



**COLLEGE ON
PHYSICS OF NANO-DEVICES**

10 - 21 July 2006

Quantum transport of chiral electrons in graphene I

Presented by:

Vladimir Falko

Lancaster University, U.K.

Quantum transport of chiral electrons in graphene

Vladimir Falko

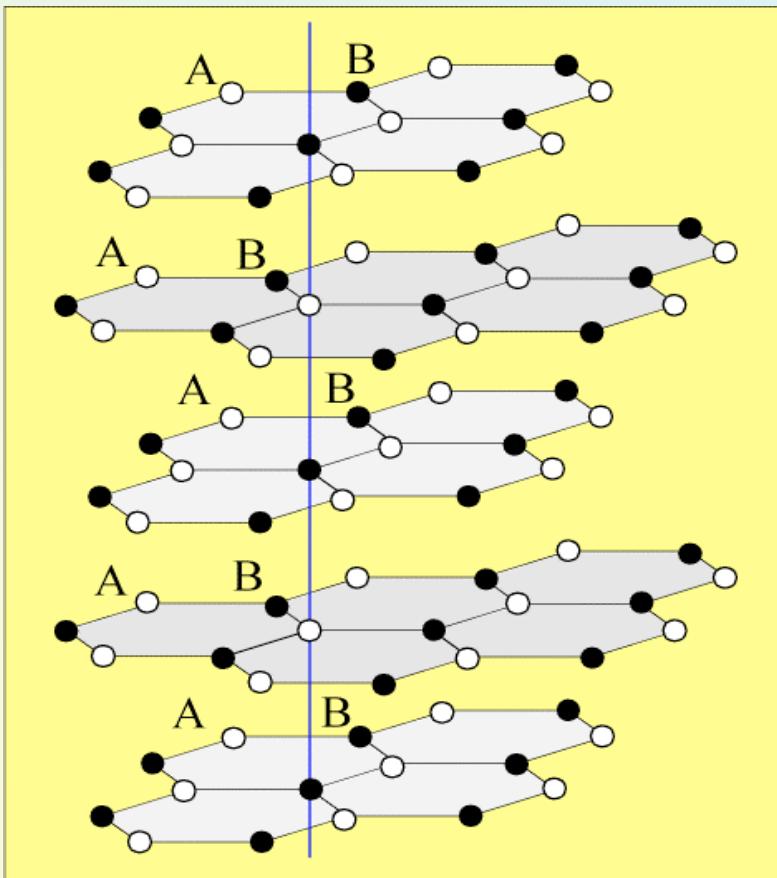
Lancaster Centre for Nanoscale Dynamics and
Mathematical Modeling



with
E.McCann, V.Cheianov
K.Kechedzhi, D.Abergel
T.Ando, B.Altshuler



Graphite



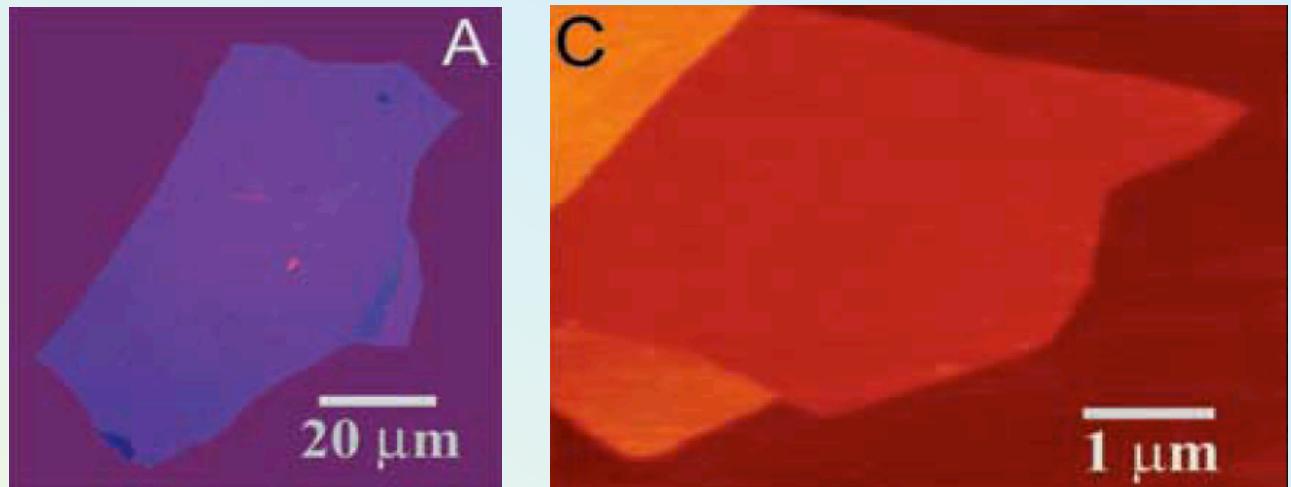
Three dimensional layered material
with hexagonal 2D layers [Bernal
(AB) stacking]

M. S. Dresselhaus and G. Dresselhaus
Adv. Phys. 51, 1 (2002)

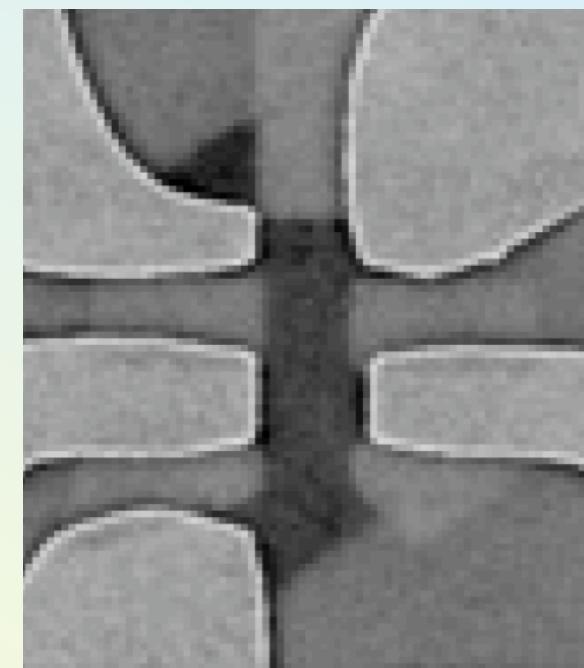
Layered poorly conducting
semimetal used in pencils

Ultra-thin graphitic films: from flakes to micro-devices

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

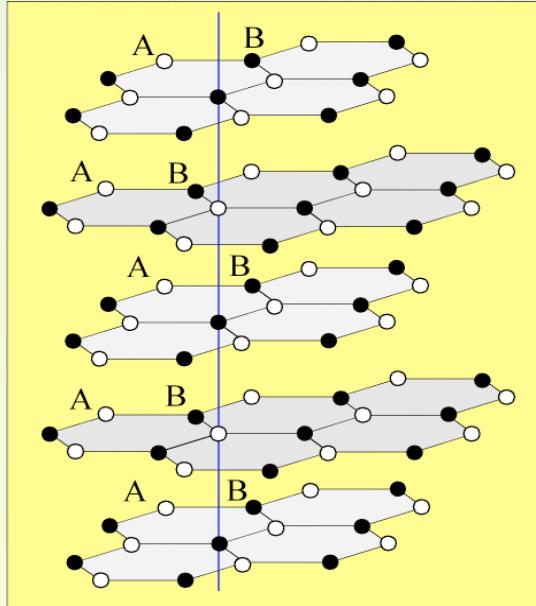


K. Novoselov et al., Nature 438, 197 (2005)
J. Bunch et al., Nano. Lett. 5, 287 (2005)
Y. Zhang et al., Phys. Rev. Lett. 94, 176803 (2005)
Y. Zhang et al., Nature 438, 201 (2005)
K. Novoselov et al, Nature Physics 2, 177 (2006)

