Graphite monolayers

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with

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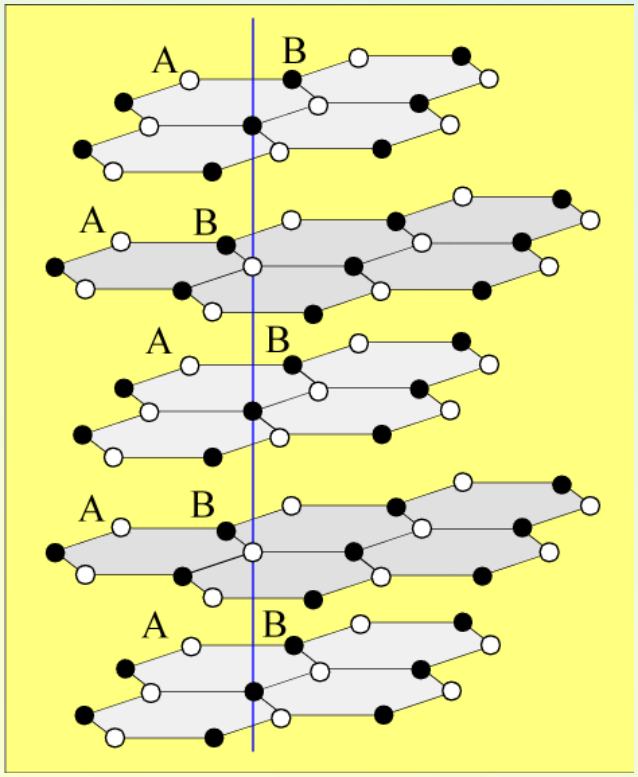
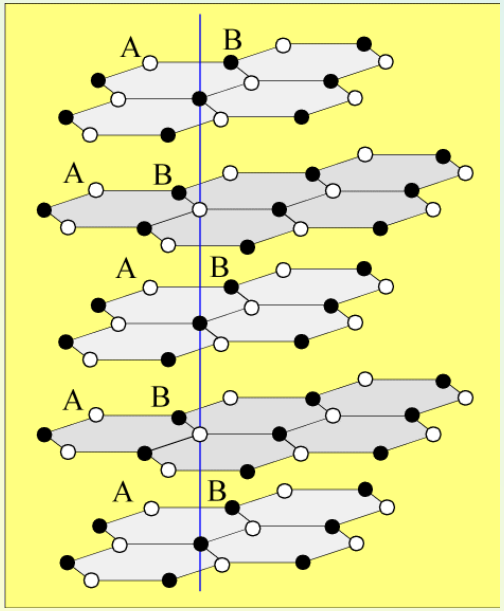
H. Suzuura, T. Ando,
B.L. Altshuler

Graphite



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

Graphite



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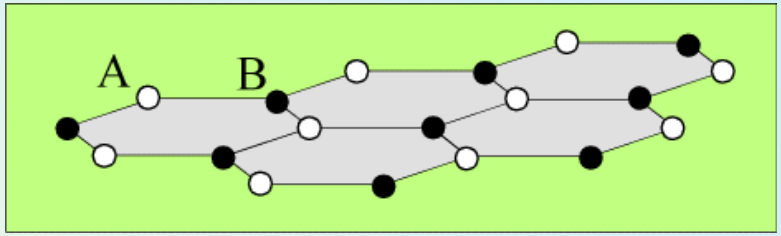
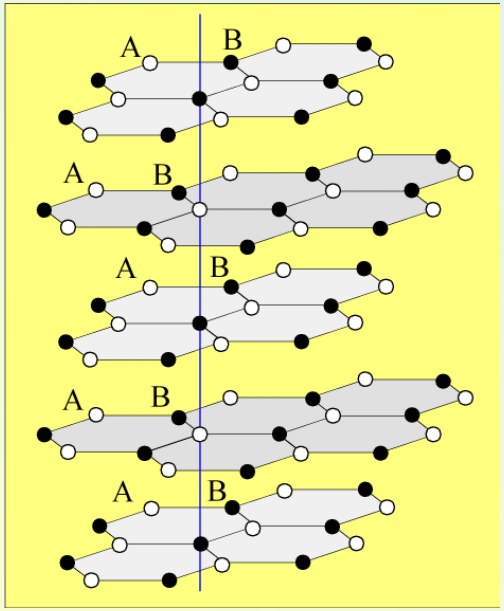


Two dimensional material;
zero gap semiconductor;
Dirac spectrum of electrons

Graphite



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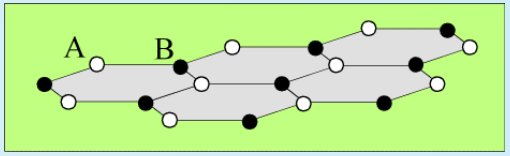
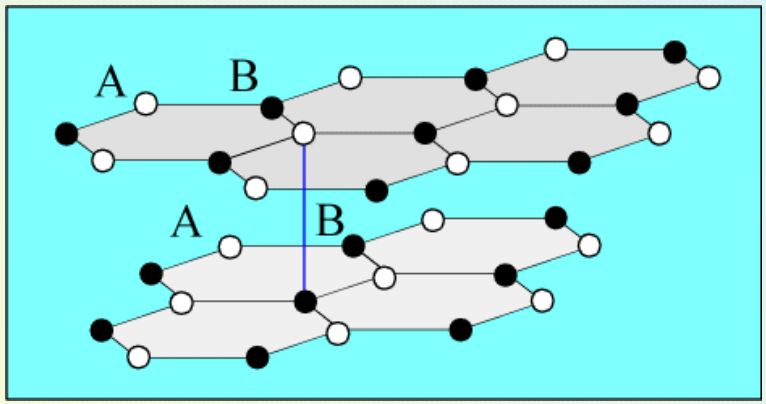


