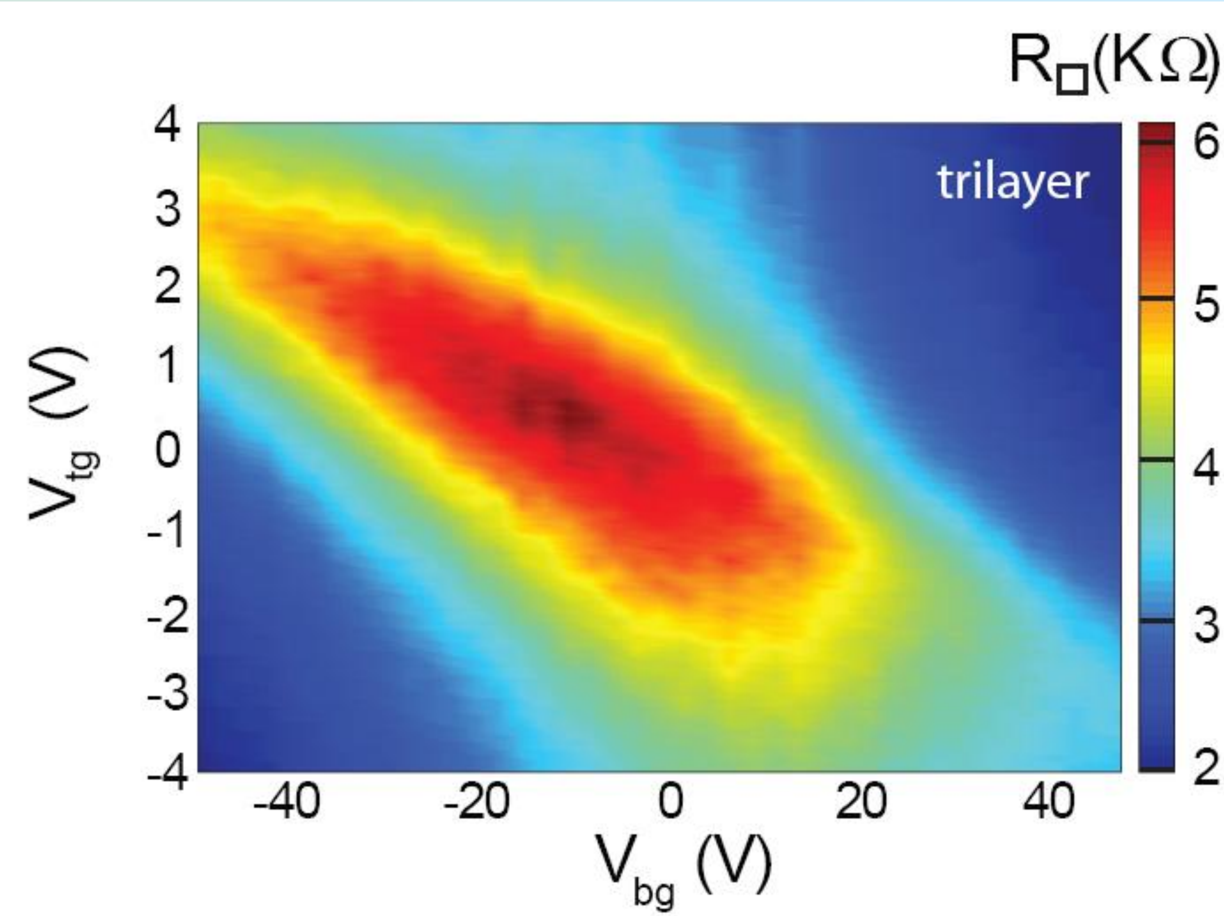
bilayer

$E_g \sim 10\, meV$

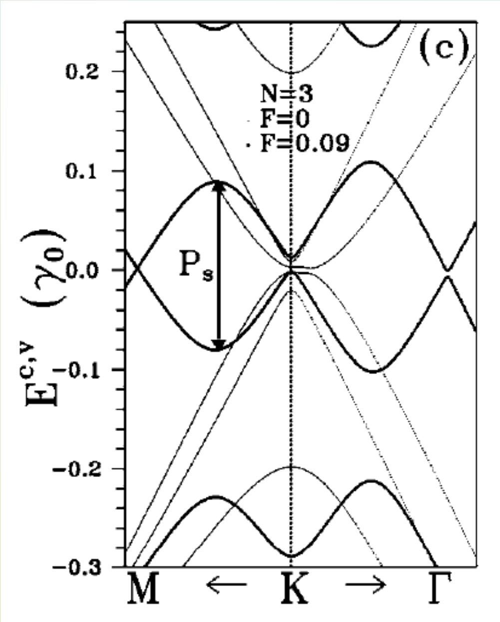
Trilayer graphene with perpendicular electric field





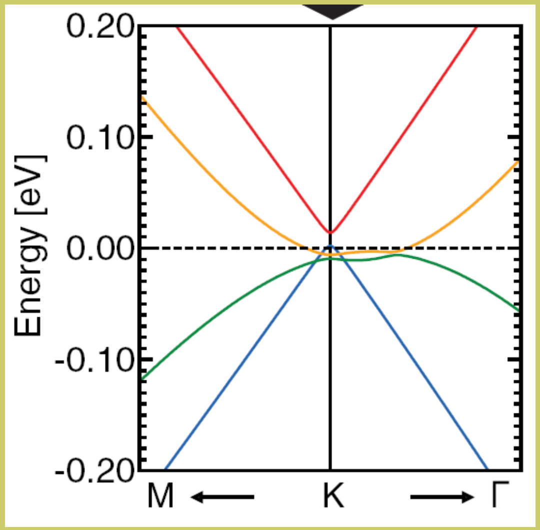


MF Craciun, S Russo, M Yamamoto, JB Oostinga,
AF Morpurgo, and S Tarucha, Nature Nanotech. **4**, 383 (2009).

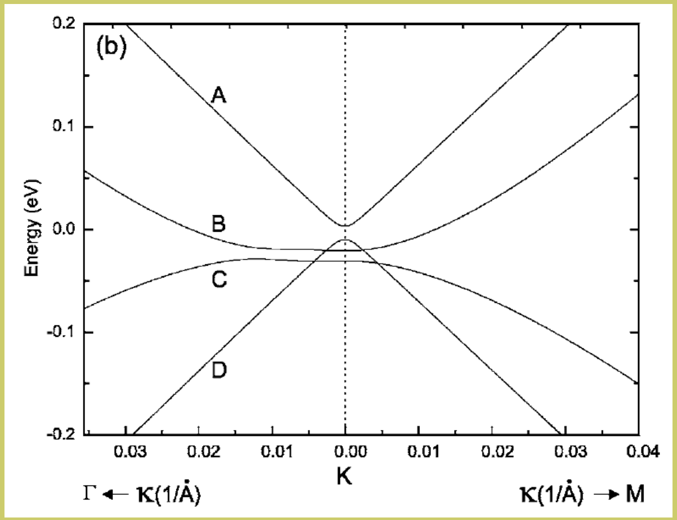


C.L. Lu *et al*, PRB **73**, 144427 (2006)
Band gap (light lines)

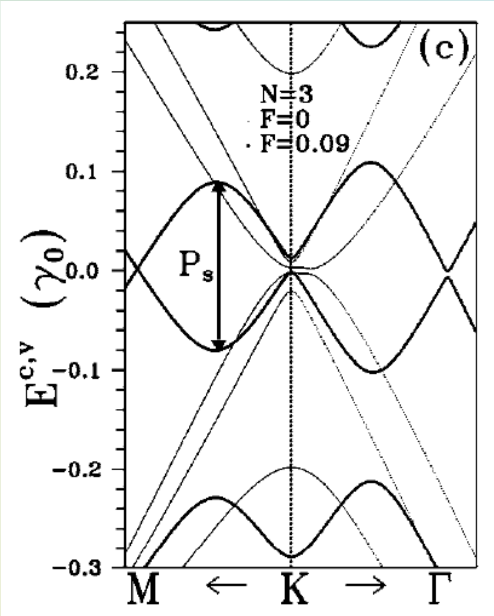
Theory of band structure of ABA-stacked trilayer graphene



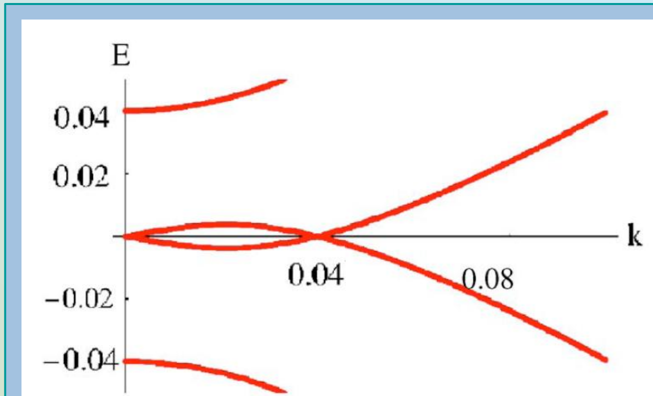
S. Latil and L. Henrard,
PRL **97**, 036803 (2006)
Band overlap



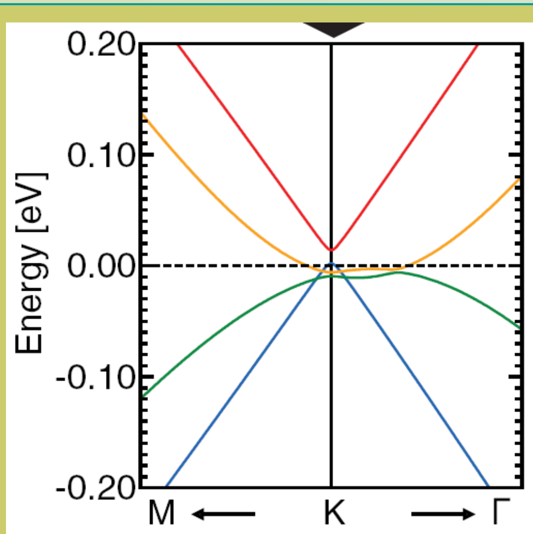
B. Partoens and F.M. Peeters,
PRB **74**, 075404 (2006)
Band overlap



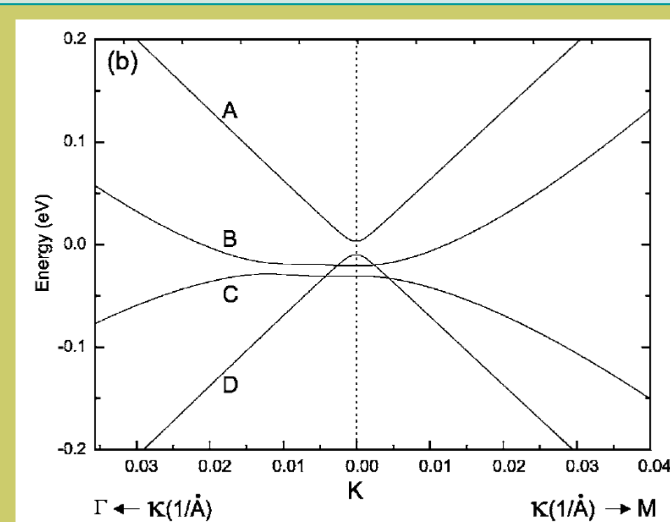
C.L. Lu *et al*, PRB **73**, 144427 (2006)
Band gap (light lines) for no electric field
Electric field (bold lines) causes crossing and anti-crossing