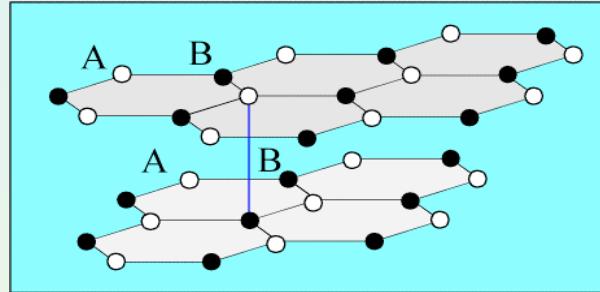


Elementary introduction in graphene physics

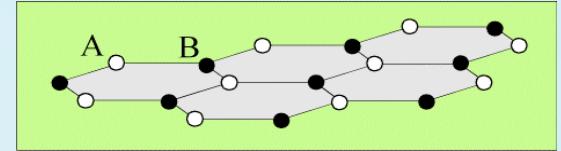
Graphite



Bilayer



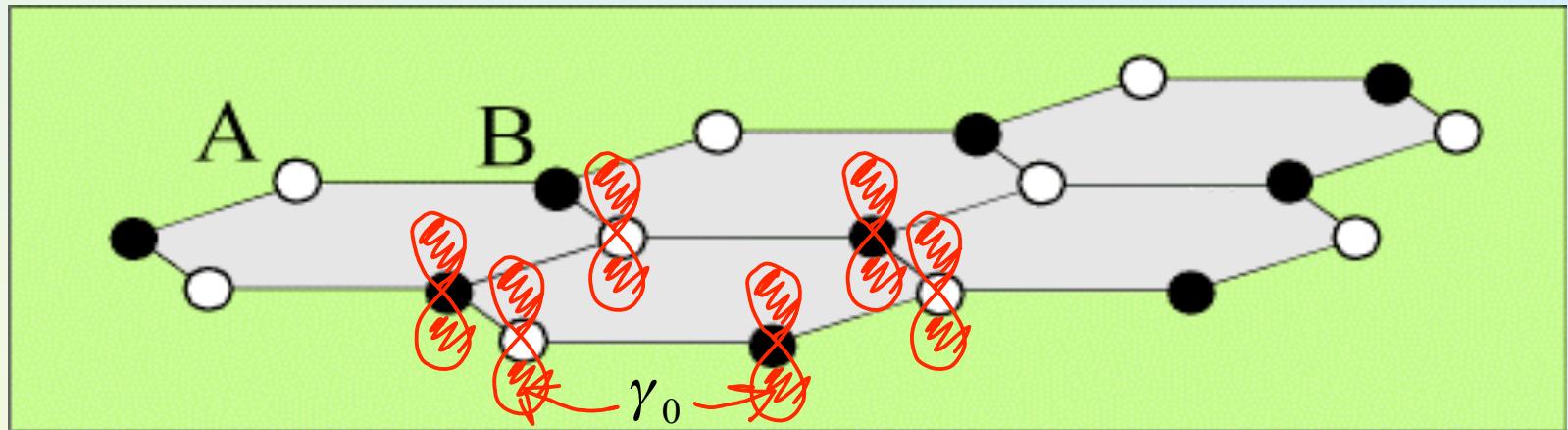
Monolayer



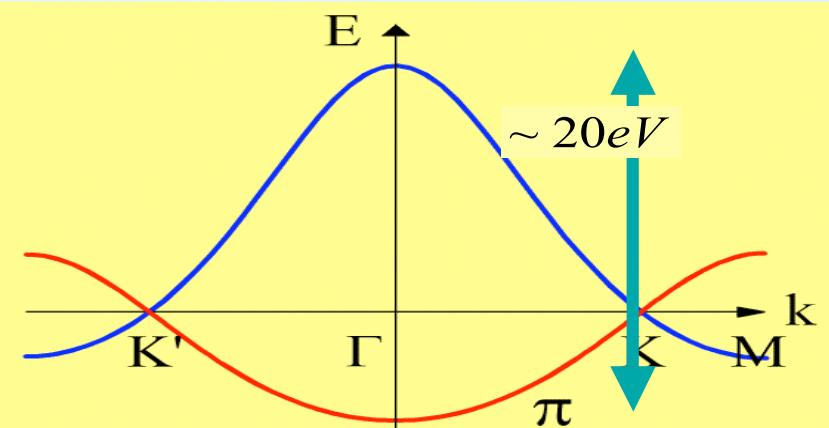
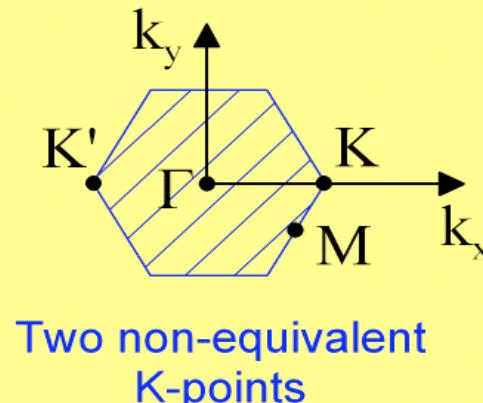
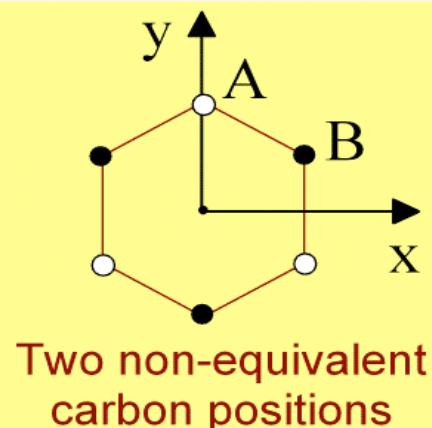
1. Tight-binding-model for the Dirac-type electron spectrum in graphene and its relation to the lattice symmetry.
2. Landau levels of chiral electrons in graphene, Quantum Hall effect in monolayers (graphene) and bilayers.
3. Chirality of carriers in graphene and Berry's phase $J\pi$, quantum transport properties of chiral 2D electrons.

Carbon has 4 electrons in the outer s-p shell

sp^2 hybridisation forms strong directed bonds which determine a honeycomb lattice structure.



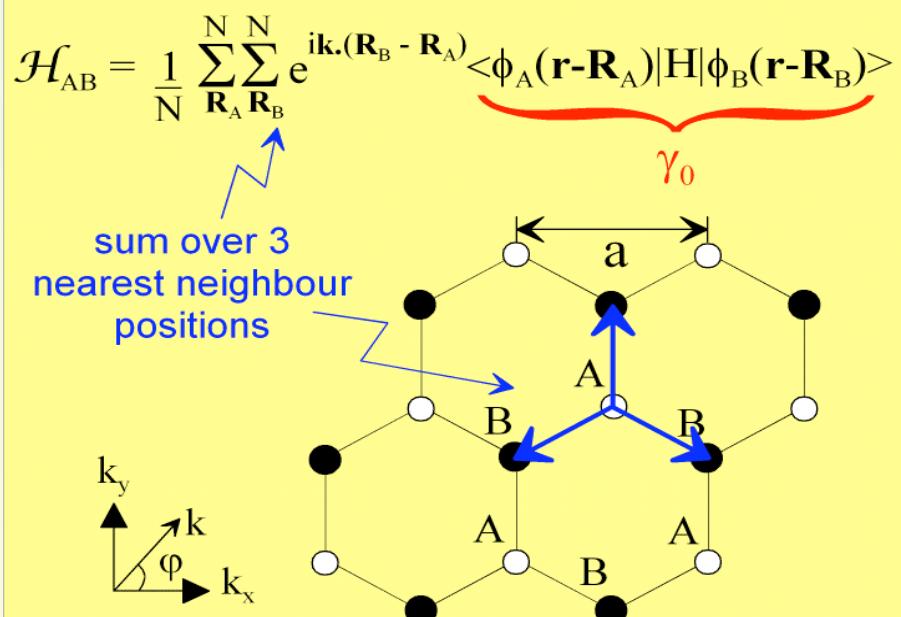
$p^z(\pi)$ orbitals determine conduction properties of graphite



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

Transfer integral on a hexagonal lattice

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



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

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

Tight binding model of a monolayer

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

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

sum over N atomic positions

jth 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 $\mathcal{H}_{ij} = \langle \Phi_i | H | \Phi_j \rangle$

Overlap integral matrix $S_{ij} = \langle \Phi_i | \Phi_j \rangle$

Column vector

$$C_j = \begin{pmatrix} C_{j1} \\ C_{j2} \end{pmatrix}$$

Eigenvalue equation

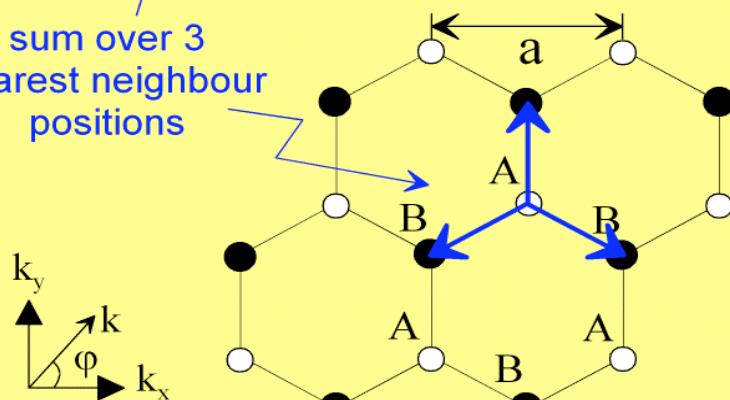
$$\mathcal{H}C_j = \varepsilon_j S C_j$$

Transfer integral on a hexagonal lattice

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

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

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

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

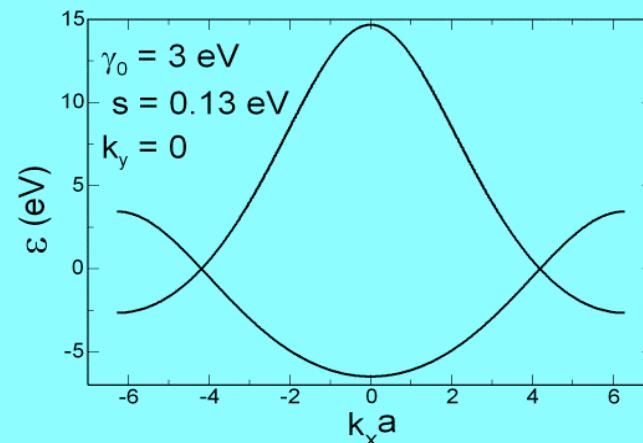
Overlap integral matrix

$$S = \begin{pmatrix} 1 & sf(\mathbf{k}) \\ sf^*(\mathbf{k}) & 1 \end{pmatrix}$$

Eigenvalue equation

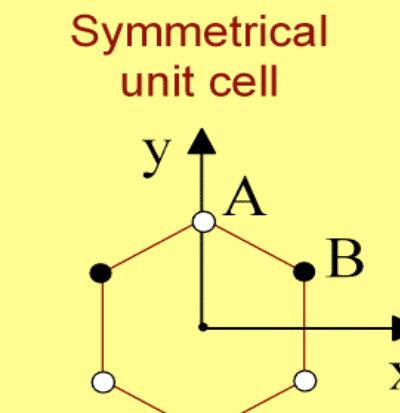
$$\mathcal{H}C_j = \varepsilon_j S C_j$$

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

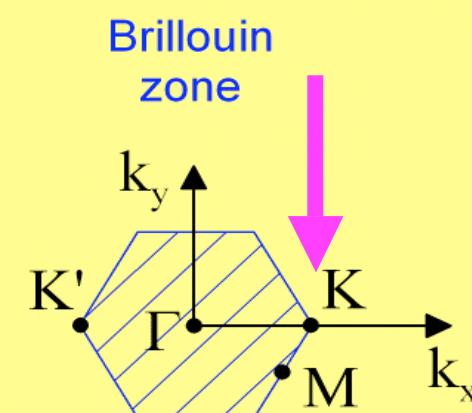


Electronic dispersion of a monolayer

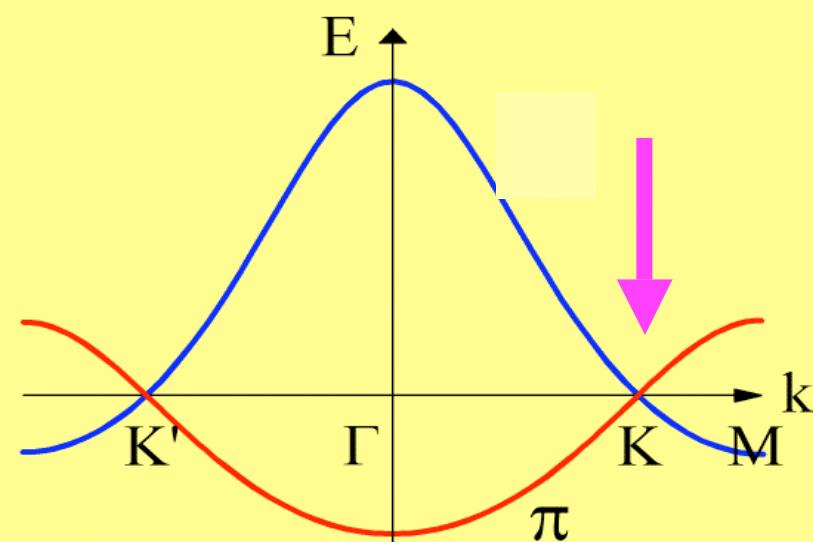
Saito *et al*, "Physical Properties of Carbon Nanotubes"
(Imperial College Press, London, 1998)