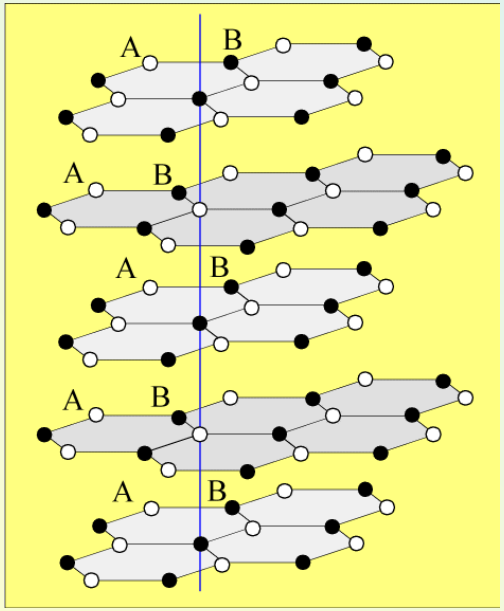
Two dimensional material; zero gap semiconductor; Dirac spectrum of electrons

Bilayer



Bilayer as a 2D material
Low energy Hamiltonian= ?

Graphite



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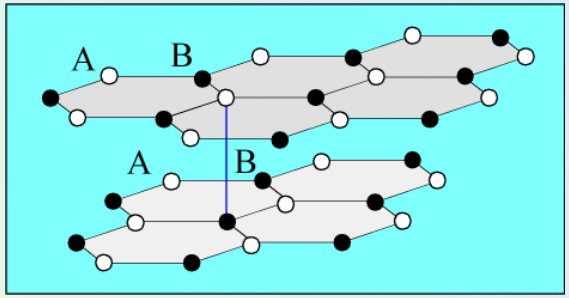
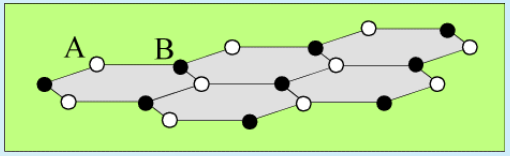


Two dimensional material;
Low energy Hamiltonian?

Monolayer

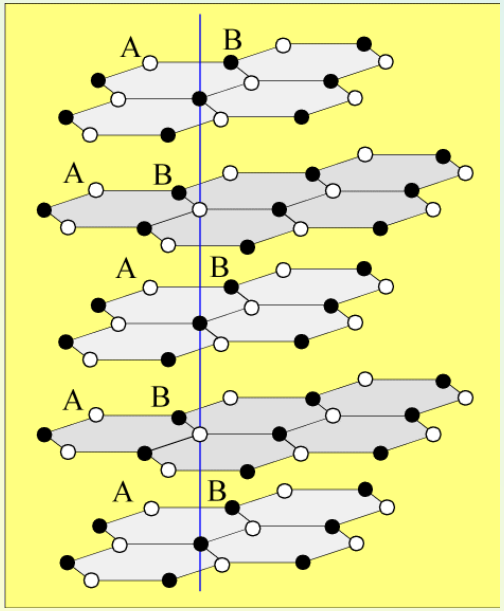


Two dimensional material;
zero gap semiconductor;
Dirac spectrum of electrons

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)
Columbia group: Zhang *et al*, Nature 438, 201 (2005).

Graphite



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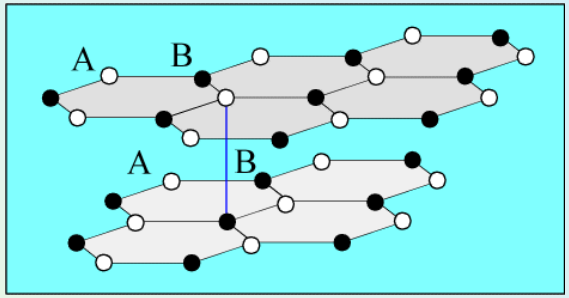
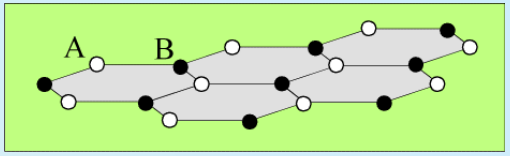


Two dimensional material; Low energy Hamiltonian?

Monolayer



Two dimensional material; zero gap semiconductor; Dirac spectrum of electrons

Lecture Overview

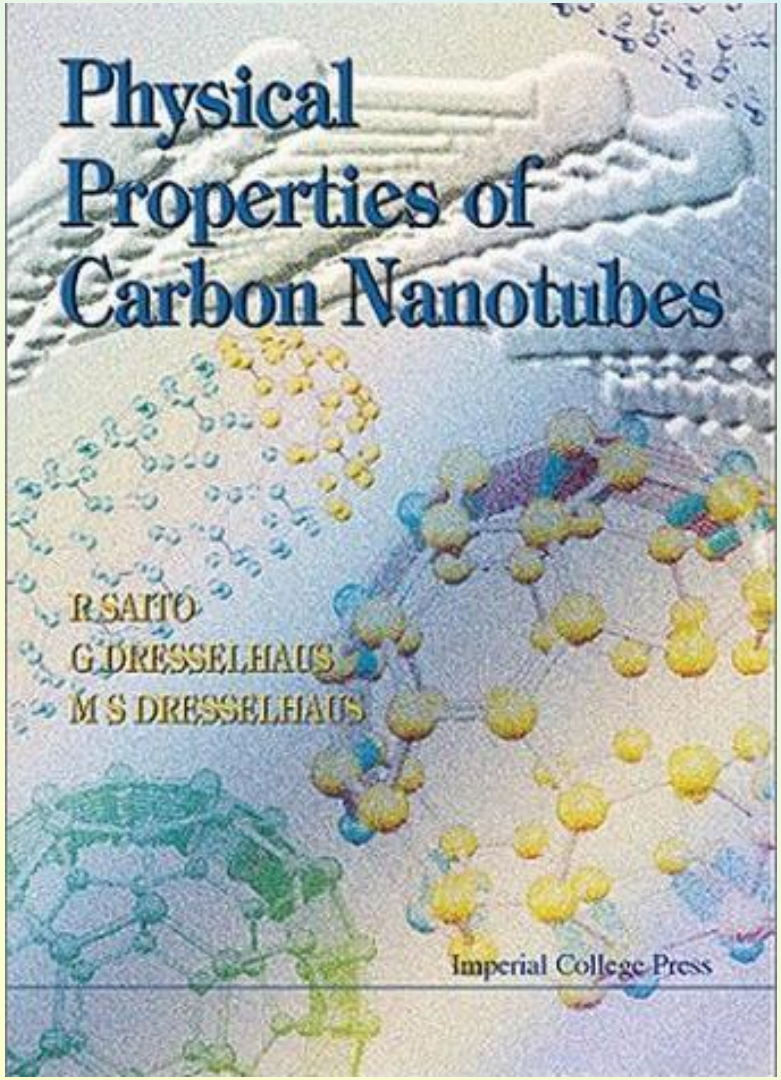
1) Tight binding model of monolayer graphene