F. Guinea *et al*, PRB **73**, 245426 (2006)
Low energy bands in an electrostatic field



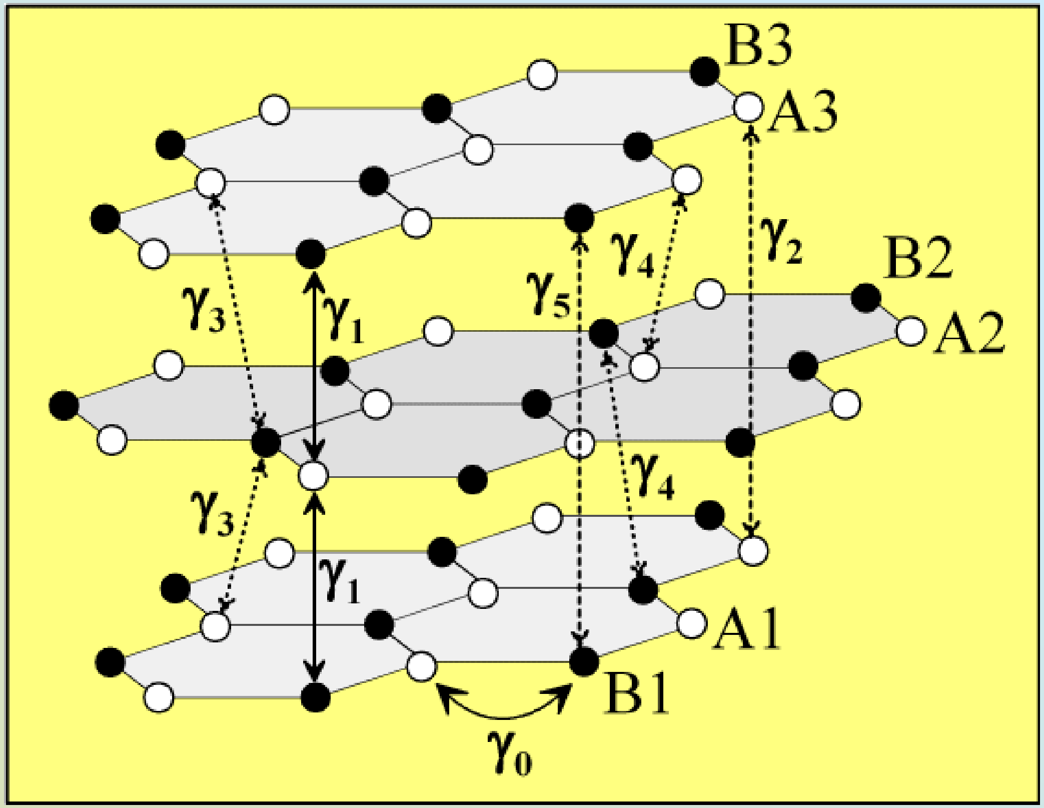
S. Latil and L. Henrard, PRL **97**, 036803 (2006)
Band overlap

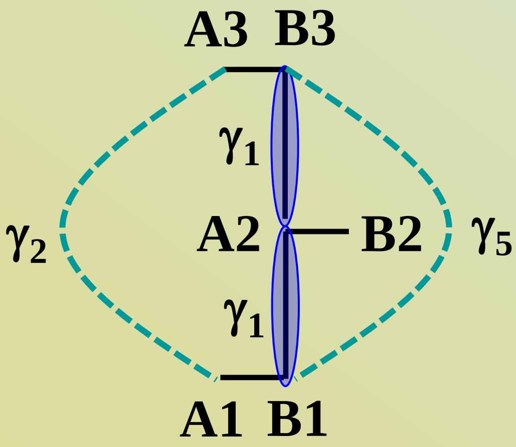


B. Partoens and F.M. Peeters, PRB **74**, 075404 (2006)
Band overlap

ABA-stacked trilayer graphene: tight-binding model

- 3 layers of carbon atoms
- 6 atoms in the unit cell (A1,B1,A2,B2,A3,B3)
- Hopping within a layer γ_0
- Interlayer coupling $\gamma_1, \gamma_3, \gamma_4$
- Next-nearest layer γ_2, γ_5





ABA-stacked trilayer graphene: tight-binding model

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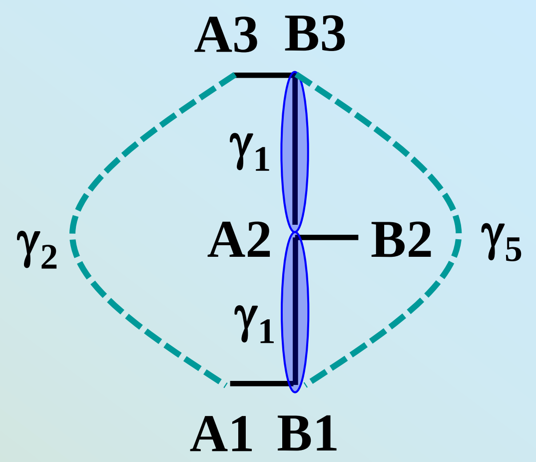


$$
\tilde{H} = \begin{array}{c} \begin{array}{cccccc} \mathbf{A1} & \mathbf{B1} & \mathbf{A2} & \mathbf{B2} & \mathbf{A3} & \mathbf{B3} \end{array} \\ \begin{pmatrix} 0 & v\pi^{+} & v_4\pi^{+} & v_3\pi & \gamma_2 & 0 \\ v\pi & 0 & \gamma_1 & v_4\pi^{+} & 0 & \gamma_5 \\ v_4\pi & \gamma_1 & 0 & v\pi^{+} & v_4\pi & \gamma_1 \\ v_3\pi^{+} & v_4\pi & v\pi & 0 & v_3\pi^{+} & v_4\pi \\ \gamma_2 & 0 & v_4\pi^{+} & v_3\pi & 0 & v\pi^{+} \\ 0 & \gamma_5 & \gamma_1 & v_4\pi^{+} & v\pi & 0 \end{pmatrix} \end{array} \begin{array}{c} \mathbf{A1} \\ \mathbf{B1} \\ \mathbf{A2} \\ \mathbf{B2} \\ \mathbf{A3} \\ \mathbf{B3} \end{array}
$$

$$\pi = p_x + ip_y$$

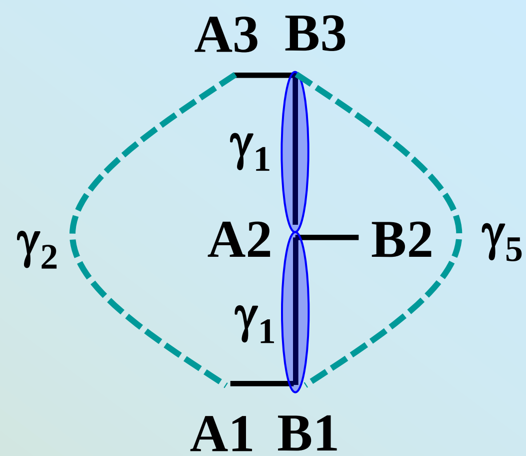
$$v = \tfrac{\sqrt{3}}{2} a\gamma_0 / \hbar$$

$$v_3 = \tfrac{\sqrt{3}}{2} a\gamma_3 / \hbar$$

$$v_4 = \tfrac{\sqrt{3}}{2} a\gamma_4 / \hbar$$

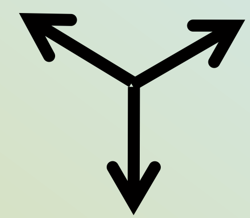
ABA-stacked trilayer graphene: tight-binding model

- 3 layers of carbon atoms
- 6 atoms in the unit cell (A1,B1,A2,B2,A3,B3)
- Hopping within a layer γ_0
- Interlayer coupling $\gamma_1,\gamma_3,\gamma_4$
- Next-nearest layer γ_2,γ_5



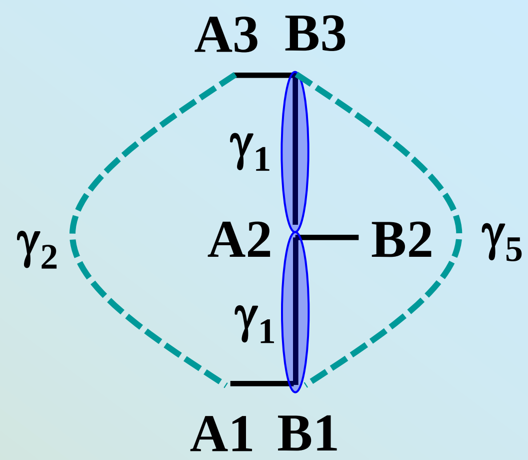
$$\tilde{H} = \begin{array}{c} \\ \\ \end{array}\begin{array}{c} \begin{array}{cccccc} A1 & B1 & A2 & B2 & A3 & B3 \end{array} \\ \begin{pmatrix} 0 & v\pi^+ & v_4\pi^+ & v_3\pi & \gamma_2 & 0 \\ v\pi & 0 & \gamma_1 & v_4\pi^+ & 0 & \gamma_5 \\ v_4\pi & \gamma_1 & 0 & v\pi^+ & v_4\pi & \gamma_1 \\ v_3\pi^+ & v_4\pi & v\pi & 0 & v_3\pi^+ & v_4\pi \\ \gamma_2 & 0 & v_4\pi^+ & v_3\pi & 0 & v\pi^+ \\ 0 & \gamma_5 & \gamma_1 & v_4\pi^+ & v\pi & 0 \end{pmatrix} \end{array} \begin{array}{c} \\ A1 \\ B1 \\ A2 \\ B2 \\ A3 \\ B3 \end{array}$$

Couplings $\gamma_0,\gamma_3,\gamma_4$ all occur between 3 nearest neighbours so appear linear in small momentum p



ABA-stacked trilayer graphene: tight-binding model

- 3 layers of carbon atoms
- 6 atoms in the unit cell (A1,B1,A2,B2,A3,B3)
- Hopping within a layer γ_0
- Interlayer coupling $\gamma_1, \gamma_3, \gamma_4$
- Next-nearest layer γ_2, γ_5

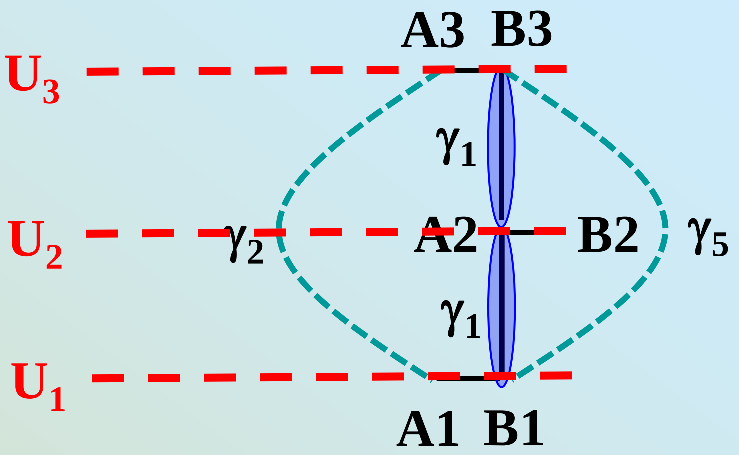


$$
\begin{array}{cc}
 & \begin{array}{cccccc} \mathbf{A1} & \mathbf{B1} & \mathbf{A2} & \mathbf{B2} & \mathbf{A3} & \mathbf{B3} \end{array} \\
\tilde{H} = & \begin{pmatrix}
0 & v\pi^{+} & v_4\pi^{+} & v_3\pi & \gamma_2 & 0 \\
v\pi & 0 & \gamma_1 & v_4\pi^{+} & 0 & \gamma_5 \\
v_4\pi & \gamma_1 & 0 & v\pi^{+} & v_4\pi & \gamma_1 \\
v_3\pi^{+} & v_4\pi & v\pi & 0 & v_3\pi^{+} & v_4\pi \\
\gamma_2 & 0 & v_4\pi^{+} & v_3\pi & 0 & v\pi^{+} \\
0 & \gamma_5 & \gamma_1 & v_4\pi^{+} & v\pi & 0
\end{pmatrix}
\begin{array}{c} \mathbf{A1} \\ \mathbf{B1} \\ \mathbf{A2} \\ \mathbf{B2} \\ \mathbf{A3} \\ \mathbf{B3} \end{array}
\end{array}
$$

Couplings $\gamma_1, \gamma_2, \gamma_5$ are vertical (with only 1 partner) so are independent of small momentum p