Two non-equivalent carbon positions



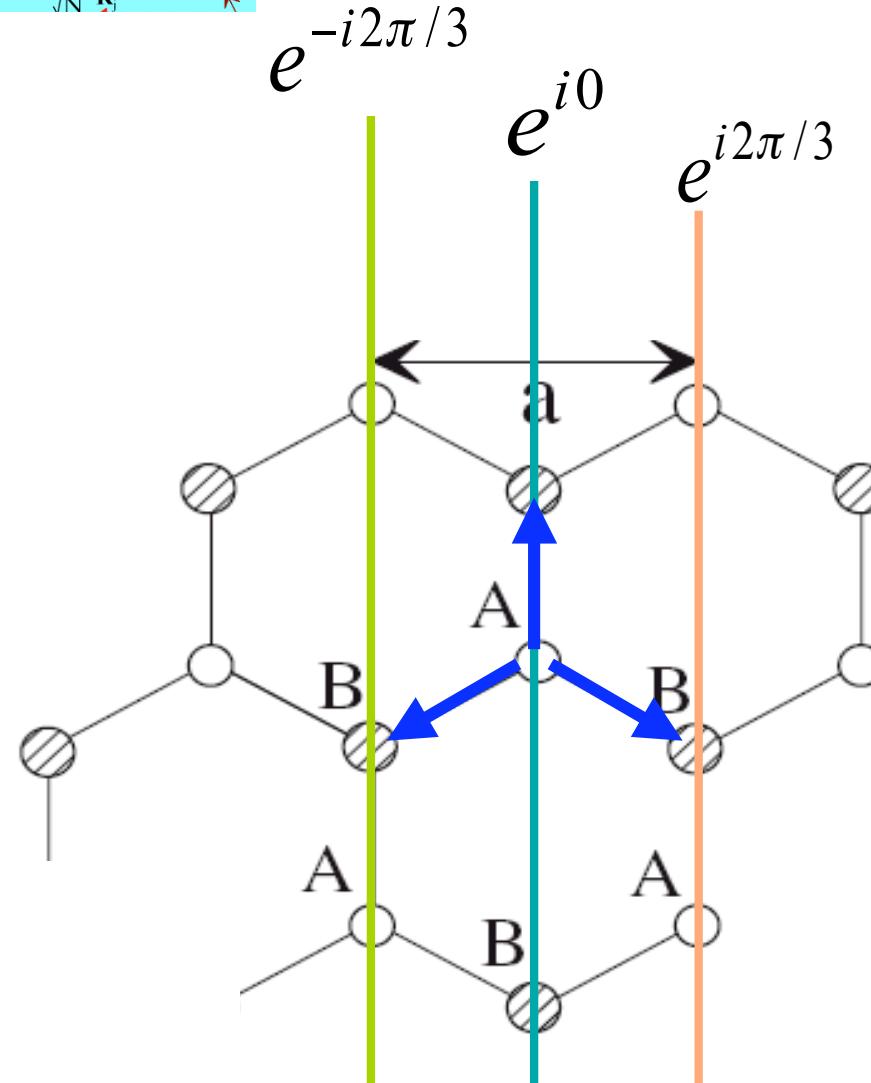
Two non-equivalent K-points



Two bands: no energy gap at the K-points

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

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



four-fold degeneracy

In the corners of the Brillouin zone,
electron states on the A and B sub-lattices
decouple and have exactly the same energy:

$$H_{AB} = -\gamma_0(e^{-i2\pi/3} + 1 + e^{i2\pi/3}) = 0$$

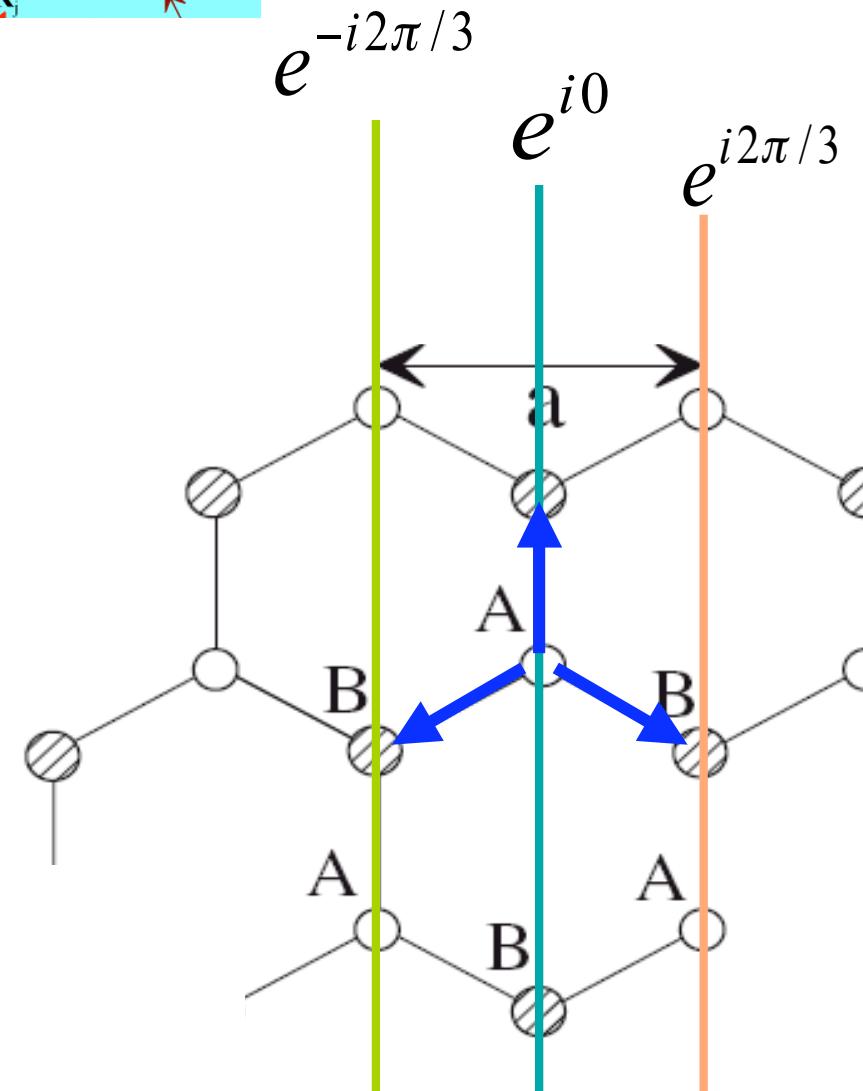
$$\varepsilon(K_+) = \varepsilon(K_-) = 0$$

$$\begin{array}{l} A + \\ B + \\ B - \\ A - \end{array} \quad \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}; \quad \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}; \quad \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}; \quad \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