2) Expansion near the K points: chiral quasiparticles and Berry phase

3) Bilayer graphene

4) Quantum Hall effect

1 Tight binding model of monolayer graphene



"Physical Properties of Carbon Nanotubes"
R Saito, G Dresselhaus and MS Dresselhaus;
Imperial College Press, 1998

1 Tight binding model of monolayer graphene

1.1 sp^2 hybridisation

Carbon has 6 electrons

- 2 are core electrons

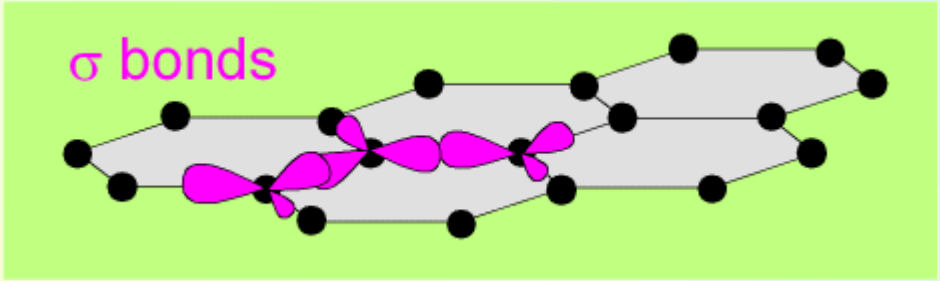
- 4 are valence electrons – one 2s and three 2p orbitals

1 Tight binding model of monolayer graphene

1.1 sp^2 hybridisation

Carbon has 6 electrons
- 2 are core electrons
- 4 are valence electrons – one 2s and three 2p orbitals

sp^2 hybridisation
- single 2s and two 2p orbitals hybridise forming three "σ bonds" in the x-y plane

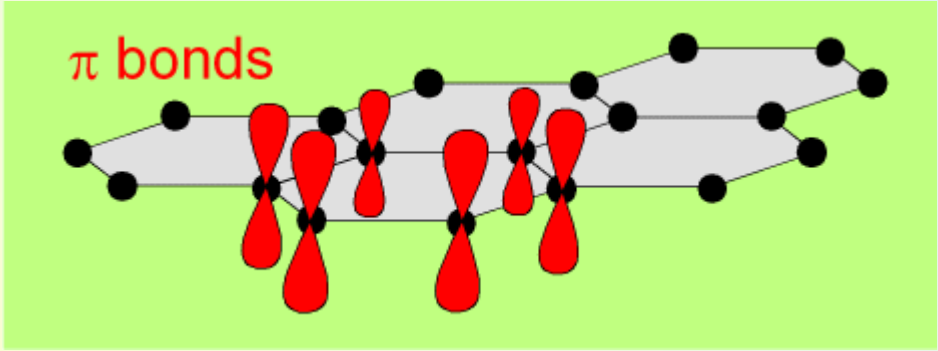


1 Tight binding model of monolayer graphene

1.1 sp^2 hybridisation

Carbon has 6 electrons
- 2 are core electrons
- 4 are valence electrons – one 2s and three 2p orbitals

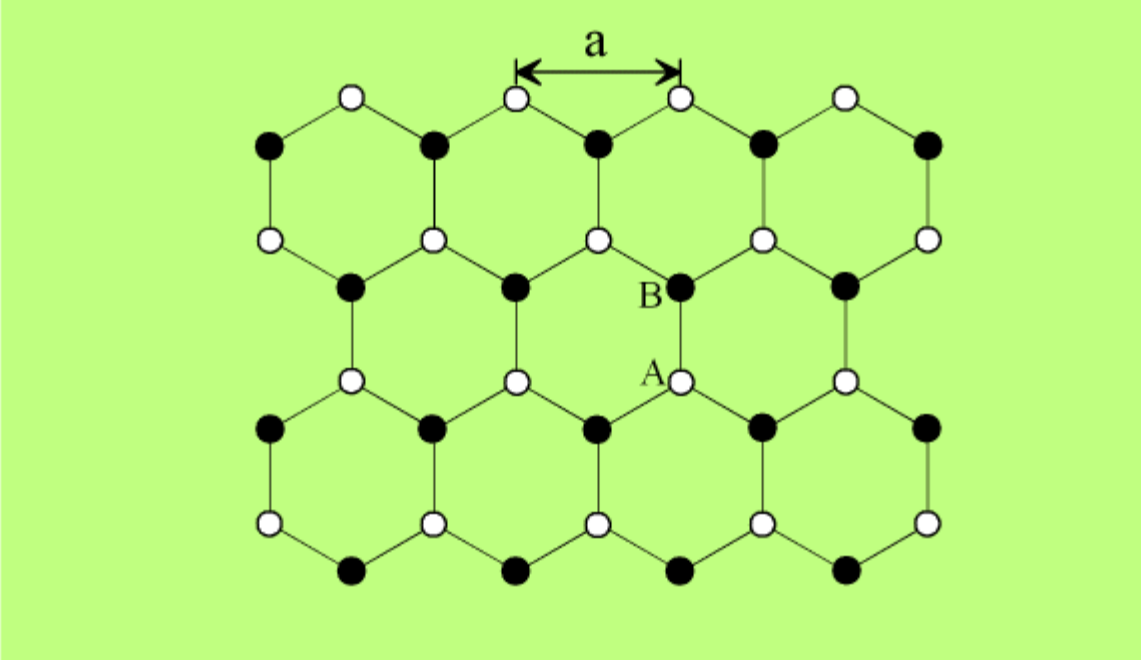
sp^2 hybridisation
- remaining $2p_z$ orbital [“π” orbital] exists perpendicular to the x-y plane