ABA-stacked trilayer graphene: tight-binding model

- 3 layers of carbon atoms
- 6 atoms in the unit cell (A1,B1,A2,B2,A3,B3)
- Hopping within a layer γ_0
- Interlayer coupling $\gamma_1,\gamma_3,\gamma_4$
- Next-nearest layer γ_2,γ_5
- Interlayer asymmetry U_1,U_2,U_3



$$
\tilde{H} = \begin{array}{c} \begin{array}{cccccc} \mathbf{A1} & \mathbf{B1} & \mathbf{A2} & \mathbf{B2} & \mathbf{A3} & \mathbf{B3} \end{array} \\ \begin{pmatrix} U_1 & v\pi^+ & v_4\pi^+ & v_3\pi & \gamma_2 & 0 \\ v\pi & U_1 & \gamma_1 & v_4\pi^+ & 0 & \gamma_5 \\ v_4\pi & \gamma_1 & U_2 & v\pi^+ & v_4\pi & \gamma_1 \\ v_3\pi^+ & v_4\pi & v\pi & U_2 & v_3\pi^+ & v_4\pi \\ \gamma_2 & 0 & v_4\pi^+ & v_3\pi & U_3 & v\pi^+ \\ 0 & \gamma_5 & \gamma_1 & v_4\pi^+ & v\pi & U_3 \end{pmatrix} \end{array} \begin{array}{c} \mathbf{A1} \\ \mathbf{B1} \\ \mathbf{A2} \\ \mathbf{B2} \\ \mathbf{A3} \\ \mathbf{B3} \end{array}
$$

ABA-stacked trilayer graphene: mirror-reflection symmetry

Introduce new basis:

$$\phi_1 = (A1 - A3)/\sqrt{2}$$ odd

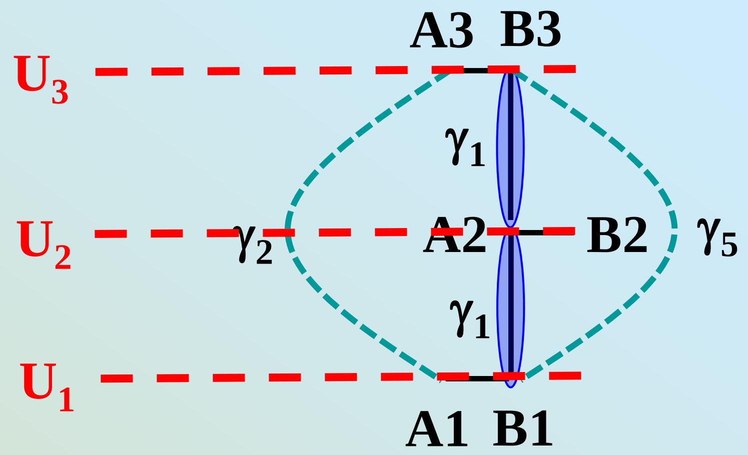
$$\phi_2 = (B1 - B3)/\sqrt{2}$$ odd

$$\phi_3 = (A1 + A3)/\sqrt{2}$$ even

$$\phi_4 = B2$$ even

$$\phi_5 = A2$$ even

$$\phi_6 = (B1 + B3)/\sqrt{2}$$ even



Introduce new asymmetry parameters:

$$\Delta_1 = (U_1 - U_3)/2$$ odd — asymmetry between outer layers

$$\Delta_2 = (U_1 - 2U_2 + U_3)/6$$ even — central layer is at different energy to the (average of the) outer ones

$$U_1 + U_2 + U_3 = 0$$ average energy is zero

ABA-stacked trilayer graphene: mirror-reflection symmetry

Monolayer block (odd)

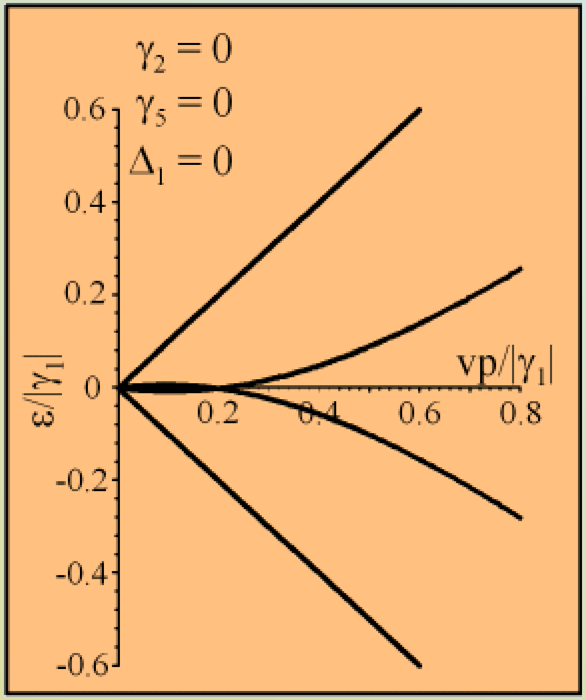
Δ_2, γ_2, γ_5 only appear on main diagonal

$$H = \begin{pmatrix} \Delta_2 - \gamma_2 & v\pi^+ & \Delta_1 & 0 & 0 & 0 \\ v\pi & \Delta_2 - \gamma_5 & 0 & 0 & 0 & \Delta_1 \\ \Delta_1 & 0 & \Delta_2 + \gamma_2 & \sqrt{2}v_3\pi & \sqrt{2}v_4\pi^+ & v\pi^+ \\ 0 & 0 & \sqrt{2}v_3\pi^+ & -2\Delta_2 & v\pi & \sqrt{2}v_4\pi \\ 0 & 0 & \sqrt{2}v_4\pi & v\pi^+ & -2\Delta_2 & \sqrt{2}\gamma_1 \\ 0 & \Delta_1 & v\pi & \sqrt{2}v_4\pi^+ & \sqrt{2}\gamma_1 & \Delta_2 + \gamma_5 \end{pmatrix}$$

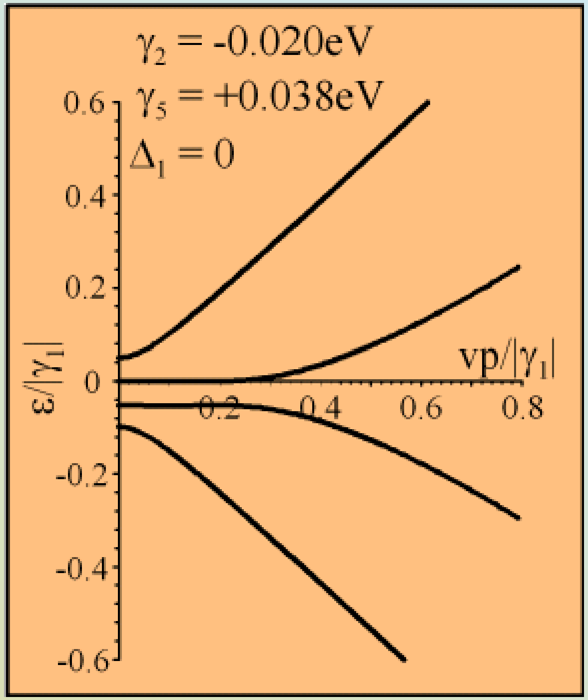
Bilayer block (even)

$$\pi = p_x + ip_y$$

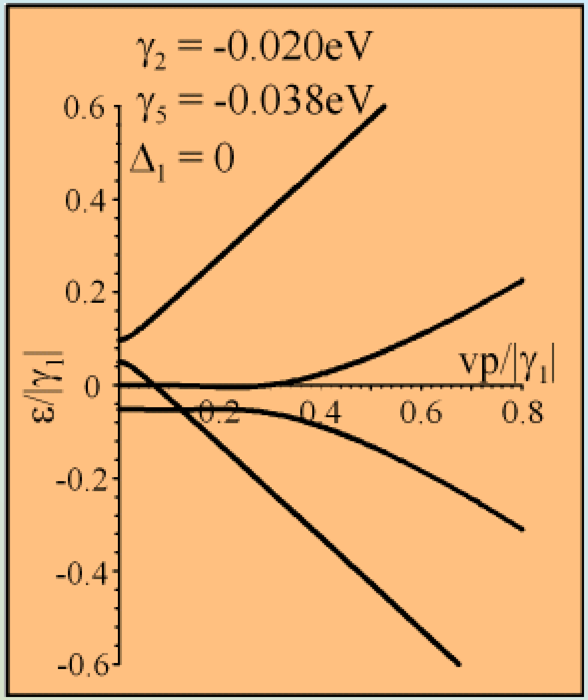
ABA-stacked trilayer graphene: next-nearest layer coupling



separate monolayer and bilayer bands (2 each at low energy, plus 2 bilayer bands at $\pm\sqrt{2}\,\gamma_1$)



γ_2, γ_5 shift the monolayer and bilayer bands...
to produce a gap



or an overlap

ABA-stacked trilayer graphene: mirror-reflection symmetry

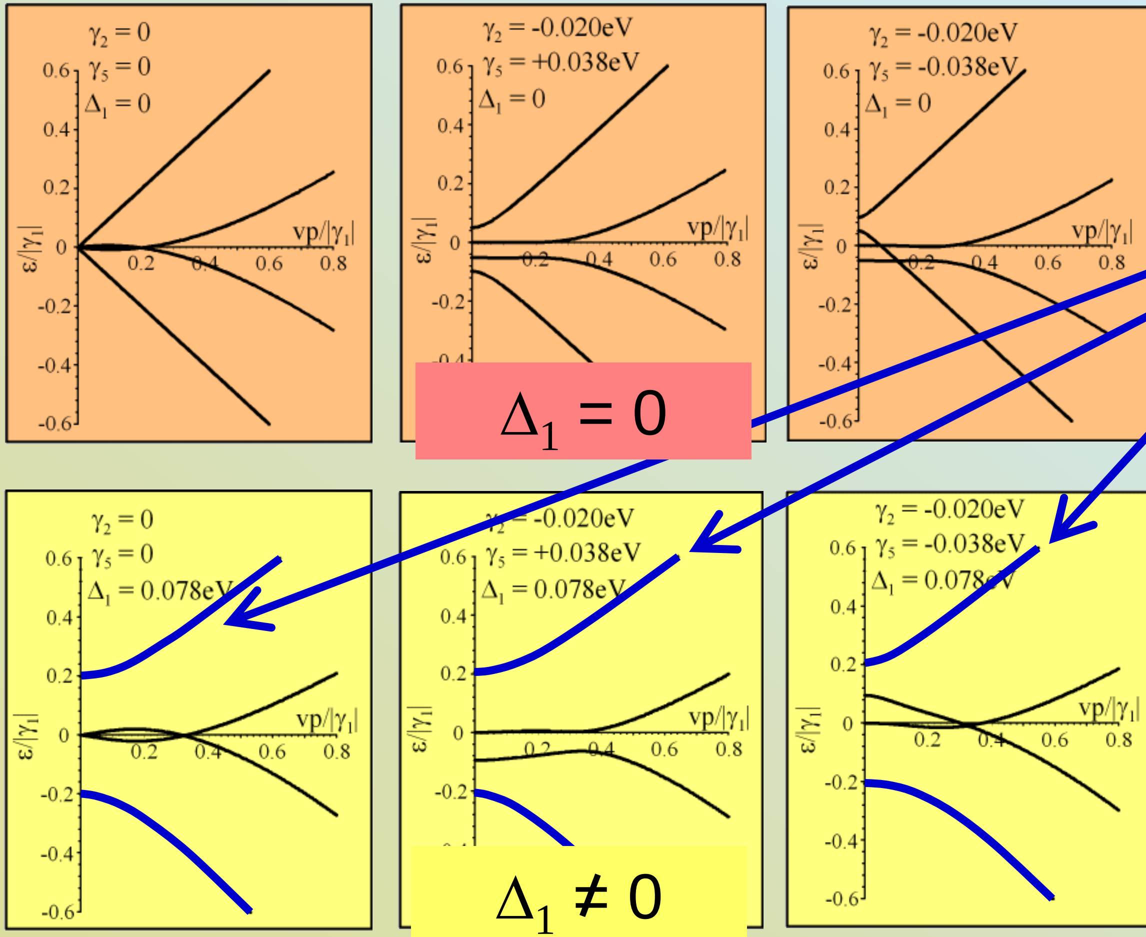
Monolayer block (odd)

$$H = \begin{pmatrix} \Delta_2 - \gamma_2 & v\pi^+ & \Delta_1 & 0 & 0 & 0 \\ v\pi & \Delta_2 - \gamma_5 & 0 & 0 & 0 & \Delta_1 \\ \Delta_1 & 0 & \Delta_2 + \gamma_2 & \sqrt{2}v_3\pi & \sqrt{2}v_4\pi^+ & v\pi^+ \\ 0 & 0 & \sqrt{2}v_3\pi^+ & -2\Delta_2 & v\pi & \sqrt{2}v_4\pi \\ 0 & 0 & \sqrt{2}v_4\pi & v\pi^+ & -2\Delta_2 & \sqrt{2}\gamma_1 \\ 0 & \Delta_1 & v\pi & \sqrt{2}v_4\pi^+ & \sqrt{2}\gamma_1 & \Delta_2 + \gamma_5 \end{pmatrix}$$