↑ valley index

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

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

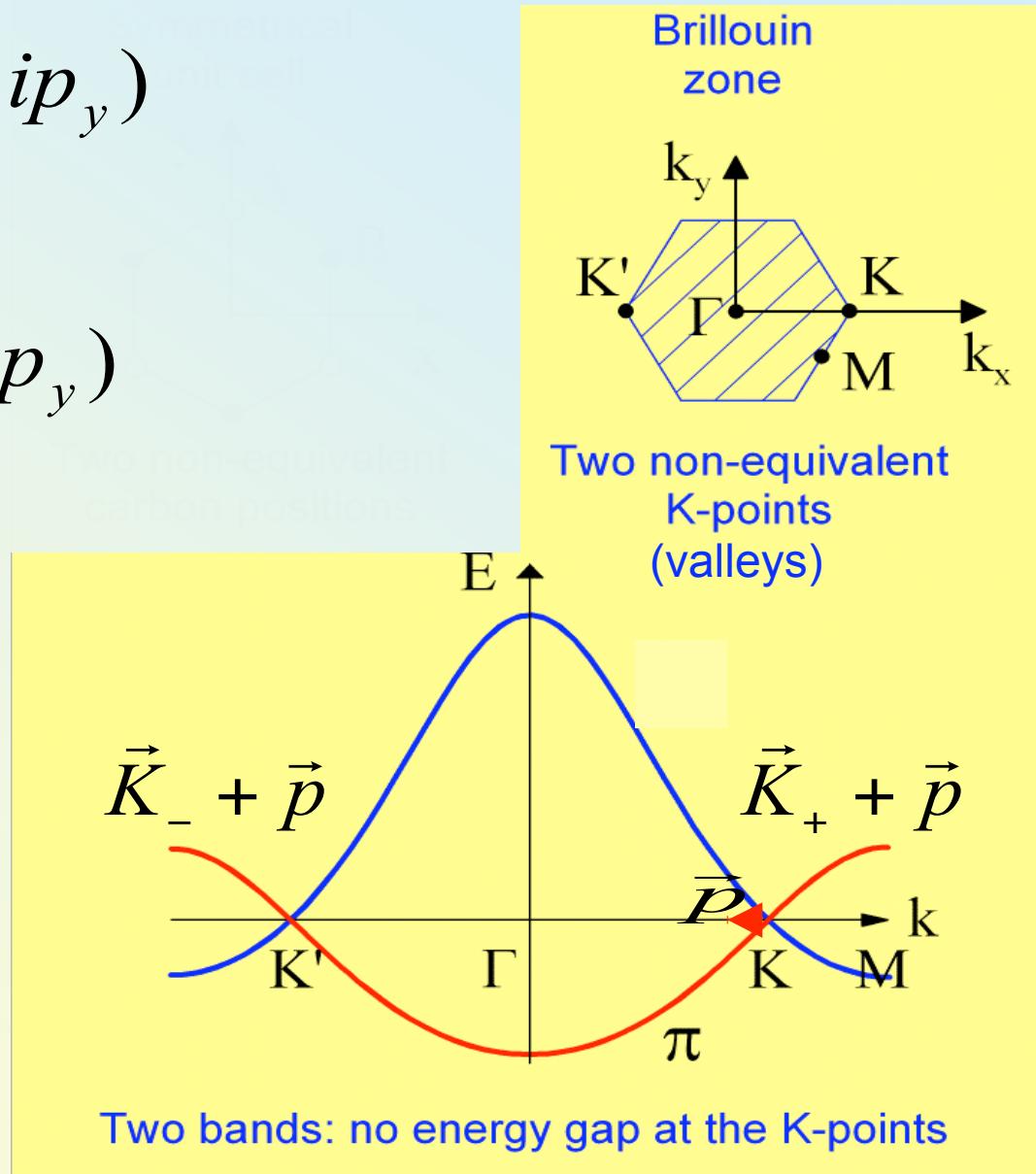


$$H_{AB,K_+} = -\gamma_0 \left[e^{-i\frac{2\pi}{3}} e^{-i(\frac{a}{2}p_x + \frac{a}{2\sqrt{3}}p_y)} + e^{i\frac{a}{\sqrt{3}}p_y} + e^{i\frac{2\pi}{3}} e^{i(\frac{a}{2}p_x - \frac{a}{2\sqrt{3}}p_y)} \right]$$

$$\approx -\frac{\sqrt{3}}{2}\gamma_0 a(p_x - ip_y)$$

$$H_{BA,K_+} \approx -\frac{\sqrt{3}}{2}\gamma_0 a(p_x + ip_y)$$

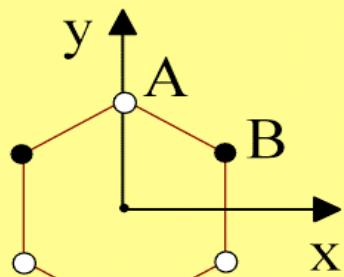
$$v = \frac{\sqrt{3}}{2}\gamma_0 a \sim 10^8 \frac{cm}{sec}$$



Electronic dispersion of a monolayer

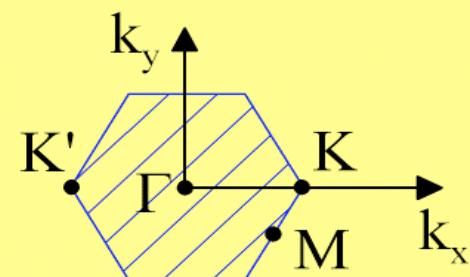
Saito *et al*, "Physical Properties of Carbon Nanotubes"
(Imperial College Press, London, 1998)

Symmetrical unit cell

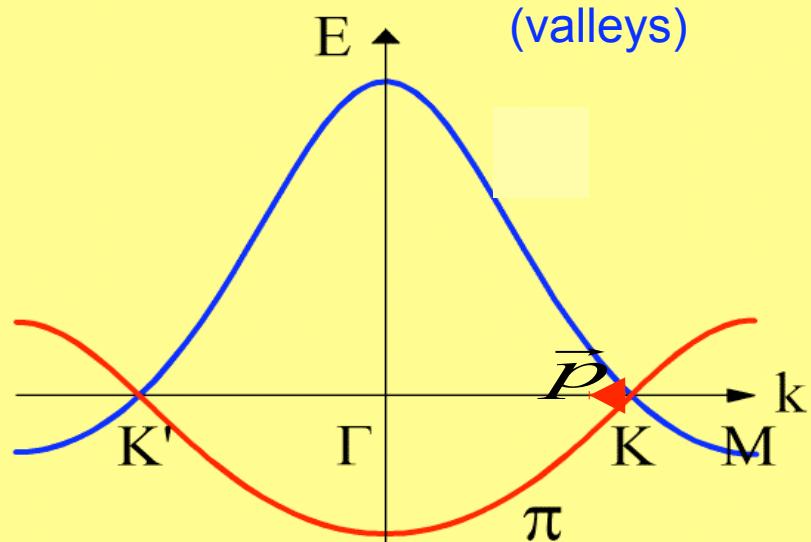


Two non-equivalent carbon positions

Brillouin zone



Two non-equivalent K-points (valleys)



Two bands: no energy gap at the K-points

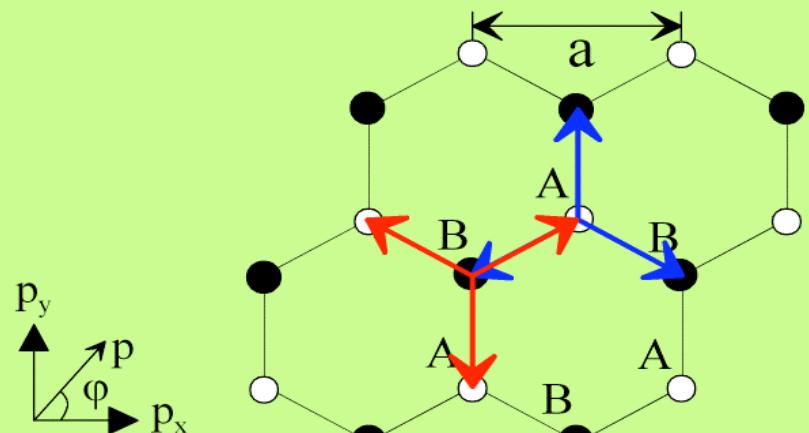
Dirac Hamiltonian of a monolayer

written in a 2 component basis of A and B sites

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

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

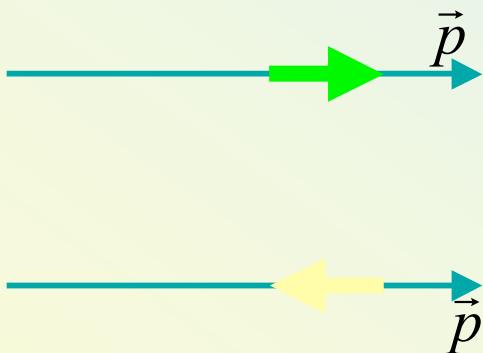
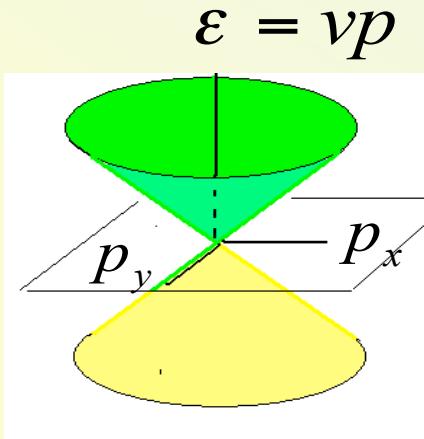
A to B hopping given by $\pi = p_x + ip_y$



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

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

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

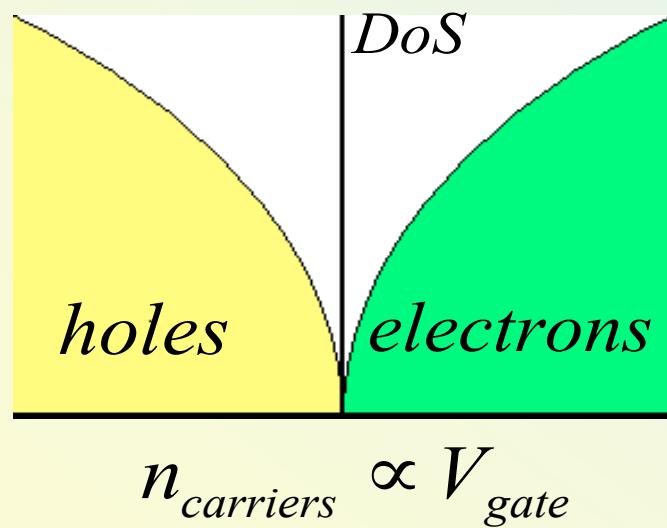
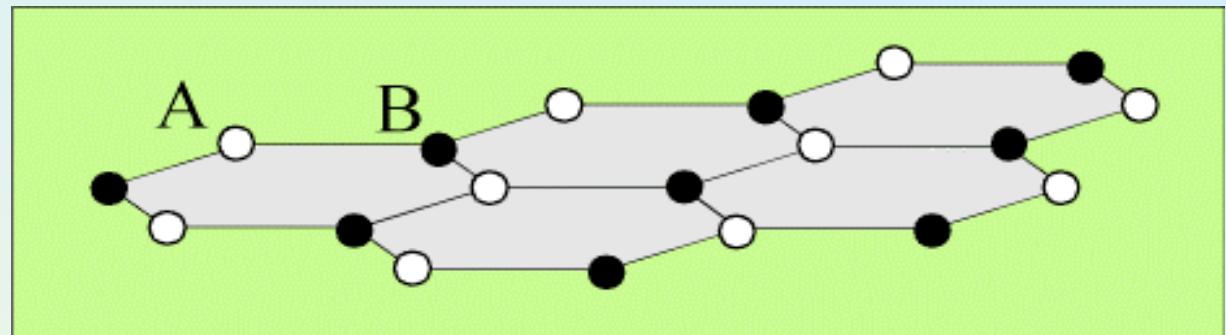


Chiral electrons
isospin direction is linked to the axis determined by the electron momentum.