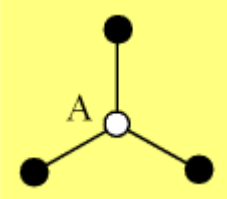


only π orbital relevant for energies of interest for transport measurements – so keep only this one orbital per site in the tight binding model

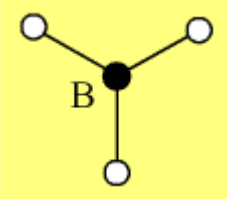
1 Tight binding model of monolayer graphene

1.2 lattice of graphene





2 different ways of orienting bonds means there are 2 different types of atomic sites [but chemically the same]



1 Tight binding model of monolayer graphene

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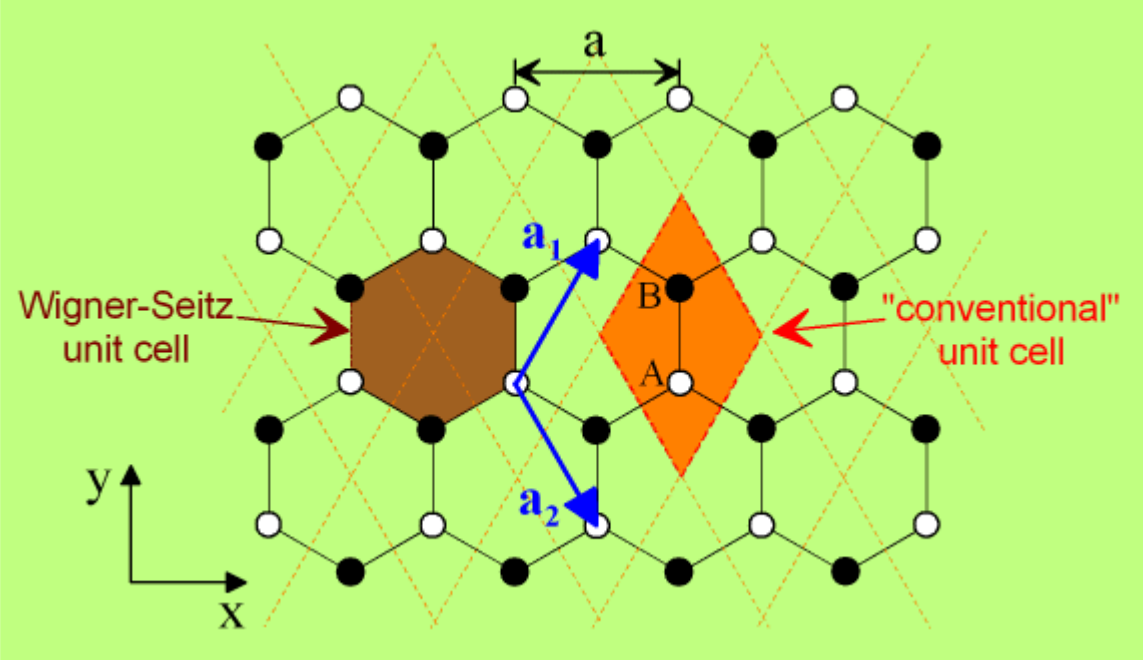
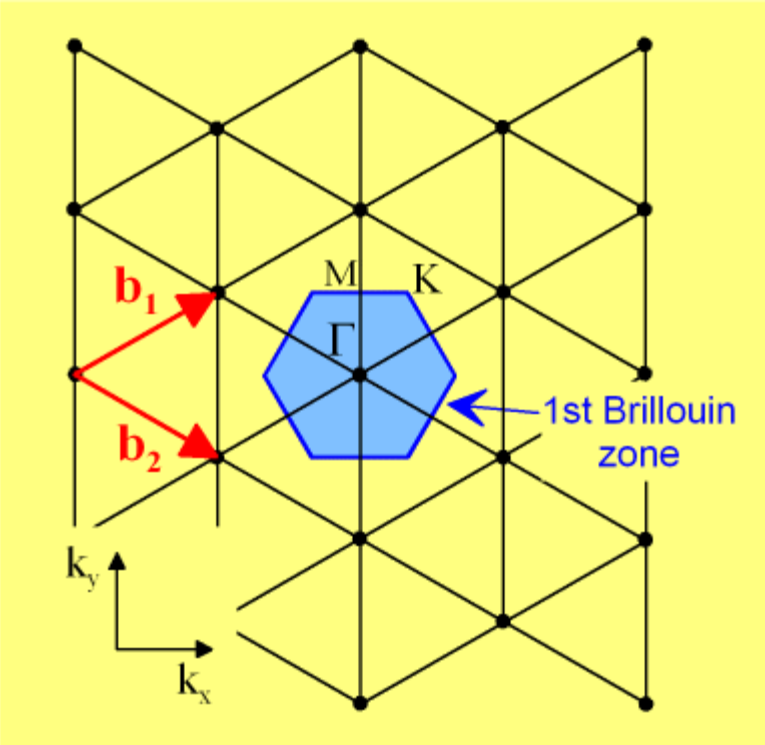


2 different atomic sites – 2 triangular sub-lattices

1 Tight binding model of monolayer graphene

1.3 reciprocal lattice



triangular reciprocal lattice

– hexagonal Brillouin zone

1 Tight binding model of monolayer graphene

1.4 Bloch functions

We take into account one π orbital per site, so there are two orbitals per unit cell.