Bilayer block (even)

Δ_1 is the only parameter to break mirror reflection symmetry so it can appear in the off-diagonal block

ABA-stacked trilayer graphene: mirror-reflection symmetry



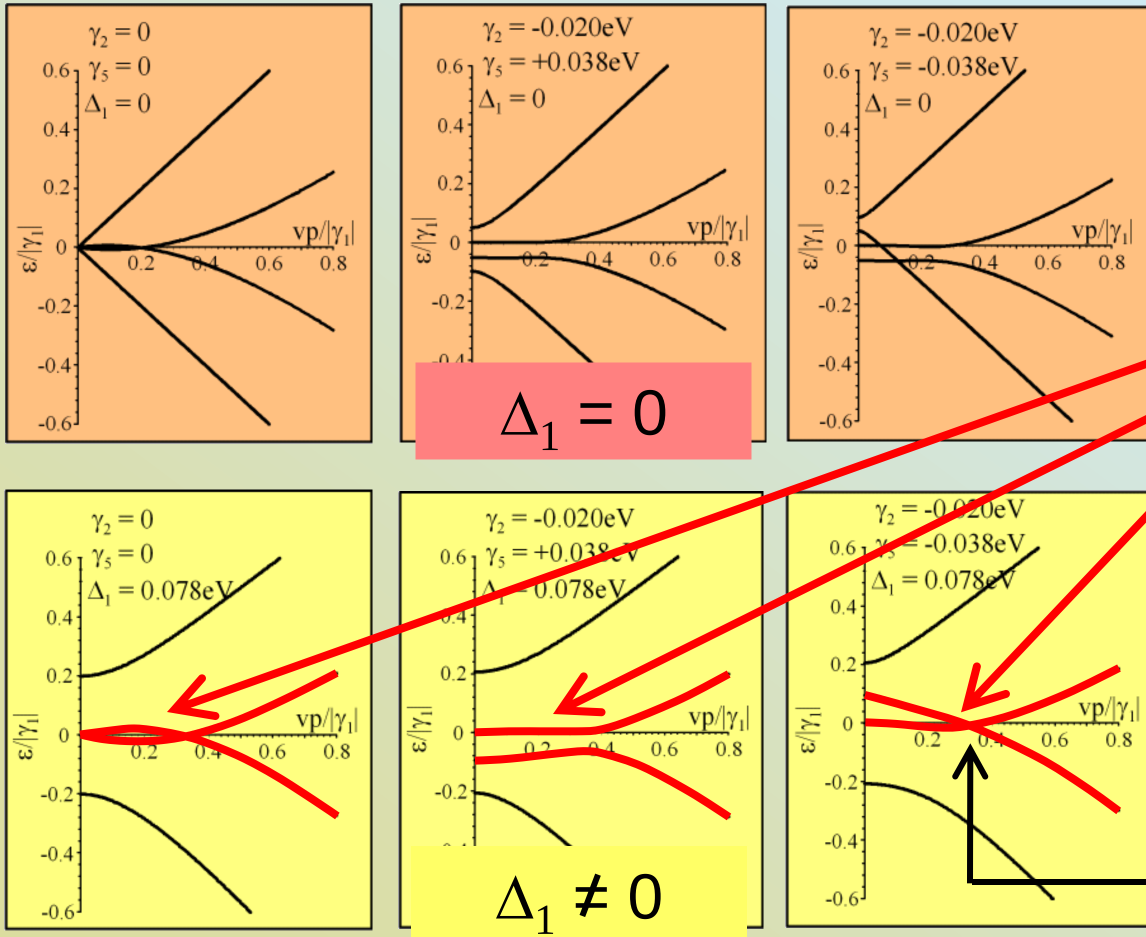
$\gamma_2 = \gamma_5 = 0$

sign(γ_2) = - sign(γ_5)

sign(γ_2) = + sign(γ_5)

- Δ_1 mixes monolayer and bilayer bands
- 2 bands go to energy $\pm\Delta_1$

ABA-stacked trilayer graphene: mirror-reflection symmetry



$\gamma_2 = \gamma_5 = 0$

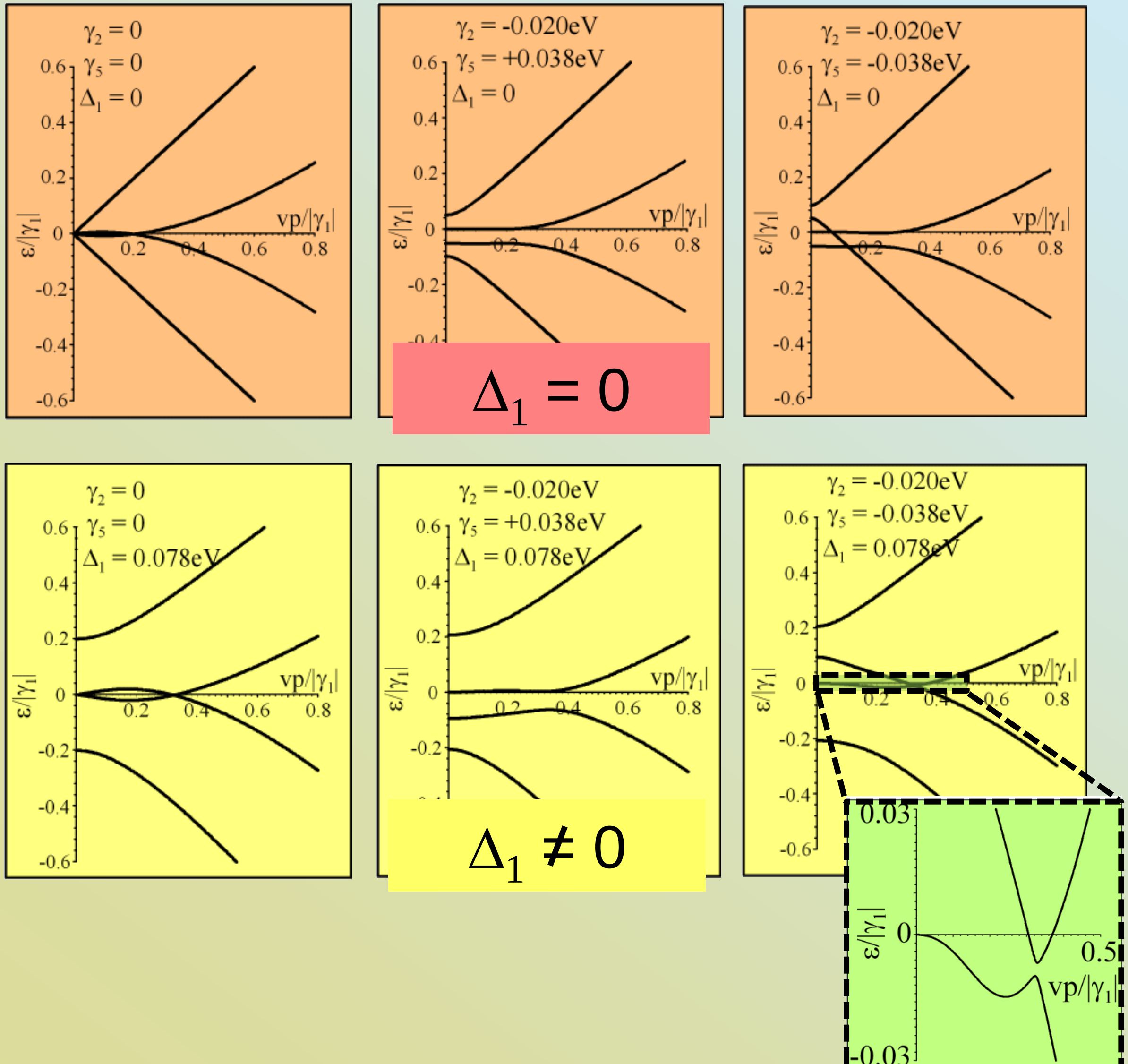
sign(γ_2) = - sign(γ_5)

sign(γ_2) = + sign(γ_5)

- Δ_1 mixes monolayer and bilayer bands
- 2 bands go to energy $\pm\Delta_1$
- 2 bands stay near zero energy

anticrossing near momentum $p \approx \Delta_1 / v$

ABA-stacked trilayer graphene: mirror-reflection symmetry



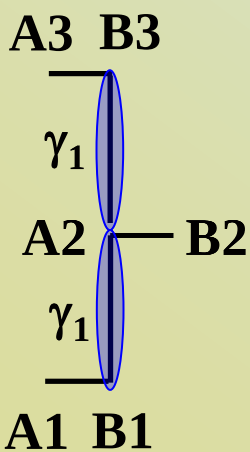
- Δ_1 mixes monolayer and bilayer bands
- 2 bands go to energy $\pm\Delta_1$
- 2 bands stay near zero energy with anti-crossing at momentum $p \approx \Delta_1 / v$
- size of hybridization gap is $\sim |\gamma_2 - \gamma_5| / 2$

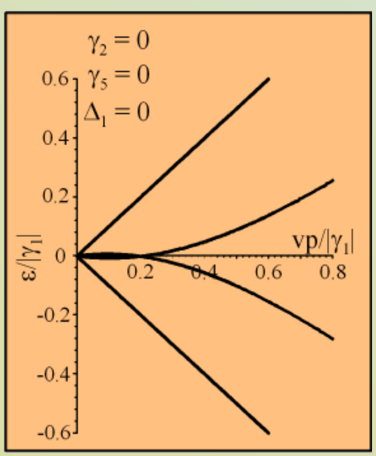
Unlike bilayer, the gap doesn't grow with Δ_1, only the position of the anticrossing p ~ Δ_1 / v

ABA-stacked trilayer graphene: low-energy effective Hamiltonian #1

$$H = \begin{pmatrix} 0 & v\pi^+ & \Delta_1 & 0 & 0 & 0 \\ v\pi & 0 & 0 & 0 & 0 & \Delta_1 \\ \Delta_1 & 0 & 0 & 0 & 0 & v\pi^+ \\ 0 & 0 & 0 & 0 & v\pi & 0 \\ 0 & 0 & 0 & v\pi^+ & 0 & \sqrt{2}\,\gamma_1 \\ 0 & \Delta_1 & v\pi & 0 & \sqrt{2}\,\gamma_1 & 0 \end{pmatrix}$$

$$\pi = p_x + ip_y$$



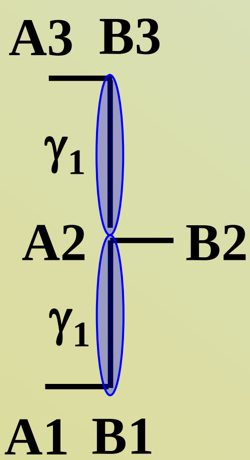


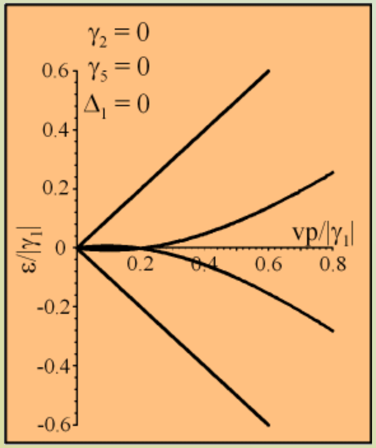
Let's simplify things by keeping only v, γ_1 and Δ_1.