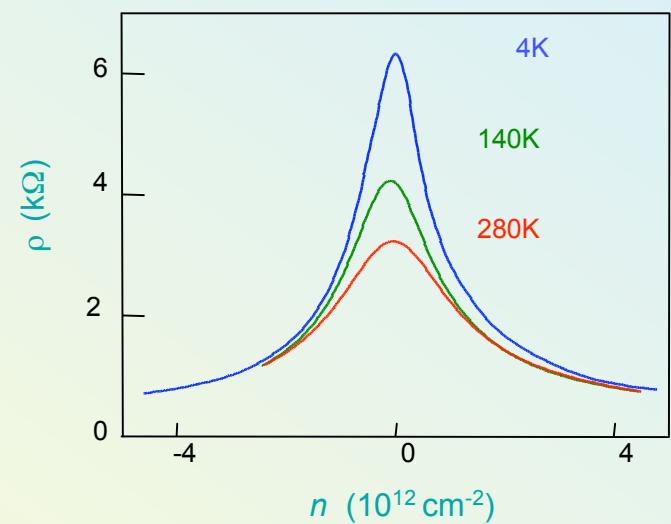
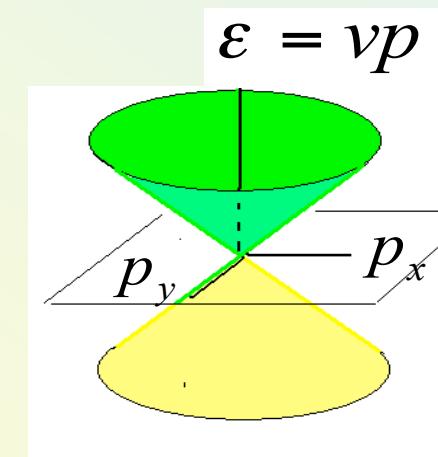
for conduction band electrons,
 $\vec{\sigma} \cdot \vec{n} = 1$

$\vec{\sigma} \cdot \vec{n} = -1$
valence band ('holes')

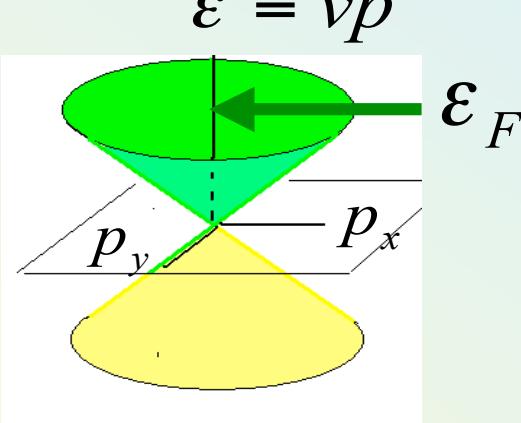
Monolayer



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



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



$$\pi = p_x + i p_y = p e^{i\varphi}$$

$$\pi^+ = p_x - i p_y = p e^{-i\varphi}$$

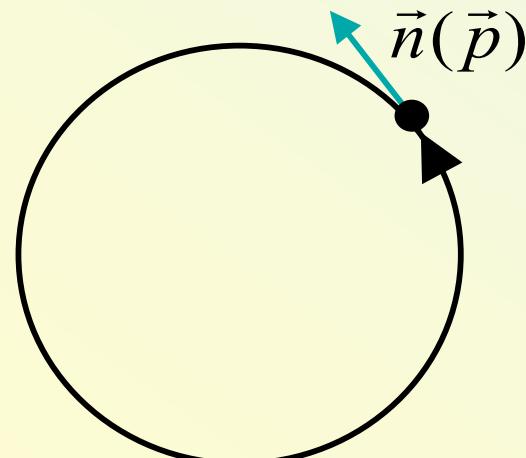
$$\hat{H}_1 = v \begin{pmatrix} 0 & \pi^+ \\ \pi^- & 0 \end{pmatrix} = v \vec{\sigma} \cdot \vec{p} = vp \vec{\sigma} \cdot \vec{n}$$

Bloch function amplitudes on the AB sites - ‘isospin’

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

Chiral electrons:
‘isospin’ direction is linked to the axis determined by the electron momentum:

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

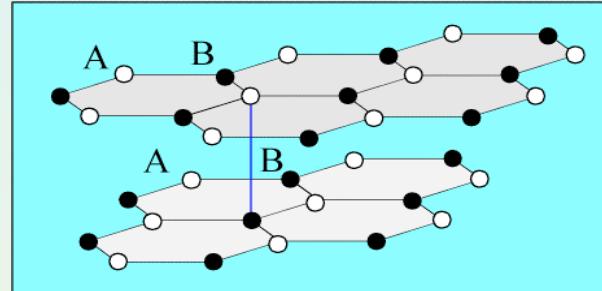


$$\psi \rightarrow e^{\frac{2\pi i}{2}\sigma_3} \psi = e^{i\pi} \psi$$

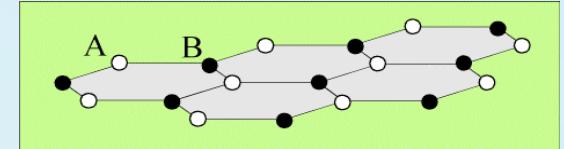
Berry phase π

Content

Bilayer



Monolayer



1. Tight-binding-model for the Dirac-type electron spectrum in graphene and its relation to the lattice symmetry.
2. Landau levels of chiral electrons in graphene, Quantum Hall effect in monolayers (graphene) and bilayers.
3. Chirality of carriers in graphene and Berry's phase $J\pi$, quantum transport properties of chiral 2D electrons.

four-fold degeneracy at $p=0$

$$\hat{H} = \begin{pmatrix} 0 & \pi^+ \\ \pi & 0 \\ & & 0 & -\pi^+ \\ & & -\pi & 0 \end{pmatrix}$$

$$\pi = p_x + ip_y$$

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

valley index

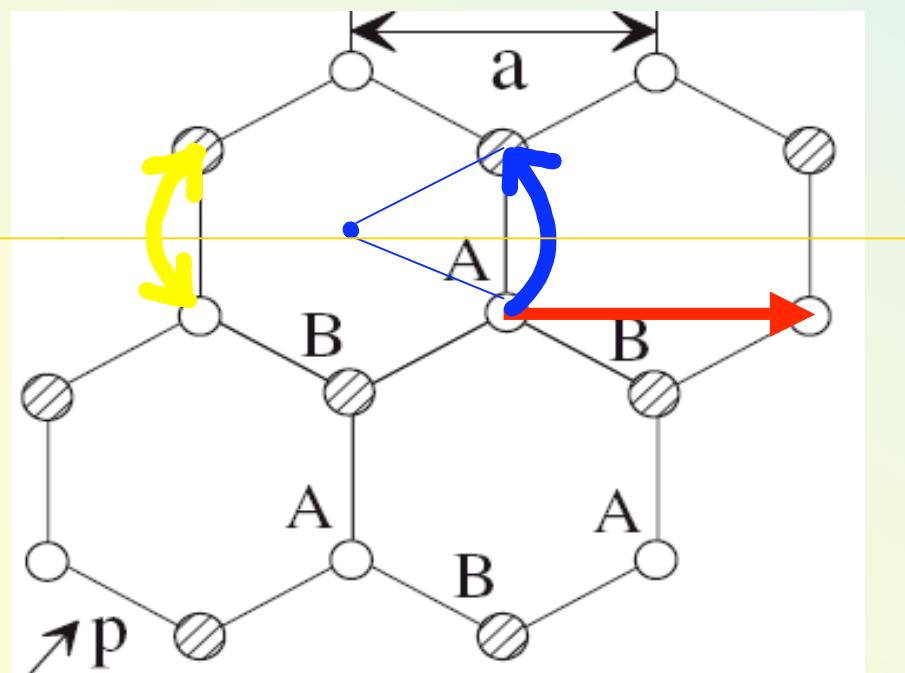
$$\begin{pmatrix} \varphi_{A,+} \\ \varphi_{B,+} \\ \varphi_{B,-} \\ \varphi_{A,-} \end{pmatrix}$$

sublattice index,
'isospin'

Also, an additional real spin degeneracy of all states

Four degenerate states in the corners of the Brillouin zone realize a 4-dimensional irreducible representation of the symmetry group of the honeycomb lattice

Generating elements: $T_{A \rightarrow A}, C_{\frac{\pi}{3}}, S_x$



$$A + \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}; B + \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}; B - \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}; A - \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

Translation $T_{A \rightarrow A}$

$$\left(e^{i\frac{4\pi}{3}} \quad e^{i\frac{4\pi}{3}} \quad e^{-i\frac{4\pi}{3}} \quad e^{-i\frac{4\pi}{3}} \right)$$

Rotation $C_{\frac{\pi}{3}}$

$$\left(e^{i\frac{2\pi}{3}} \quad e^{-i\frac{2\pi}{3}} \quad e^{i\frac{2\pi}{3}} \quad e^{-i\frac{2\pi}{3}} \right)$$

Mirror reflection S_x

$$\left(\begin{array}{cccc} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{array} \right)$$

$A \longleftrightarrow B$

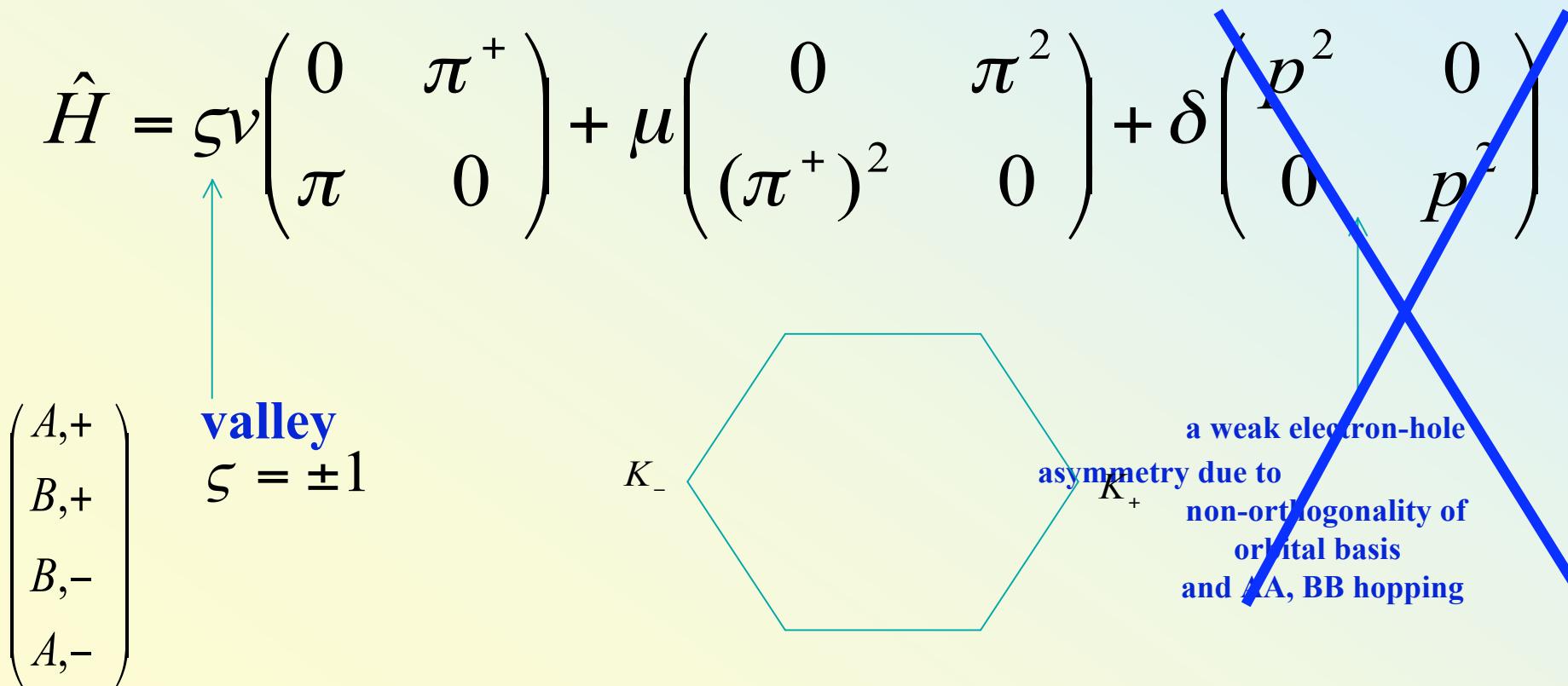
To write down the monolayer Hamiltonian describing electrons near the K-points, one has to construct all possible invariants using 4x4 matrices (with sublattice and valley indices) acting within the 4-dimensional representation and the momentum operator, \vec{p} .
(phenomenology)