Bloch functions

$$\Phi_A\left(\vec{k},\vec{r}\right)=\frac{1}{\sqrt{N}}\sum_{\vec{R}_A}^{N} e^{i\vec{k}.\vec{R}_A}\varphi_A\left(\vec{r}-\vec{R}_A\right)$$

$$\Phi_B\left(\vec{k},\vec{r}\right)=\frac{1}{\sqrt{N}}\sum_{\vec{R}_B}^{N} e^{i\vec{k}.\vec{R}_B}\varphi_B\left(\vec{r}-\vec{R}_B\right)$$

sum over all type B atomic sites in N unit cells

atomic wavefunction

1 Tight binding model of monolayer graphene

1.4 Bloch functions

We take into account one π orbital per site, so there are two orbitals per unit cell.

Bloch functions : label with j = 1 [A sites] or 2 [B sites]

$$\Phi_j\left(\vec{k},\vec{r}\right)=\frac{1}{\sqrt{N}}\sum_{\vec{R}_j}^{N} e^{i\vec{k}.\vec{R}_j}\varphi_j\left(\vec{r}-\vec{R}_j\right)$$

sum over all type j atomic sites in N unit cells

atomic wavefunction

1 Tight binding model of monolayer graphene

1.5 Secular equation

Eigenfunction Ψ_j (for j = 1 or 2) is written as a linear combination of Bloch functions:

$$\Psi_j\left(\vec{k},\vec{r}\right)=\sum_{j'=1}^{2}C_{jj'}\left(\vec{k}\right)\Phi_{j'}\left(\vec{k},\vec{r}\right)$$

Eigenvalue E_j (for j = 1 or 2) is written as :

$$E_j\left(\vec{k}\right)=\frac{\left\langle\Psi_j\middle|H\middle|\Psi_j\right\rangle}{\left\langle\Psi_j\middle|\Psi_j\right\rangle}$$

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substitute expression in terms of Bloch functions

$$E_j\left(\vec{k}\right)=\frac{\sum_{i,l}^{2}C_{ji}^{*}C_{jl}\left\langle\Phi_i\middle|H\middle|\Phi_l\right\rangle}{\sum_{i,l}^{2}C_{ji}^{*}C_{jl}\left\langle\Phi_i\middle|\Phi_l\right\rangle}\equiv\frac{\sum_{i,l}^{2}H_{il}C_{ji}^{*}C_{jl}}{\sum_{i,l}^{2}S_{il}C_{ji}^{*}C_{jl}}$$

defining transfer integral matrix elements $H_{il}=\left\langle\Phi_i\middle|H\middle|\Phi_l\right\rangle;$ **and overlap integral matrix elements** $S_{il}=\left\langle\Phi_i\middle|\Phi_l\right\rangle$

1 Tight binding model of monolayer graphene

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1 Tight binding model of monolayer graphene

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$$E_j\left(\vec{k}\right)=\frac{\sum_{i,l}^{2} H_{il}C_{ji}^{*}C_{jl}}{\sum_{i,l}^{2} S_{il}C_{ji}^{*}C_{jl}}$$

If the H_{il} and S_{il} are known, we can find the energy by minimising with respect to C_{jm}^{*}:

$$\frac{\partial E_j}{\partial C_{jm}^{*}}=\frac{\sum_{l}^{2} H_{ml}C_{jl}}{\sum_{i,l}^{2} S_{il}C_{ji}^{*}C_{jl}}-\frac{\sum_{i,l}^{2} H_{il}C_{ji}^{*}C_{jl}\sum_{l}^{2} S_{ml}C_{jl}}{\left(\sum_{i,l}^{2} S_{il}C_{ji}^{*}C_{jl}\right)^{2}}$$

$$\frac{\partial E_j}{\partial C_{jm}^{*}}=0 \quad\Rightarrow\quad \sum_{l=1}^{2} H_{ml}C_{jl}=E_j\sum_{l=1}^{2} S_{ml}C_{jl}$$

1 Tight binding model of monolayer graphene

1.5 Secular equation

$$\sum_{l=1}^{2} H_{ml} C_{jl} = E_j \sum_{l=1}^{2} S_{ml} C_{jl}$$

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$$\sum_{l=1}^{2} H_{ml} C_{jl} = E_j \sum_{l=1}^{2} S_{ml} C_{jl}$$

Explicitly write out sums:

$$m=1 \quad \Rightarrow \quad H_{11}C_{j1} + H_{12}C_{j2} = E_j\left(S_{11}C_{1l} + S_{12}C_{2l}\right)$$

$$m=2 \quad \Rightarrow \quad H_{21}C_{j1} + H_{22}C_{j2} = E_j\left(S_{21}C_{1l} + S_{22}C_{2l}\right)$$

1 Tight binding model of monolayer graphene

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Write as a matrix equation:

$$\begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \begin{pmatrix} C_{j1} \\ C_{j2} \end{pmatrix} = E_j \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} C_{j1} \\ C_{j2} \end{pmatrix}$$

$$HC_j = E_j S C_j$$

1 Tight binding model of monolayer graphene

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$$HC_j = E_j S C_j$$

Secular equation gives the eigenvalues:

$$\det\left(H - ES\right) = 0$$

1 Tight binding model of monolayer graphene

1.6 Calculation of transfer and overlap integrals

$$H_{ij} = \left\langle \Phi_i \middle| H \middle| \Phi_j \right\rangle; \qquad S_{ij} = \left\langle \Phi_i \middle| \Phi_j \right\rangle \qquad \Phi_j\left(\vec{k},\vec{r}\right) = \frac{1}{\sqrt{N}} \sum_{\vec{R}_j}^{N} e^{i\vec{k}.\vec{R}_j} \varphi_j\left(\vec{r} - \vec{R}_j\right)$$

1 Tight binding model of monolayer graphene

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Diagonal matrix element

$$H_{AA} = \langle \Phi_A | H | \Phi_A \rangle = \frac{1}{N} \sum_{\vec{R}_{Ai}}^{N} \sum_{\vec{R}_{Aj}}^{N} e^{i\vec{k}.(\vec{R}_{Aj} - \vec{R}_{Ai})} \langle \varphi_A(\vec{r} - \vec{R}_{Ai}) | H | \varphi_A(\vec{r} - \vec{R}_{Aj}) \rangle$$