ABA-stacked trilayer graphene: low-energy effective Hamiltonian #1

$$H = \begin{pmatrix} 0 & v\pi^{+} & \Delta_1 & 0 & 0 & 0 \\ v\pi & 0 & 0 & 0 & 0 & \Delta_1 \\ \Delta_1 & 0 & 0 & 0 & 0 & v\pi^{+} \\ 0 & 0 & 0 & 0 & v\pi & 0 \\ 0 & 0 & 0 & v\pi^{+} & 0 & \sqrt{2}\,\gamma_1 \\ 0 & \Delta_1 & v\pi & 0 & \sqrt{2}\,\gamma_1 & 0 \end{pmatrix}$$

$$\pi = p_x + ip_y$$





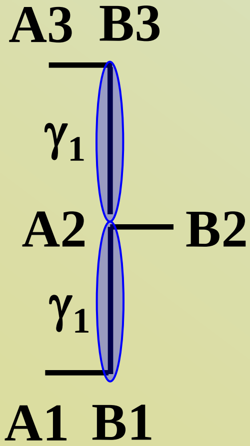
There are four bands near zero energy (at $\varepsilon << \gamma_1$) so we can eliminate the "high-energy" bilayer components:

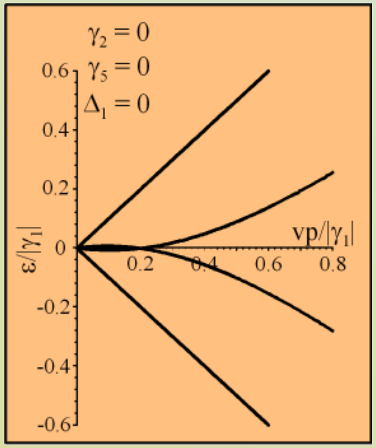
$$\phi_5 = A2$$

$$\phi_6 = (B1 + B3)/\sqrt{2}$$

ABA-stacked trilayer graphene: low-energy effective Hamiltonian #1

$$H = \begin{pmatrix} 0 & v\pi^{+} & \Delta_1 & 0 \\ v\pi & 0 & 0 & -\dfrac{\Delta_1 v\pi^{+}}{\sqrt{2}\gamma_1} \\ \Delta_1 & 0 & 0 & -\dfrac{\left(v\pi^{+}\right)^2}{\sqrt{2}\gamma_1} \\ 0 & -\dfrac{\Delta_1 v\pi}{\sqrt{2}\gamma_1} & -\dfrac{\left(v\pi\right)^2}{\sqrt{2}\gamma_1} & 0 \end{pmatrix}$$



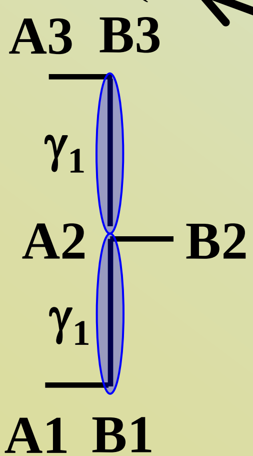


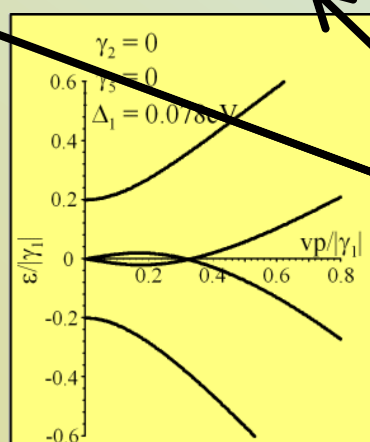
Effective Hamiltonian describing four bands near zero energy

(at $\varepsilon << \gamma_1$)

ABA-stacked trilayer graphene: low-energy effective Hamiltonian #2: large Δ_1

$$H = \begin{pmatrix} 0 & v\pi^{+} & \Delta_1 & 0 \\ v\pi & 0 & 0 & -\dfrac{\Delta_1 v\pi^{+}}{\sqrt{2}\gamma_1} \\ \Delta_1 & 0 & 0 & -\dfrac{\left(v\pi^{+}\right)^2}{\sqrt{2}\gamma_1} \\ 0 & -\dfrac{\Delta_1 v\pi}{\sqrt{2}\gamma_1} & -\dfrac{\left(v\pi\right)^2}{\sqrt{2}\gamma_1} & 0 \end{pmatrix}$$





For large Δ_1 there are two bands near zero energy (at $\varepsilon \ll \Delta_1 \ll \gamma_1$) so we can eliminate another two components: $\phi_1 = (A1 - A3)/\sqrt{2}$

$\phi_3 = (A1 + A3)/\sqrt{2}$

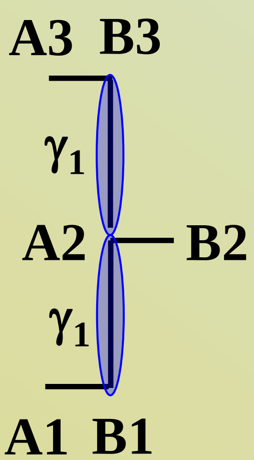
ABA-stacked trilayer graphene: low-energy effective Hamiltonian #2: large Δ_1

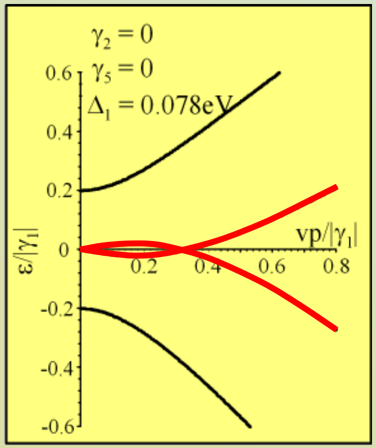
$$H = \begin{pmatrix} 0 & -\left(1+\frac{v^2\pi\pi^+}{\Delta_1^2}\right)^{-1/2}\left(1-\frac{v^2\pi\pi^+}{\Delta_1^2}\right)\frac{\Delta_1 v\pi^+}{\sqrt{2}\gamma_1} \\ -\frac{\Delta_1 v\pi}{\sqrt{2}\gamma_1}\left(1-\frac{v^2\pi\pi^+}{\Delta_1^2}\right)\left(1+\frac{v^2\pi\pi^+}{\Delta_1^2}\right)^{-1/2} & 0 \end{pmatrix}$$

in basis of $\phi_2 = (B1 - B3)/\sqrt{2}$ and $\phi_4 = B2$

chiral quasiparticles even for large asymmetry

$$\boxed{\psi = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{-i\phi/2} \\ \mp e^{+i\phi/2} \end{pmatrix}}$$





For large Δ_1 there are two bands near zero energy (at $\varepsilon \ll \Delta_1 \ll \gamma_1$).

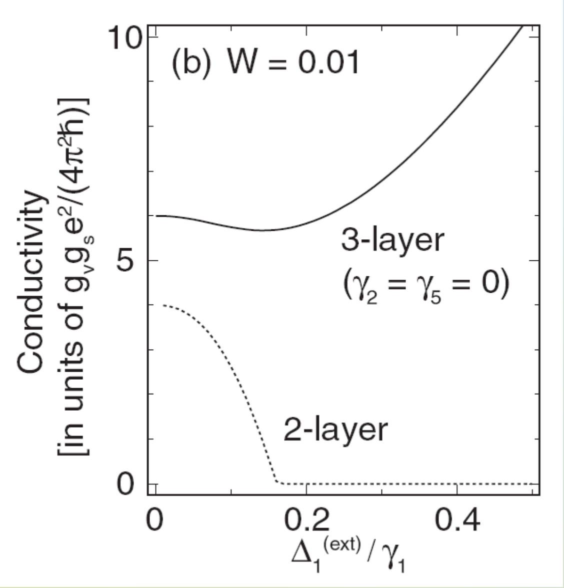
$$\gamma_2 = \gamma_3 = \gamma_4 = \gamma_5 = \Delta_2 = 0$$

$$\varepsilon \approx \pm \frac{vp}{\sqrt{2}\gamma_1}\frac{\left(v^2p^2 - \Delta_1^2\right)}{\sqrt{v^2p^2 + \Delta_1^2}}$$

Summary of ABA-trilayer

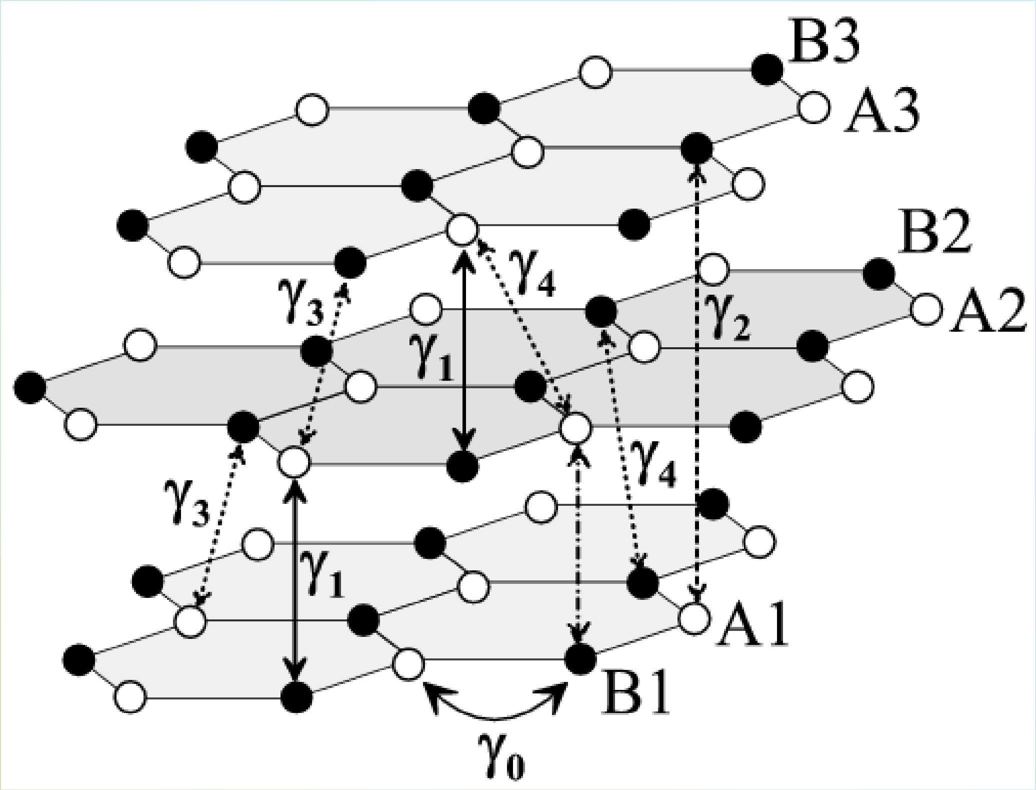
- ABA-stacked trilayer graphene:
  - Interlayer asymmetry Δ_1 hybridises low-energy linear and parabolic bands
  - Two low-energy bands with an anti-crossing and gap << Δ_1
  - The bands still support chiral quasiparticles
  - Density of states and minimal conductivity increase with Δ_1

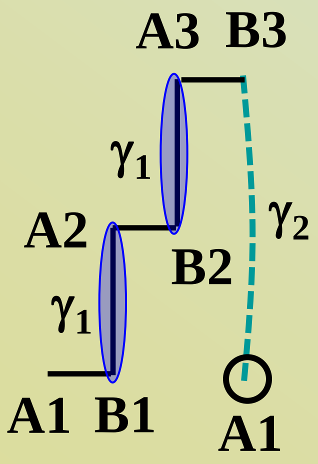
Mikito Koshino and E McCann, Phys Rev B **79**, 125443 (2009).