Alternatively, one can apply the tight-binding model including the dominant next-neighbor (AB) hop and also longer-distance (AA) hops and to expand to higher order in $pa \ll 1$ (or π, π).⁺
(microscopy)

$$H_{AB,K_+} = -\gamma_0 \left[e^{-i\frac{2\pi}{3}} e^{-i(\frac{a}{2}p_x + \frac{a}{2\sqrt{3}}p_y)} + e^{i\frac{a}{\sqrt{3}}p_y} + e^{i\frac{2\pi}{3}} e^{i(\frac{a}{2}p_x - \frac{a}{2\sqrt{3}}p_y)} \right]$$

$$\approx \frac{\sqrt{3}}{2} \gamma_0 a (p_x - ip_y) - \frac{\gamma_0 a^2}{8} (p_x + ip_y)^2$$

higher order invariants (expansion terms)



$$\hat{H} = \zeta v \begin{pmatrix} 0 & \pi^+ \\ \pi & 0 \end{pmatrix} + \mu \begin{pmatrix} 0 & \pi^2 \\ (\pi^+)^2 & 0 \end{pmatrix}$$

higher order invariant

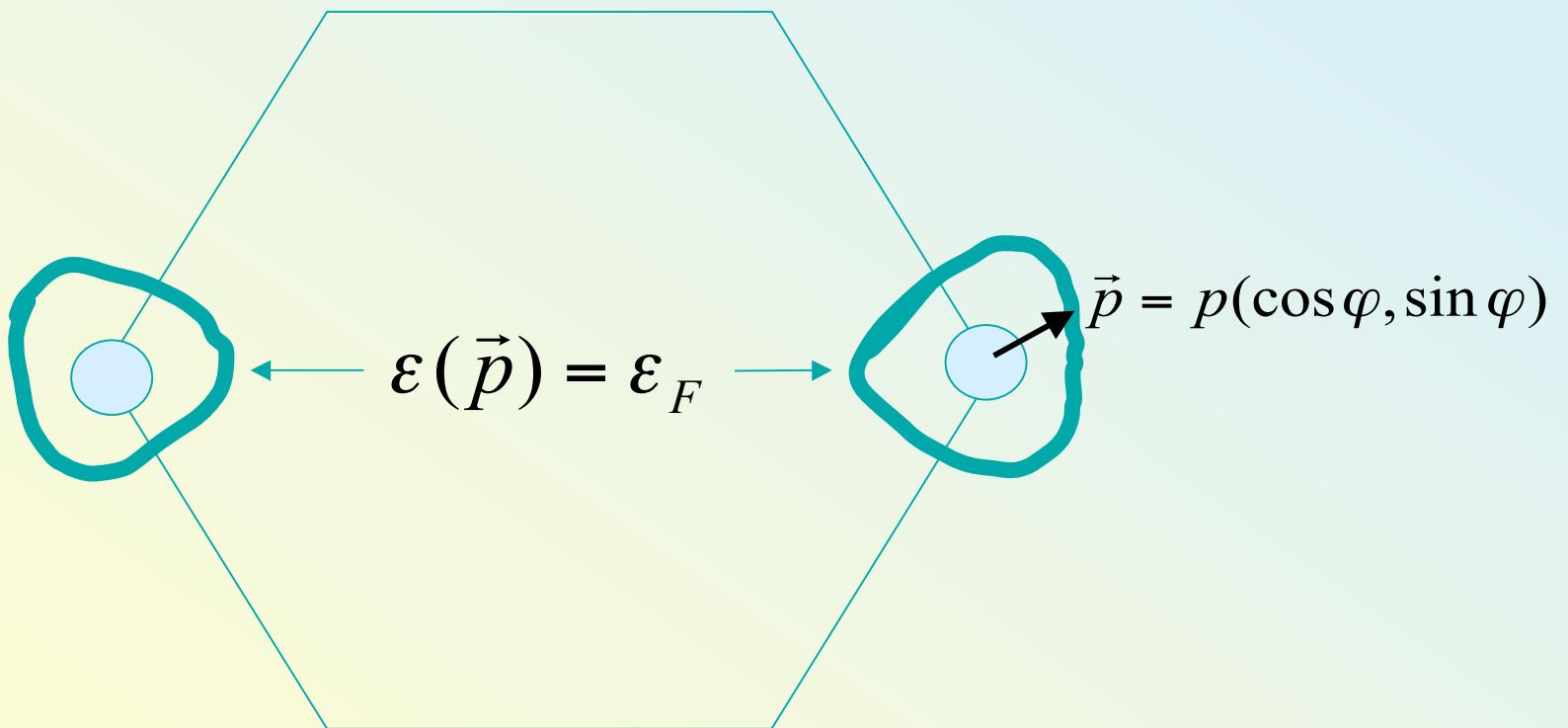
‘trigonal warping’: centre-asymmetric

valley

$$\zeta = \pm 1$$

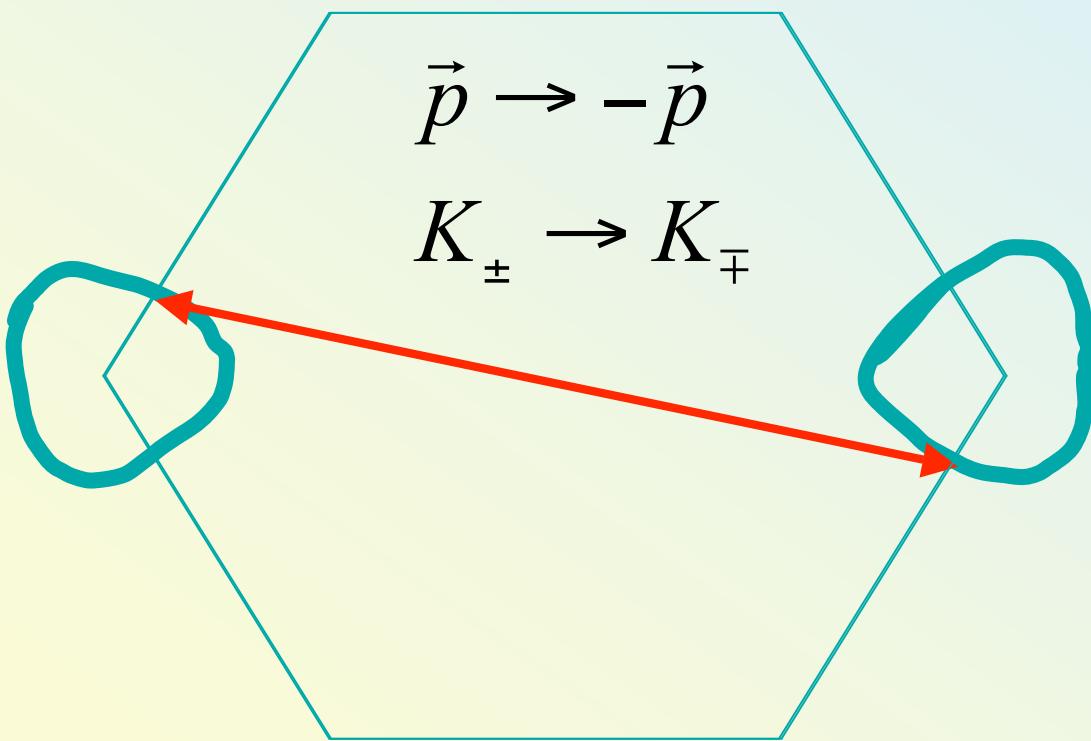
$$\pi = p_x + ip_y = pe^{i\varphi}$$

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