Same site only:

$$\begin{aligned} H_{AA} &= \frac{1}{N} \sum_{\vec{R}_{Ai}}^{N} \langle \varphi_A(\vec{r} - \vec{R}_{Ai}) | H | \varphi_A(\vec{r} - \vec{R}_{Ai}) \rangle \\ &= \langle \varphi_A(\vec{r} - \vec{R}_{Ai}) | H | \varphi_A(\vec{r} - \vec{R}_{Ai}) \rangle \\ &\equiv \varepsilon_0 \end{aligned}$$

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$$= \langle \varphi_A(\vec{r} - \vec{R}_{Ai}) | H | \varphi_A(\vec{r} - \vec{R}_{Ai}) \rangle$$

$$\equiv \varepsilon_0$$

A and B sites are chemically identical:

$$H_{AA} = H_{BB} = \varepsilon_0$$

1 Tight binding model of monolayer graphene

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Same site only:

$$H_{AA} = \frac{1}{N} \sum_{\vec{R}_{Ai}}^{N} \langle \varphi_A(\vec{r} - \vec{R}_{Ai}) | H | \varphi_A(\vec{r} - \vec{R}_{Ai}) \rangle$$

$$= \langle \varphi_A(\vec{r} - \vec{R}_{Ai}) | H | \varphi_A(\vec{r} - \vec{R}_{Ai}) \rangle$$

$$\equiv \varepsilon_0$$

$$S_{AA} = \frac{1}{N} \sum_{\vec{R}_{Ai}}^{N} \langle \varphi_A(\vec{r} - \vec{R}_{Ai}) | \varphi_A(\vec{r} - \vec{R}_{Ai}) \rangle$$

$$= \langle \varphi_A(\vec{r} - \vec{R}_{Ai}) | \varphi_A(\vec{r} - \vec{R}_{Ai}) \rangle$$

$$\equiv 1$$

A and B sites are chemically identical:

$$H_{AA} = H_{BB} = \varepsilon_0 \qquad S_{AA} = S_{BB} = 1$$

1 Tight binding model of monolayer graphene

1.6 Calculation of transfer and overlap integrals

Off-diagonal matrix element

$$H_{AB} = \left\langle \Phi_A \middle| H \middle| \Phi_B \right\rangle = \frac{1}{N} \sum_{\vec{R}_{Ai}}^{N} \sum_{\vec{R}_{Bj}}^{N} e^{i\vec{k}.\left(\vec{R}_{Bj} - \vec{R}_{Ai}\right)} \left\langle \varphi_A\left(\vec{r} - \vec{R}_{Ai}\right) \middle| H \middle| \varphi_B\left(\vec{r} - \vec{R}_{Bj}\right) \right\rangle$$

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1.6 Calculation of transfer and overlap integrals

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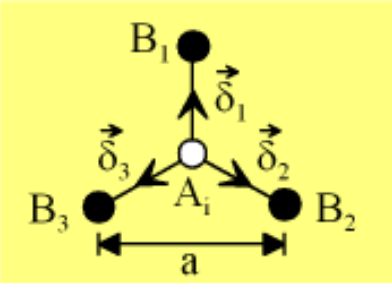
Every A site has 3 B nearest neighbours:



$$\vec{\delta}_1 = R_{B1} - R_{Ai} = \left(0, \frac{a}{\sqrt{3}}\right); \quad \vec{\delta}_2 = R_{B2} - R_{Ai} = \left(\frac{a}{2}, -\frac{a}{2\sqrt{3}}\right);$$

$$\vec{\delta}_3 = R_{B3} - R_{Ai} = \left(-\frac{a}{2}, -\frac{a}{2\sqrt{3}}\right)$$

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1.6 Calculation of transfer and overlap integrals

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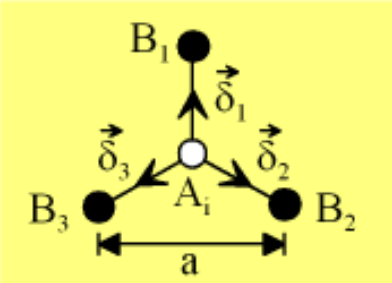
Every A site has 3 B nearest neighbours:



$$\vec{\delta}_1 = R_{B1} - R_{Ai} = \left(0, \frac{a}{\sqrt{3}}\right); \quad \vec{\delta}_2 = R_{B2} - R_{Ai} = \left(\frac{a}{2}, -\frac{a}{2\sqrt{3}}\right);$$

$$\vec{\delta}_3 = R_{B3} - R_{Ai} = \left(-\frac{a}{2}, -\frac{a}{2\sqrt{3}}\right)$$

$$H_{AB} = \frac{1}{N} \sum_{\vec{R}_{Ai}}^{N} \left[\sum_{\vec{\delta}_j=1}^{3} e^{i\vec{k}.\vec{\delta}_j} \left\langle \varphi_A(\vec{r} - \vec{R}_{Ai}) \middle| H \middle| \varphi_B(\vec{r} - \vec{R}_{Bj}) \right\rangle \right] = \sum_{\vec{\delta}_j=1}^{3} e^{i\vec{k}.\vec{\delta}_j} \left\langle \varphi_A(\vec{r} - \vec{R}_{Ai}) \middle| H \middle| \varphi_B(\vec{r} - \vec{R}_{Bj}) \right\rangle$$

1 Tight binding model of monolayer graphene

1.6 Calculation of transfer and overlap integrals

Off-diagonal matrix element

$$H_{AB} = \langle \Phi_A | H | \Phi_B \rangle = \frac{1}{N} \sum_{\vec{R}_{Ai}}^{N} \sum_{\vec{R}_{Bj}}^{N} e^{i\vec{k}.(\vec{R}_{Bj} - \vec{R}_{Ai})} \left\langle \varphi_A(\vec{r} - \vec{R}_{Ai}) \middle| H \middle| \varphi_B(\vec{r} - \vec{R}_{Bj}) \right\rangle$$