ABC-stacked trilayer graphene: tight-binding model

- 3 layers of carbon atoms
- 6 atoms in the unit cell (A1,B1,A2,B2,A3,B3)
- Hopping within a layer γ_0
- Interlayer coupling $\gamma_1, \gamma_3, \gamma_4$
- Next-nearest layer γ_2





ABC-stacked trilayer graphene: tight-binding model

- 3 layers of carbon atoms
- 6 atoms in the unit cell
  (A1,B1,A2,B2,A3,B3)
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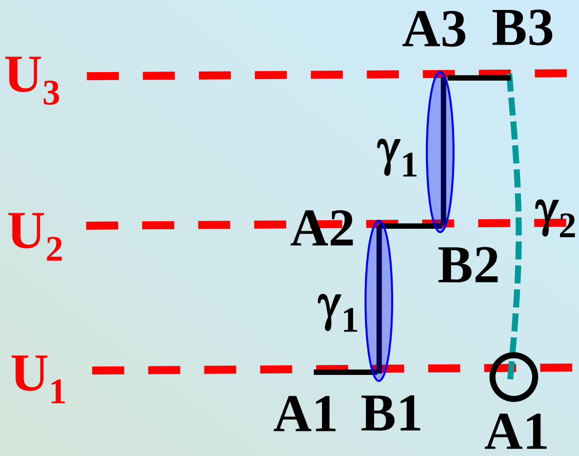
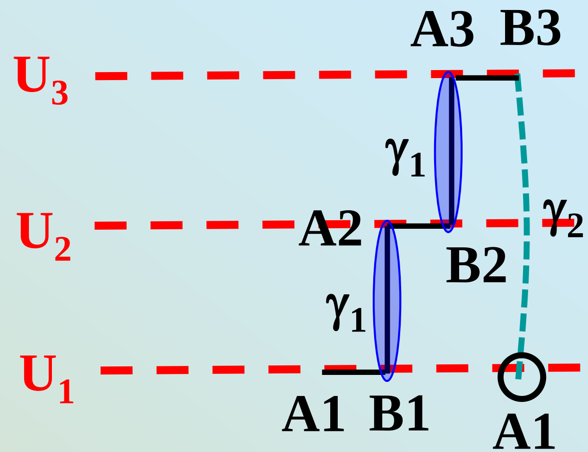
- Interlayer coupling $\gamma_1,\gamma_3,\gamma_4$
- Next-nearest layer γ_2
- Interlayer asymmetry U_1,U_2,U_3



$$\begin{array}{ccc}
 & \begin{array}{cccccc} \mathbf{A1} & \mathbf{B1} & \mathbf{A2} & \mathbf{B2} & \mathbf{A3} & \mathbf{B3} \end{array} & \\
H = & \begin{pmatrix}
U_1 & v\pi^+ & v_4\pi^+ & v_3\pi & 0 & \gamma_2/2 \\
v\pi & U_1 & \gamma_1 & v_4\pi^+ & 0 & 0 \\
v_4\pi & \gamma_1 & U_2 & v\pi^+ & v_4\pi^+ & v_3\pi \\
v_3\pi^+ & v_4\pi & v\pi & U_2 & \gamma_1 & v_4\pi^+ \\
0 & 0 & v_4\pi & \gamma_1 & U_3 & v\pi^+ \\
\gamma_2/2 & 0 & v_3\pi^+ & v_4\pi & v\pi & U_3
\end{pmatrix} & \begin{array}{c} \mathbf{A1} \\ \mathbf{B1} \\ \mathbf{A2} \\ \mathbf{B2} \\ \mathbf{A3} \\ \mathbf{B3} \end{array}
\end{array}$$

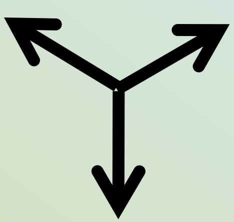
ABC-stacked trilayer graphene: tight-binding model

- 3 layers of carbon atoms
- 6 atoms in the unit cell
  (A1,B1,A2,B2,A3,B3)
- Hopping within a layer γ_0
- Interlayer coupling $\gamma_1,\gamma_3,\gamma_4$
- Next-nearest layer γ_2
- Interlayer asymmetry U_1,U_2,U_3



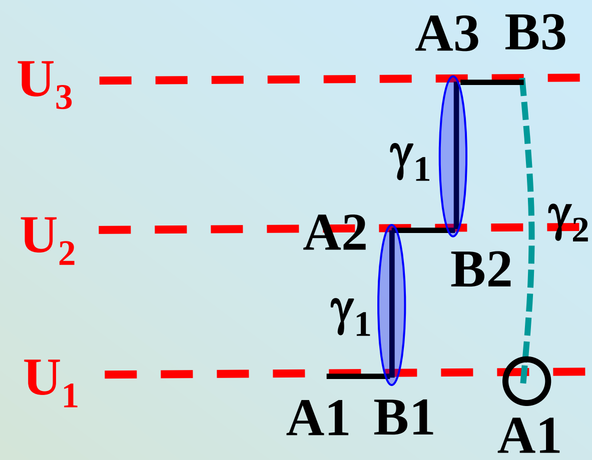
$$
H = \begin{array}{c}
\begin{array}{cccccc} \mathbf{A1} & \mathbf{B1} & \mathbf{A2} & \mathbf{B2} & \mathbf{A3} & \mathbf{B3} \end{array} \\
\begin{pmatrix}
U_1 & v\pi^+ & v_4\pi^+ & v_3\pi & 0 & \gamma_2/2 \\
v\pi & U_1 & \gamma_1 & v_4\pi^+ & 0 & 0 \\
v_4\pi & \gamma_1 & U_2 & v\pi^+ & v_4\pi^+ & v_3\pi \\
v_3\pi^+ & v_4\pi & v\pi & U_2 & \gamma_1 & v_4\pi^+ \\
0 & 0 & v_4\pi & \gamma_1 & U_3 & v\pi^+ \\
\gamma_2/2 & 0 & v_3\pi^+ & v_4\pi & v\pi & U_3
\end{pmatrix}
\end{array}
\begin{array}{c} \mathbf{A1} \\ \mathbf{B1} \\ \mathbf{A2} \\ \mathbf{B2} \\ \mathbf{A3} \\ \mathbf{B3} \end{array}
$$

Couplings $\gamma_0,\gamma_3,\gamma_4$ all occur between 3 nearest neighbours so appear linear in small momentum p



ABC-stacked trilayer graphene: tight-binding model

- 3 layers of carbon atoms
- 6 atoms in the unit cell (A1,B1,A2,B2,A3,B3)
- Hopping within a layer γ_0
- Interlayer coupling $\gamma_1, \gamma_3, \gamma_4$
- Next-nearest layer γ_2
- Interlayer asymmetry U_1, U_2, U_3

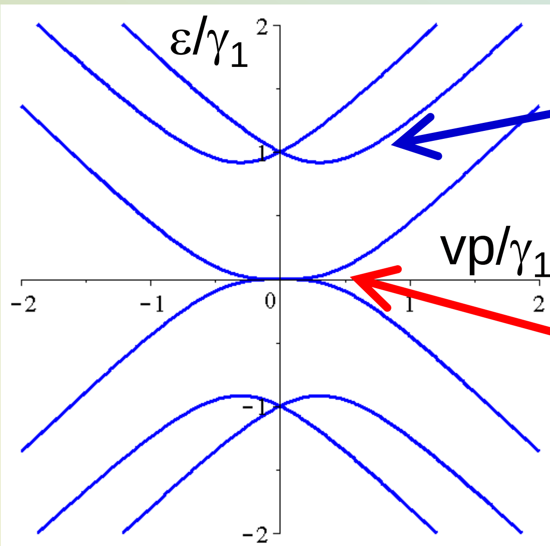


$$H = \begin{array}{cc} \begin{array}{cccccc} \mathbf{A1} & \mathbf{B1} & \mathbf{A2} & \mathbf{B2} & \mathbf{A3} & \mathbf{B3} \end{array} & \\ \begin{pmatrix} U_1 & v\pi^+ & v_4\pi^+ & v_3\pi & 0 & \gamma_2/2 \\ v\pi & U_1 & \gamma_1 & v_4\pi^+ & 0 & 0 \\ v_4\pi & \gamma_1 & U_2 & v\pi^+ & v_4\pi^+ & v_3\pi \\ v_3\pi^+ & v_4\pi & v\pi & U_2 & \gamma_1 & v_4\pi^+ \\ 0 & 0 & v_4\pi & \gamma_1 & U_3 & v\pi^+ \\ \gamma_2/2 & 0 & v_3\pi^+ & v_4\pi & v\pi & U_3 \end{pmatrix} & \begin{array}{c} \mathbf{A1} \\ \mathbf{B1} \\ \mathbf{A2} \\ \mathbf{B2} \\ \mathbf{A3} \\ \mathbf{B3} \end{array} \end{array}$$

Couplings γ_1,and γ_2 are vertical (with only 1 partner) so are independent of small momentum p

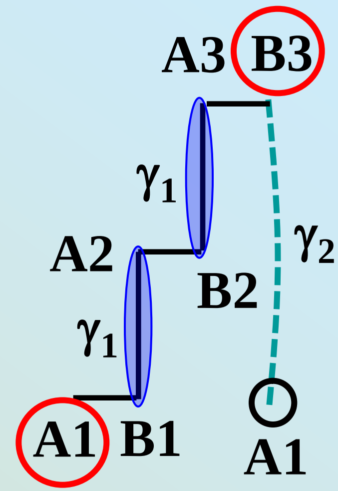
ABC-stacked trilayer graphene: tight-binding model

$$\gamma_2 = \gamma_3 = \gamma_4 = U_1 = U_2 = U_3 = 0$$



high-energy bands created by B1A2 and B2A3 dimers

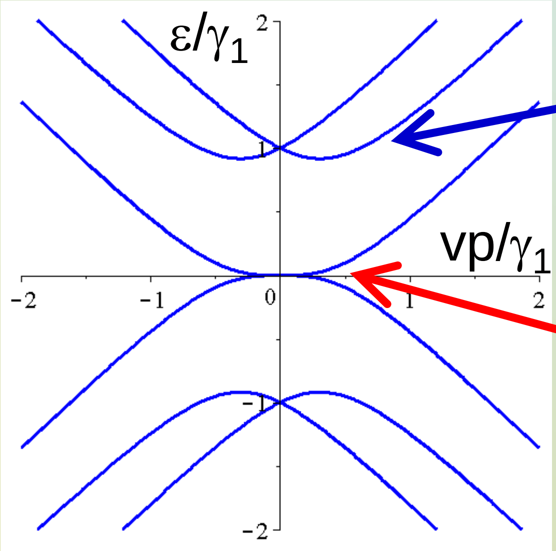
low-energy bands created by effective hopping A1 to B3: cubic generalisation of bilayer bands



F. Guinea *et al*, PRB **73**, 245426 (2006);
S. Latil and L. Henrard, PRL **97**, 036803 (2006);
C.-L. Lu *et al*, APL **89**, 221910 (2006);
M. Aoki and H. Amawashi, SSC **142**, 123 (2007).

ABC-stacked trilayer graphene: tight-binding model

$$\gamma_2 = \gamma_3 = \gamma_4 = U_1 = U_2 = U_3 = 0$$



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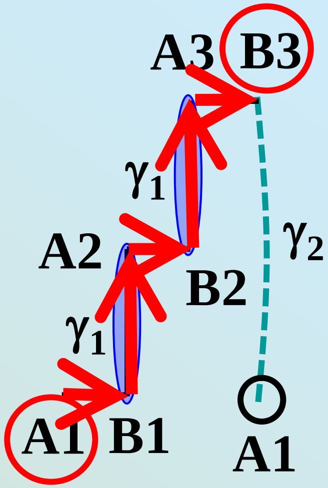


$$\hat{H}^{(eff)}_{ABC} = \frac{v^3}{\gamma_1^2}\begin{pmatrix} 0 & \left(p_x - ip_y\right)^3 \\ \left(p_x + ip_y\right)^3 & 0 \end{pmatrix}$$

chirality related to Berry's phase 3π

F. Guinea *et al*, PRB **73**, 245426 (2006);
J.L. Manes, F. Guinea, and M.A. Vozmediano, PRB **75**, 155424 (2007);
H. Min and A.H. MacDonald, PRB **77**, 155416 (2008).