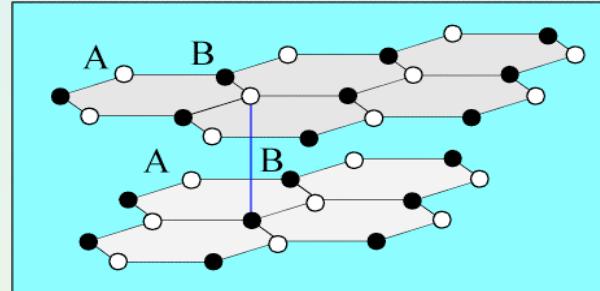
Time-inversion symmetry

$$t \rightarrow -t$$

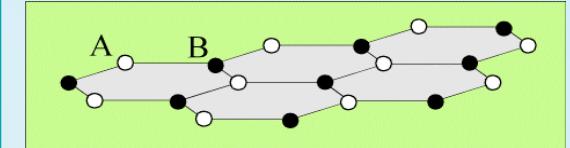


Content

Bilayer

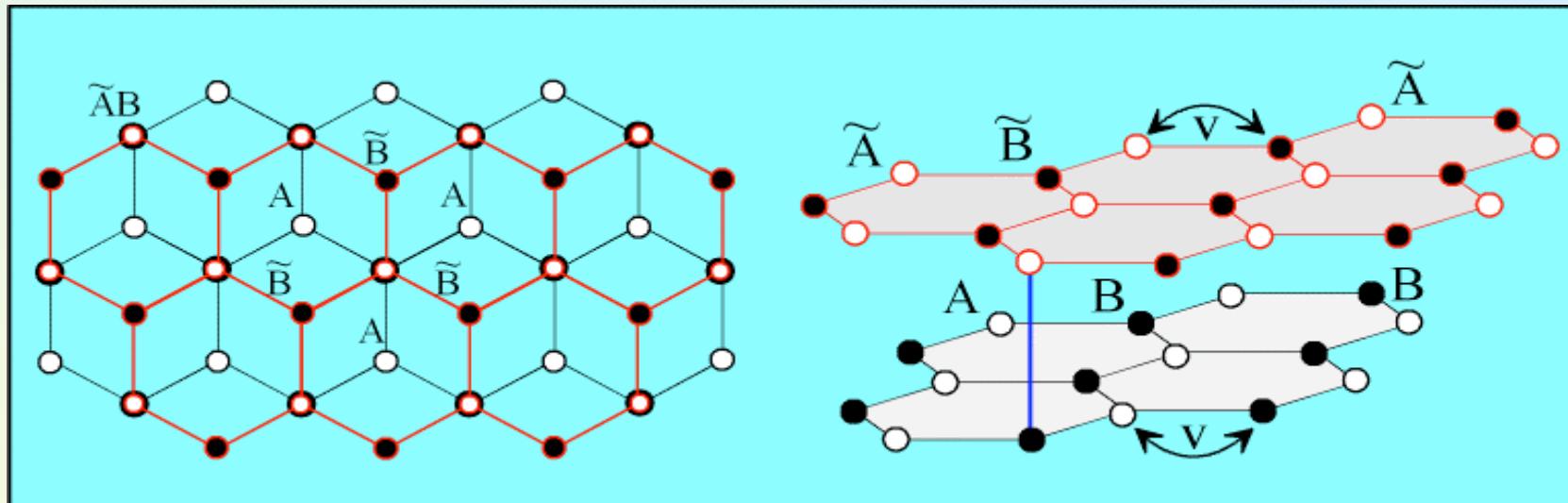


Monolayer



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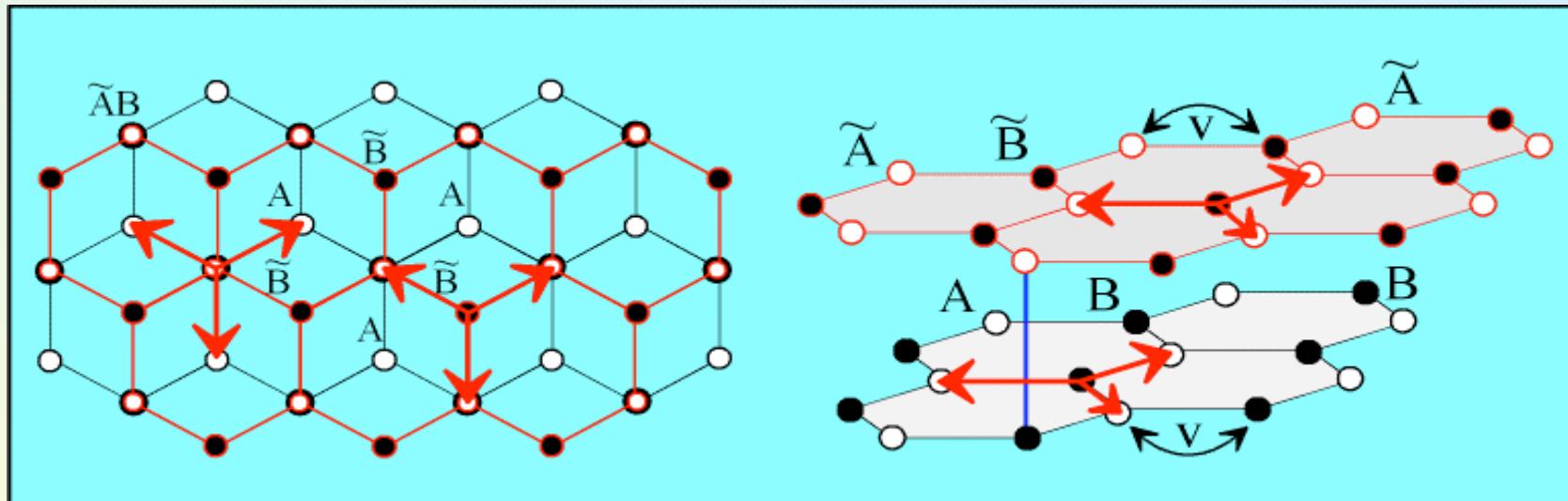
Bilayer [Bernal (AB) stacking]



4 atoms
per unit cell

$$\mathcal{H} = \begin{pmatrix} & & & \\ & & & \\ & & & \\ & & & \end{pmatrix} \begin{matrix} \tilde{A} & \tilde{B} & \tilde{\tilde{A}} & \tilde{B} \\ A & B & \tilde{A} & B \end{matrix}$$

Bilayer [Bernal (AB) stacking]



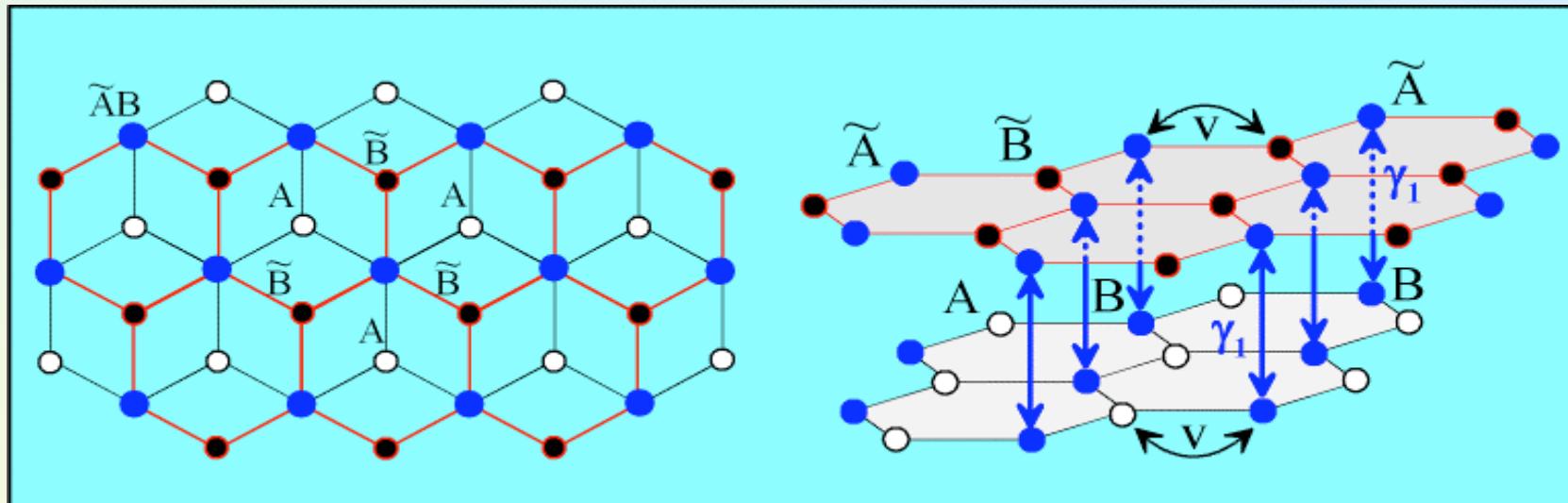
(B to A) and (\tilde{B} to \tilde{A})

hopping
given by

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

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

Bilayer [Bernal (AB) stacking]

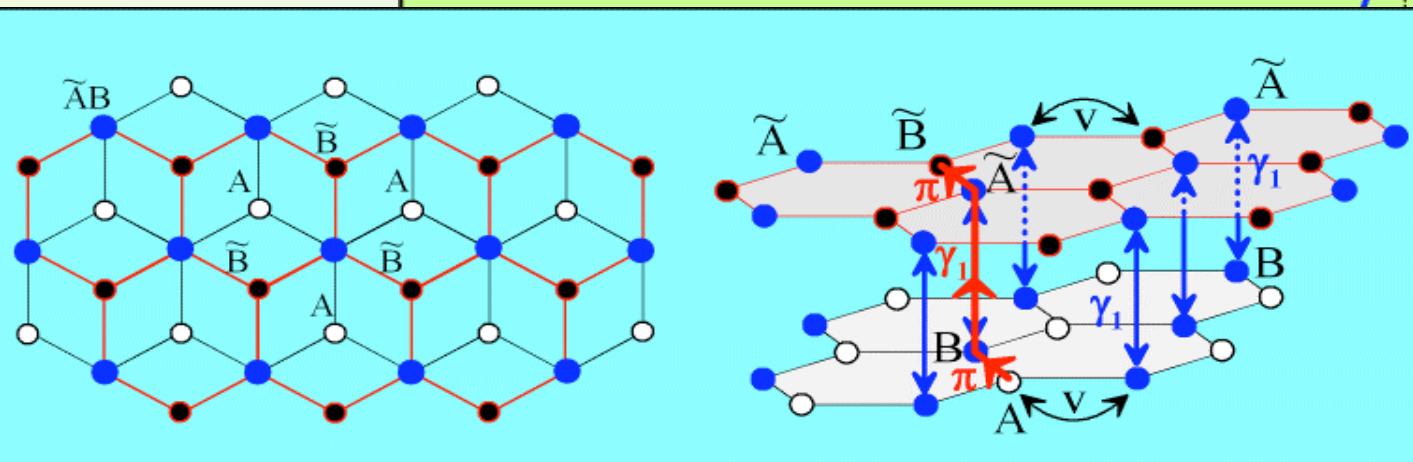
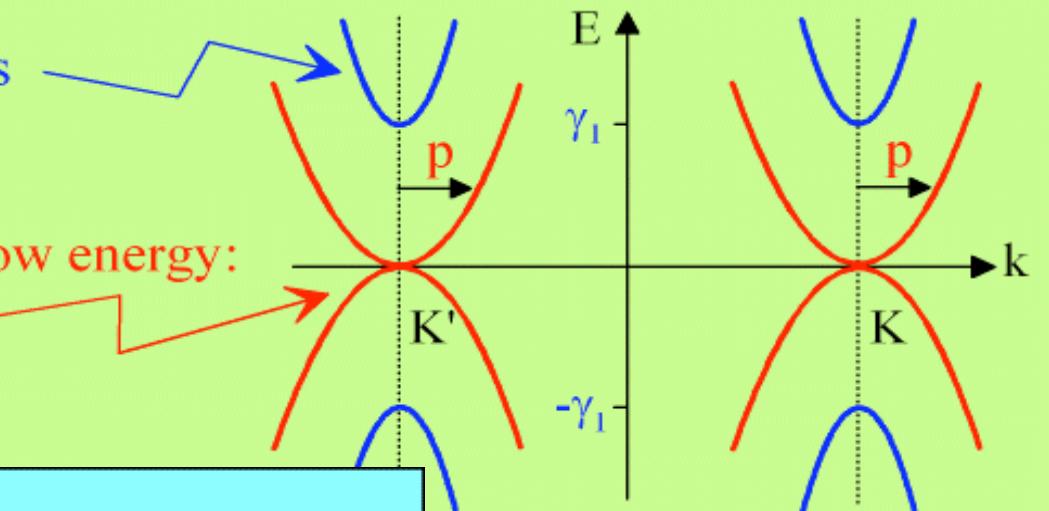