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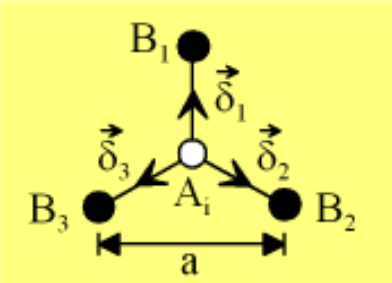

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Parameterise nearest neighbour transfer integral:

$$\gamma_0 = -\left\langle \varphi_A(\vec{r} - \vec{R}_{Ai}) \middle| H \middle| \varphi_B(\vec{r} - \vec{R}_{Bj}) \right\rangle$$

$$\Rightarrow \quad H_{AB} = -\gamma_0 f(\vec{k}); \qquad f(\vec{k}) = \sum_{\vec{\delta}_j=1}^{3} e^{i\vec{k}.\vec{\delta}_j}$$

1 Tight binding model of monolayer graphene

1.6 Calculation of transfer and overlap integrals

Off-diagonal matrix element

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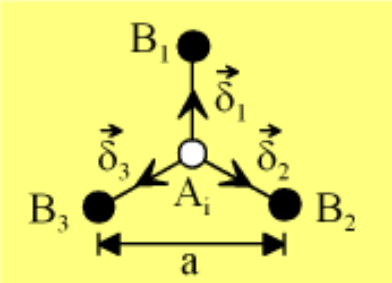

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$$H_{AB} = \frac{1}{N} \sum_{\vec{R}_{Ai}}^{N} \left[\sum_{\vec{\delta}_j=1}^{3} e^{i\vec{k}.\vec{\delta}_j} \left\langle \varphi_A(\vec{r} - \vec{R}_{Ai}) \middle| H \middle| \varphi_B(\vec{r} - \vec{R}_{Bj}) \right\rangle \right] = \sum_{\vec{\delta}_j=1}^{3} e^{i\vec{k}.\vec{\delta}_j} \left\langle \varphi_A(\vec{r} - \vec{R}_{Ai}) \middle| H \middle| \varphi_B(\vec{r} - \vec{R}_{Bj}) \right\rangle$$

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$$\gamma_0 = -\left\langle \varphi_A(\vec{r} - \vec{R}_{Ai}) \middle| H \middle| \varphi_B(\vec{r} - \vec{R}_{Bj}) \right\rangle$$

$$s = \left\langle \varphi_A(\vec{r} - \vec{R}_{Ai}) \middle| \varphi_B(\vec{r} - \vec{R}_{Bj}) \right\rangle$$

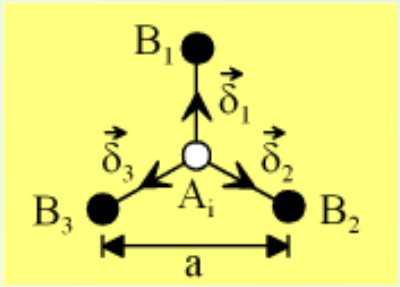
$$\Rightarrow \quad H_{AB} = -\gamma_0 f(\vec{k}); \qquad f(\vec{k}) = \sum_{\vec{\delta}_j=1}^{3} e^{i\vec{k}.\vec{\delta}_j}$$

$$\Rightarrow \quad S_{AB} = s\, f(\vec{k})$$

1 Tight binding model of monolayer graphene

1.6 Calculation of transfer and overlap integrals

Off-diagonal matrix element



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$$\vec{\delta}_3 = R_{B3} - R_{Ai} = \left(-\frac{a}{2}, -\frac{a}{2\sqrt{3}}\right)$$

$$f\left(\vec{k}\right) = \sum_{\vec{\delta}_j=1}^{3} e^{i\vec{k}.\vec{\delta}_j} = e^{ik_y a/\sqrt{3}} + 2e^{-ik_y a/2\sqrt{3}} \cos\left(\frac{k_x a}{2}\right)$$

1 Tight binding model of monolayer graphene

1.7 Calculation of energy

$$H=\begin{pmatrix}\varepsilon_0 & -\gamma_0 f\left(\vec{k}\right)\\ -\gamma_0 f^{*}\left(\vec{k}\right) & \varepsilon_0\end{pmatrix};\quad S=\begin{pmatrix}1 & sf\left(\vec{k}\right)\\ sf^{*}\left(\vec{k}\right) & 1\end{pmatrix}$$

1 Tight binding model of monolayer graphene

1.7 Calculation of energy

$$H=\begin{pmatrix}\varepsilon_0 & -\gamma_0 f\left(\vec{k}\right)\\ -\gamma_0 f^*\left(\vec{k}\right) & \varepsilon_0\end{pmatrix};\quad S=\begin{pmatrix}1 & sf\left(\vec{k}\right)\\ sf^*\left(\vec{k}\right) & 1\end{pmatrix}$$

Secular equation gives the eigenvalues:

$$\det\left(H-ES\right)=0$$

$$\det\begin{pmatrix}\varepsilon_0-E & -\left(\gamma_0+Es\right)f\left(\vec{k}\right)\\ -\left(\gamma_0+Es\right)f^*\left(\vec{k}\right) & \varepsilon_0-E\end{pmatrix}=0$$

$$\left(E-\varepsilon_0\right)^2-\left(\gamma_0+Es\right)^2\left|f\left(\vec{k}\right)\right|^2=0$$

1 Tight binding model of monolayer graphene

1.7 Calculation of energy

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$$\left(E-\varepsilon_0\right)^2-\left(\gamma_0+Es\right)^2\left|f\left(\vec{k}\right)\right|^2=0$$

$$E=\frac{\varepsilon_0\pm\gamma_0\left|f\left(\vec{k}\right)\right|}{1\mp s\left|f\left(\vec{k}\right)\right|}$$