AB-stacked bilayer

$$\hat{H}^{(eff)}_{bilayer} =$$

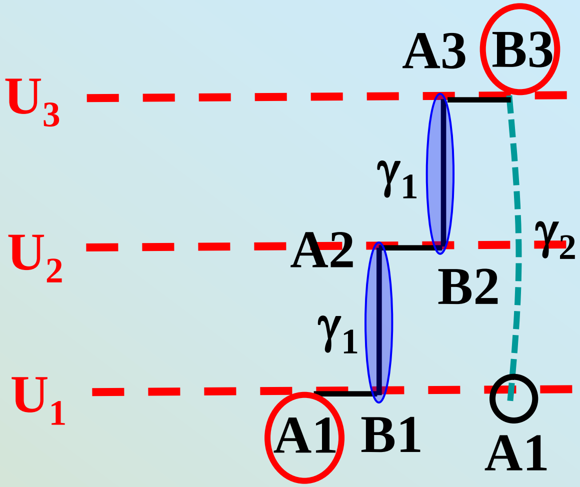
ABC-stacked trilayer

$$\hat{H}^{(eff)}_{ABC} =$$

$-\frac{v^2}{\gamma_1}\begin{pmatrix} 0 & (p_x - ip_y)^2 \\ (p_x + ip_y)^2 & 0 \end{pmatrix}$	chirality	$\frac{v^3}{\gamma_1^2}\begin{pmatrix} 0 & (p_x - ip_y)^3 \\ (p_x + ip_y)^3 & 0 \end{pmatrix}$
$+v_3\begin{pmatrix} 0 & p_x + ip_y \\ p_x - ip_y & 0 \end{pmatrix}$	trigonal warping	
$+\frac{2vv_4 p^2}{\gamma_1}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	γ_4: e-h asymmetry	
$+\Delta\left[1 - \frac{2v^2p^2}{\gamma_1^2}\right]\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	asymmetry gap	

ABC-stacked trilayer graphene: interlayer asymmetry

- 3 layers of carbon atoms
- 6 atoms in the unit cell (A1,B1,A2,B2,A3,B3)
- Hopping within a layer γ_0
- Interlayer coupling $\gamma_1,\gamma_3,\gamma_4$
- Next-nearest layer γ_2
- Interlayer asymmetry U_1,U_2,U_3



New asymmetry parameters:

$$\Delta_1 = (U_1 - U_3)/2$$

breaks symmetry between A1 and B3 sites, opening a gap

$$\Delta_2 = (U_1 - 2U_2 + U_3)/6$$

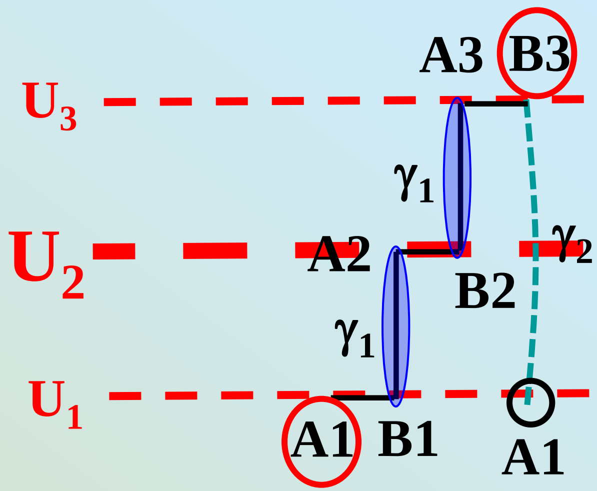
$$\Delta_1 \left[1 - \frac{v^2 p^2}{\gamma_1^2}\right] \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

in A1/B3 basis

F. Guinea *et al*, PRB **73**, 245426 (2006);
M. Aoki and H. Amawashi, SSC **142**, 123 (2007).

ABC-stacked trilayer graphene: interlayer asymmetry

- 3 layers of carbon atoms
- 6 atoms in the unit cell (A1,B1,A2,B2,A3,B3)
- Hopping within a layer γ_0
- Interlayer coupling $\gamma_1, \gamma_3, \gamma_4$
- Next-nearest layer γ_2
- Interlayer asymmetry U_1, U_2, U_3



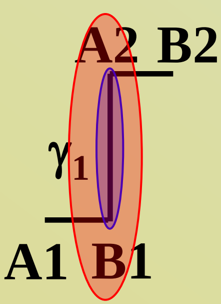
New asymmetry parameters:

$$\Delta_1 = (U_1 - U_3)/2$$

$$\Delta_2 = (U_1 - 2U_2 + U_3)/6$$

The central layer is at a different potential to the outer layers: it introduces e-h asymmetry

$$\Delta_2 \left[1 - \frac{3v^2 p^2}{\gamma_1^2}\right] \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$



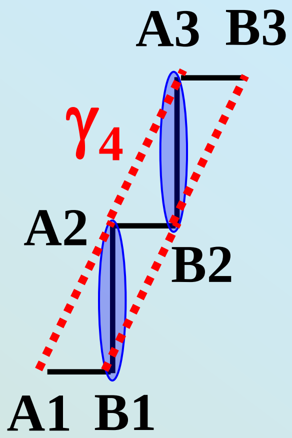
In a bilayer, a similar term is produced by asymmetry between the dimer (B1A2) and non-dimer sites (A1B2)

$$\Delta_{graphite} \left[1 - \frac{2v^2 p^2}{\gamma_1^2}\right] \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

AB-stacked bilayer		ABC-stacked trilayer
$\hat{H}^{(eff)}_{bilayer} =$		$\hat{H}^{(eff)}_{ABC} =$
$-\frac{v^2}{\gamma_1}\begin{pmatrix} 0 & (p_x - ip_y)^2 \\ (p_x + ip_y)^2 & 0 \end{pmatrix}$	chirality	$\frac{v^3}{\gamma_1^2}\begin{pmatrix} 0 & (p_x - ip_y)^3 \\ (p_x + ip_y)^3 & 0 \end{pmatrix}$
$+v_3\begin{pmatrix} 0 & p_x + ip_y \\ p_x - ip_y & 0 \end{pmatrix}$	trigonal warping	
$+\frac{2vv_4 p^2}{\gamma_1}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	γ_4: e-h asymmetry	
$+\Delta\left[1-\frac{2v^2p^2}{\gamma_1^2}\right]\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	asymmetry gap	$+\Delta_1\left[1-\frac{v^2p^2}{\gamma_1^2}\right]\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
$+\Delta_{graphite}\left[1-\frac{2v^2p^2}{\gamma_1^2}\right]\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	more e-h asymmetry	$+\Delta_2\left[1-\frac{3v^2p^2}{\gamma_1^2}\right]\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

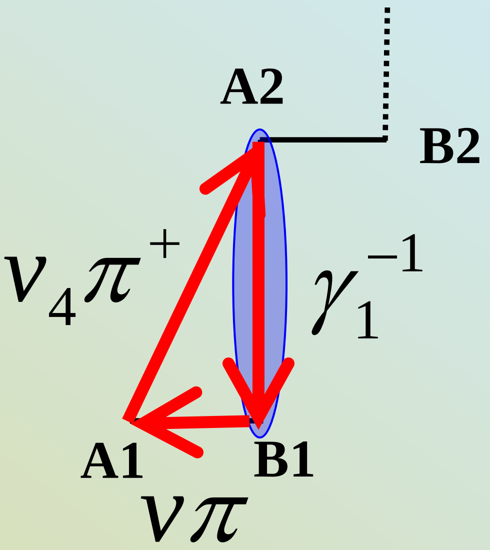
ABC-stacked trilayer graphene: role of γ_4

- 3 layers of carbon atoms
- 6 atoms in the unit cell (A1,B1,A2,B2,A3,B3)
- Hopping within a layer γ_0
- Interlayer coupling $\gamma_1, \gamma_3, \gamma_4$
- Next-nearest layer γ_2
- Interlayer asymmetry U_1, U_2, U_3



It creates the same term in the effective Hamiltonian as for the bilayer, describing electron-hole asymmetry

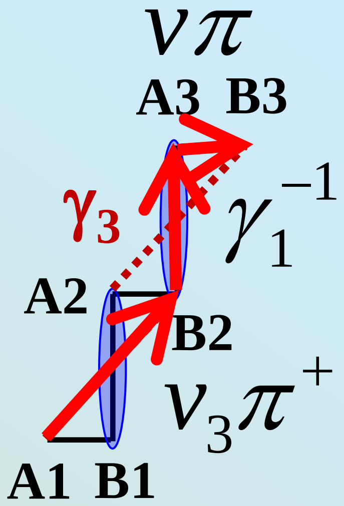
$$\frac{2vv_4p^2}{\gamma_1}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$$



This term only involves the outer two layers, so it will have the same form in all N-layer ABC multilayers (N>1).

ABC-stacked trilayer graphene: role of γ_3

- 3 layers of carbon atoms
- 6 atoms in the unit cell (A1,B1,A2,B2,A3,B3)
- Hopping within a layer γ_0
- Interlayer coupling $\gamma_1, \gamma_3, \gamma_4$
- Next-nearest layer γ_2
- Interlayer asymmetry U_1, U_2, U_3

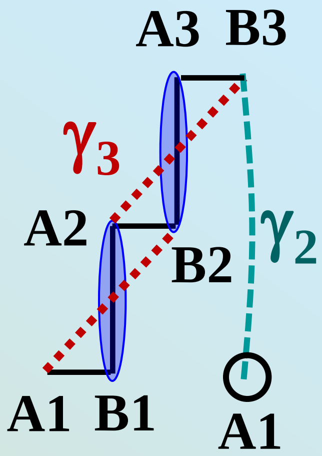


"skew" interlayer coupling γ_3 contributes to trigonal warping

$$-\frac{2vv_3p^2}{\gamma_1}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

ABC-stacked trilayer graphene: role of γ_3 and γ_2

- 3 layers of carbon atoms
- 6 atoms in the unit cell (A1,B1,A2,B2,A3,B3)
- Hopping within a layer γ_0
- Interlayer coupling γ_1,γ_3,γ_4
- Next-nearest layer γ_2
- Interlayer asymmetry U_1,U_2,U_3



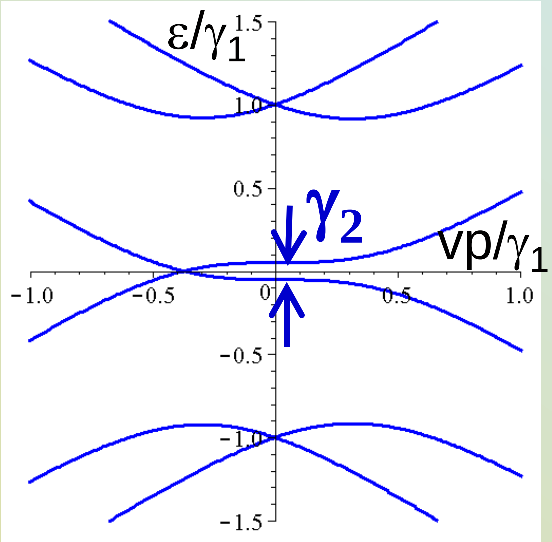
"skew" interlayer coupling γ_3 contributes to trigonal warping

$$-\frac{2vv_3p^2}{\gamma_1}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$$

vertical, next-nearest layer coupling γ_2 contributes to trigonal warping

$$\frac{\gamma_2}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$$

ABC-stacked trilayer graphene: role of γ_3 and γ_2



Even though coupling γ_2 may be small ($|\gamma_2| \sim$ 20meV?) , the γ_2 term is important because it doesn't vanish at the K point.

S. Latil and L. Henrard, PRL **97**, 036803 (2006);
C.-L. Lu *et al*, APL **89**, 221910 (2006);
M. Aoki and H. Amawashi, SSC **142**, 123 (2007).