Bilayer Hamiltonian $H = \begin{pmatrix} A & \tilde{B} & \tilde{A} & B \\ 0 & 0 & 0 & v\pi^+ \\ 0 & 0 & v\pi & 0 \\ 0 & v\pi^+ & 0 & \gamma_1 \\ v\pi & 0 & \gamma_1 & 0 \end{pmatrix} \begin{matrix} A \\ \tilde{B} \\ \tilde{A} \\ B \end{matrix}$

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

Quadratic dispersion at low energy:

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



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

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

$$\text{mass } m = \gamma_1 / v^2$$

A to \tilde{B} hopping

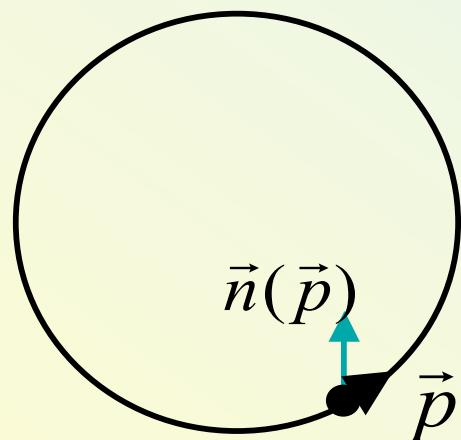
- bottom layer A \rightarrow B (factor π)
- switch layers via dimer $B\tilde{A}$ (γ_1^{-1})
- top layer $\tilde{A} \rightarrow \tilde{B}$ (factor π)

$$\pi = p_x + ip_y$$

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

$$\begin{aligned}\boldsymbol{\pi} &= p_x + i p_y = p e^{i\varphi} \\ \boldsymbol{\pi}^+ &= p_x - i p_y = p e^{-i\varphi}\end{aligned}$$

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



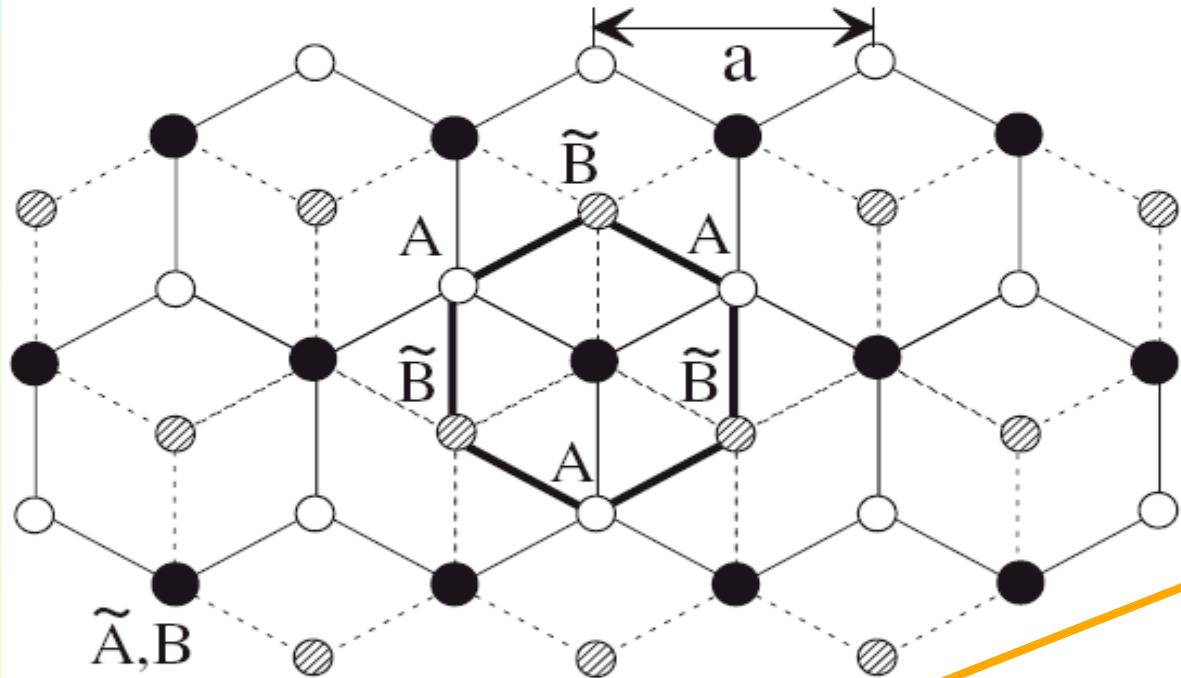
$$\psi \rightarrow e^{2 \times 2\pi \frac{i}{2} \sigma_3} \psi = e^{i 2\pi} \psi$$

Berry phase 2π

(for a monolayer = π)

Monolayer:

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



$$\pi = p_x + i p_y$$

$$-\frac{v^2}{\gamma_1} \begin{pmatrix} 0 & (\pi^\dagger)^2 \\ \pi^2 & 0 \end{pmatrix}$$

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

$$\hat{H}_2 = -\frac{1}{2m} [\sigma_x (p_x^2 - p_y^2) + \sigma_y (p_x p_y + p_y p_x)] + v_3 (\sigma_x p_x - \sigma_y p_y)$$

$$\sigma v_3 \begin{pmatrix} 0 & \pi \\ \pi^+ & 0 \end{pmatrix}$$

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

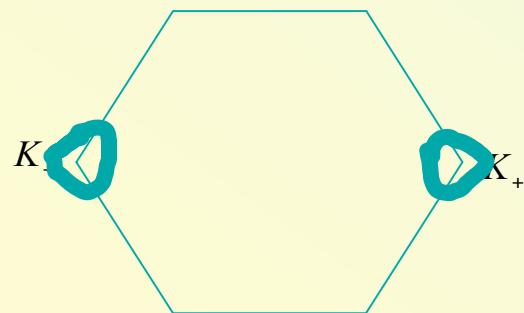
$$\hat{H}_2 = -\frac{1}{2m} [\sigma_x (p_x^2 - p_y^2) + \sigma_y (p_x p_y + p_y p_x)]$$

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

‘trigonal warping’

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

strong magnetic field
 $\lambda_B^{-1} \sim p \gg m v_3$



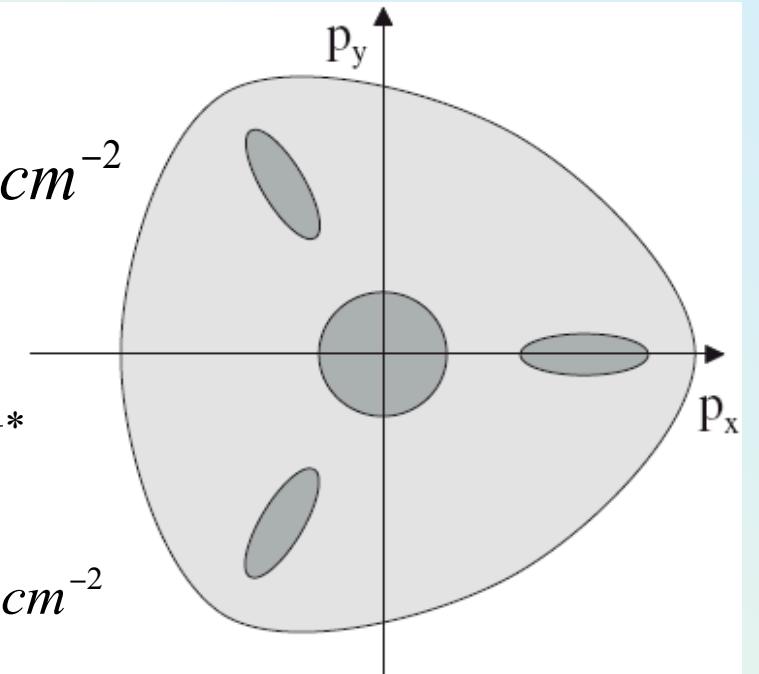
■ $0 < \varepsilon < \frac{\gamma_1}{2} \left(\frac{v_3}{v} \right)^2$
 $N < N_L \sim 10^{11} \text{ cm}^{-2}$

■ $\frac{\gamma_1}{2} \left(\frac{v_3}{v} \right)^2 < \varepsilon < \gamma_1$
 $N_L < N < 8N^*$

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

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

Lifshitz transition



Summary of Lecture 1

chiral electrons in graphene monolayer and bilayer

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

valley

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

dominant at a high magnetic field
and in high-density structures

$$\begin{pmatrix} A \\ B \\ B \\ A \end{pmatrix} \zeta = +1$$

$$\begin{pmatrix} A \\ \tilde{B} \\ \tilde{B} \\ A \end{pmatrix} \zeta = -1$$

‘trigonal warping’

Lecture 2: applications to transport properties