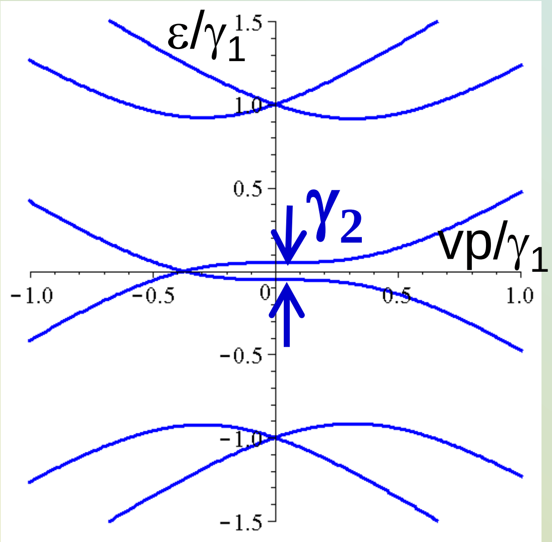
"skew" interlayer coupling γ_3 contributes to trigonal warping

$$-\frac{2vv_3p^2}{\gamma_1}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

vertical, next-nearest layer coupling γ_2 contributes to trigonal warping

$$\frac{\gamma_2}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

ABC-stacked trilayer graphene: role of γ_3 and γ_2



Even though coupling γ_2 may be small ($|\gamma_2| \sim$ 20meV?) , the γ_2 term is important because it doesn't vanish at the K point.

It sets the energy scale for the Lifshitz transition: $$\varepsilon_L \approx \frac{\gamma_2}{2} \sim 10\,meV$$

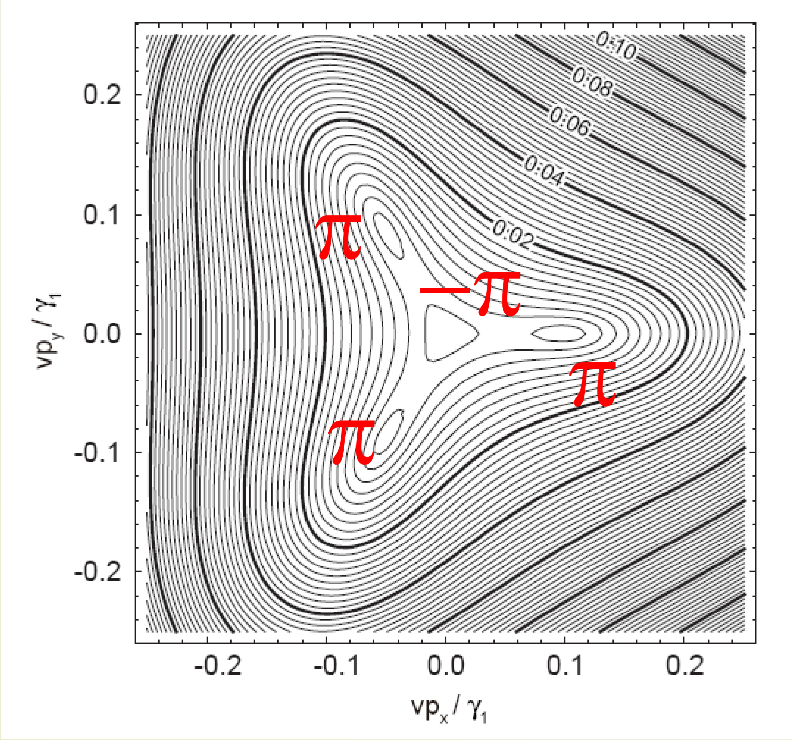
cf. bilayer $$\varepsilon_L \approx \frac{\gamma_1}{4}\left(\frac{v_3}{v}\right)^2 \sim 1meV$$

"skew" interlayer coupling γ_3 contributes to trigonal warping $$-\frac{2vv_3p^2}{\gamma_1}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

vertical, next-nearest layer coupling γ_2 contributes to trigonal warping $$\frac{\gamma_2}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Trigonal warping and Berry's phase

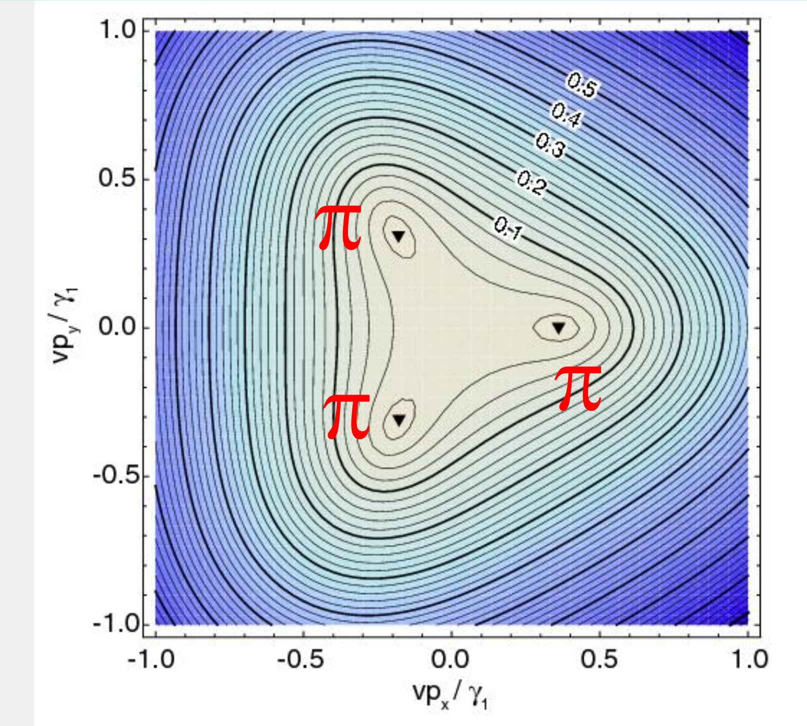
bilayer
Berry's phase 2π



central pocket

$$\varepsilon_L \approx \frac{\gamma_1}{4}\left(\frac{v_3}{v}\right)^2 \sim 1meV$$

ABC-trilayer
Berry's phase 3π

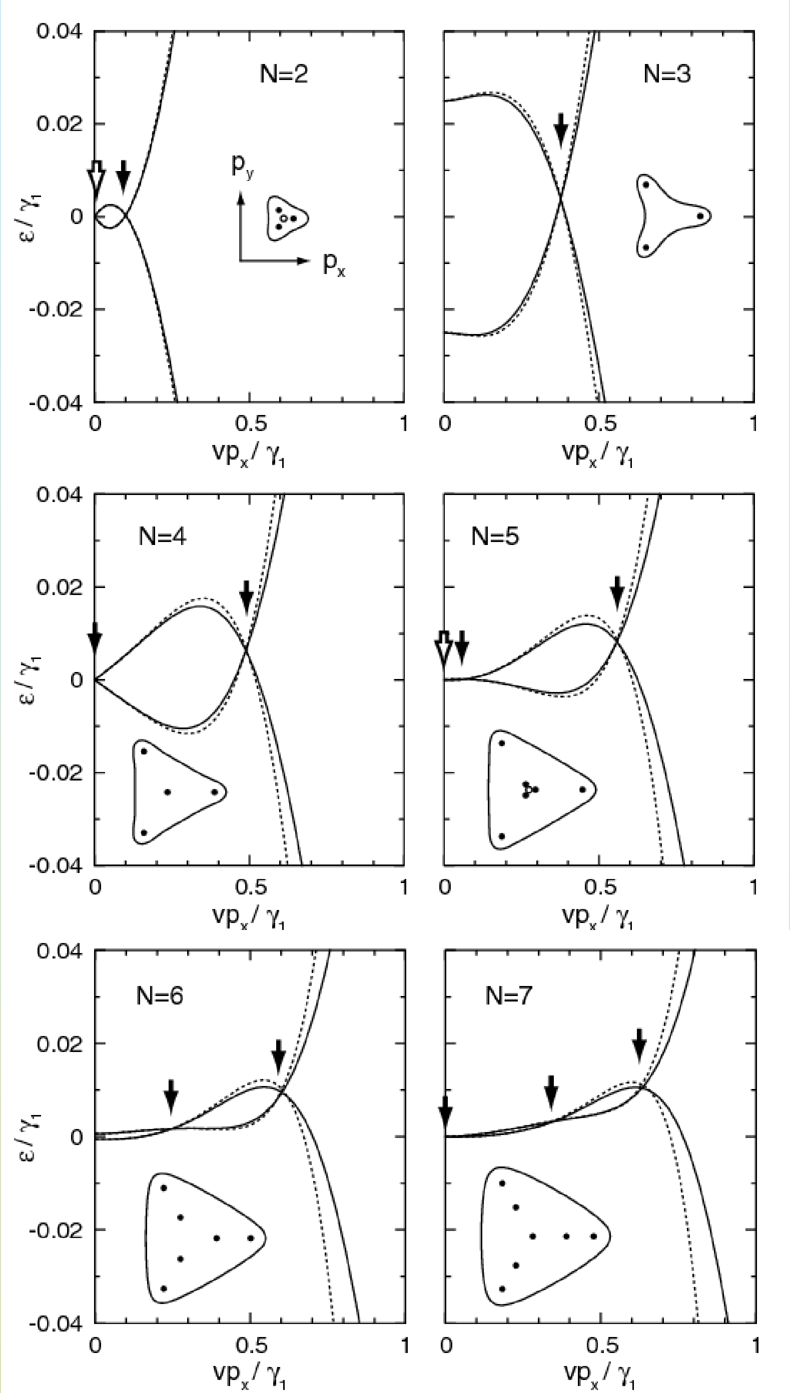


no central pocket

$$\varepsilon_L \approx \frac{\gamma_2}{2} \sim 10\,meV$$

Trigonal warping and Berry's phase

for N layers of
ABC-stacked multilayers
(with Berry phase Nπ)



AB-stacked bilayer		ABC-stacked trilayer
$\hat{H}^{(eff)}_{bilayer} =$		$\hat{H}^{(eff)}_{ABC} =$
$-\frac{v^2}{\gamma_1}\begin{pmatrix} 0 & (p_x - ip_y)^2 \\ (p_x + ip_y)^2 & 0 \end{pmatrix}$	chirality	$\frac{v^3}{\gamma_1^2}\begin{pmatrix} 0 & (p_x - ip_y)^3 \\ (p_x + ip_y)^3 & 0 \end{pmatrix}$
$+v_3\begin{pmatrix} 0 & p_x + ip_y \\ p_x - ip_y & 0 \end{pmatrix}$	trigonal warping	$+\left[-\frac{2vv_3p^2}{\gamma_1} + \frac{\gamma_2}{2}\right]\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
$+\frac{2vv_4p^2}{\gamma_1}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	γ_4: e-h asymmetry	$+\frac{2vv_4p^2}{\gamma_1}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
$+\Delta\left[1-\frac{2v^2p^2}{\gamma_1^2}\right]\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	asymmetry gap	$+\Delta_1\left[1-\frac{v^2p^2}{\gamma_1^2}\right]\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
$+\Delta_{graphite}\left[1-\frac{2v^2p^2}{\gamma_1^2}\right]\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	more e-h asymmetry	$+\Delta_2\left[1-\frac{3v^2p^2}{\gamma_1^2}\right]\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

Summary

- Trilayers aren't the same as monolayers or bilayers

- ABA-stacked trilayer:
  - Combination of "monolayer" and "bilayer" bands
  - Interlayer asymmetry Δ_1 hybridises them
  - Two low-energy bands still support chiral quasiparticles

- ABC-stacked trilayer:
  - Cubic generalisation of monolayer and bilayer
  - Lifshitz transition at relatively large energy ~ $\gamma_2/2$ ~ 10meV
  - Lifshitz transition into 3 pockets (3π) not 4 (2π) as in bilayer.

Mikito Koshino and E. McCann, Physical Review B **79**, 125443 (2009).
Mikito Koshino and E. McCann, arXiv:0906.4634