1 Tight binding model of monolayer graphene

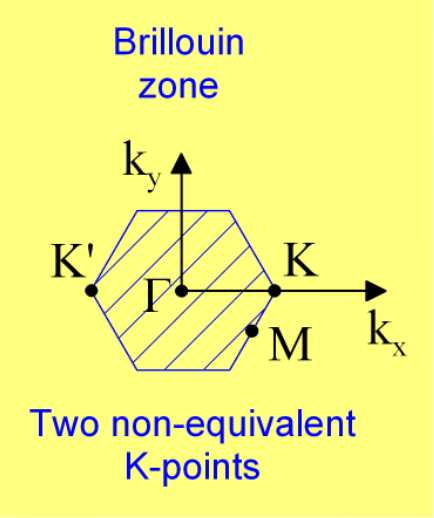
1.7 Calculation of energy

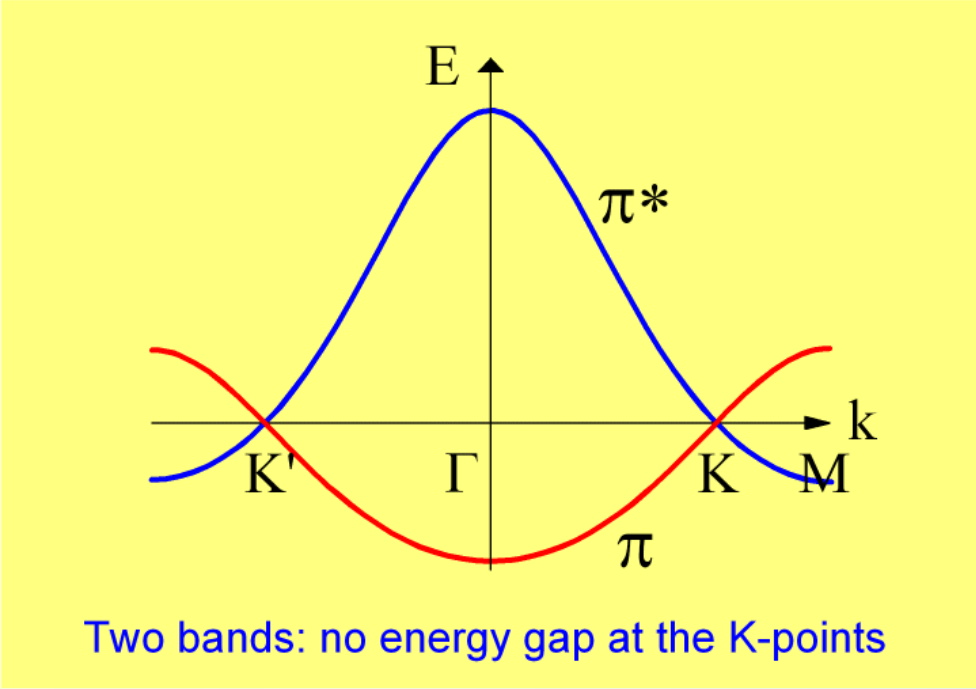
$$E = \frac{\varepsilon_0 \pm \gamma_0 \left| f\left(\vec{k}\right) \right|}{1 \mp s \left| f\left(\vec{k}\right) \right|}$$

Typical parameter values [quoted in Saito *et al*]:

$$\varepsilon_0 = 0,\ \gamma_0 = 3.033eV,\ s = 0.129$$

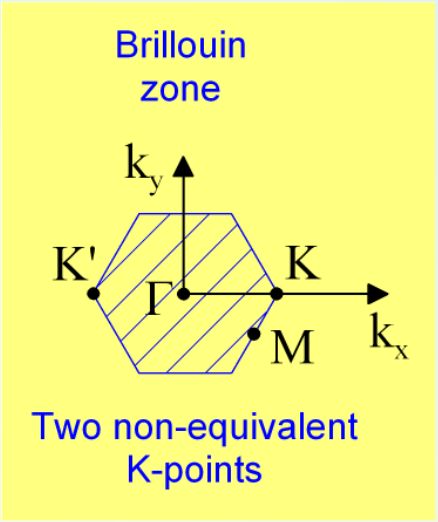
$$f\left(\vec{k}\right) = e^{ik_y a/\sqrt{3}} + 2e^{-ik_y a/2\sqrt{3}} \cos\left(\frac{k_x a}{2}\right)$$





2 Expansion near the K points

2.1 Exactly at the K point



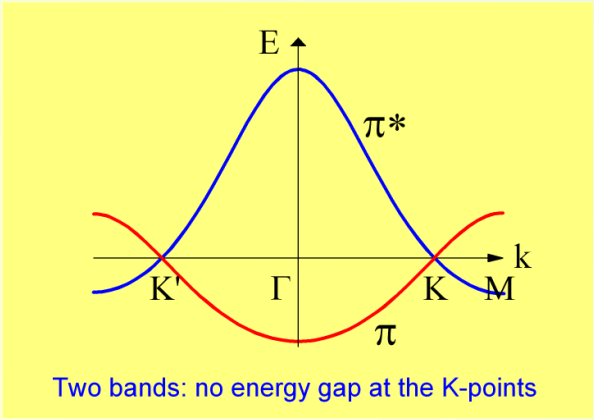
$$\vec{K} = \left(\frac{4\pi}{3a}, 0\right)$$

$$\vec{\delta}_1 = \left(0, \frac{a}{\sqrt{3}}\right); \quad \Rightarrow \quad K.\vec{\delta}_1 = 0$$

$$\vec{\delta}_2 = \left(\frac{a}{2}, -\frac{a}{2\sqrt{3}}\right); \quad \Rightarrow \quad K.\vec{\delta}_2 = \frac{2\pi}{3}$$

$$\vec{\delta}_3 = \left(-\frac{a}{2}, -\frac{a}{2\sqrt{3}}\right); \quad \Rightarrow \quad K.\vec{\delta}_3 = -\frac{2\pi}{3}$$

$$f\left(\vec{K}\right) = \sum_{\vec{\delta}_j=1}^{3} e^{i\vec{K}.\vec{\delta}_j} = e^0 + e^{2\pi i/3} + e^{-2\pi i/3} = 0$$



At the corners of the Brillouin zone (K points), electron states on the A and B sub-lattices decouple and have exactly the same energy

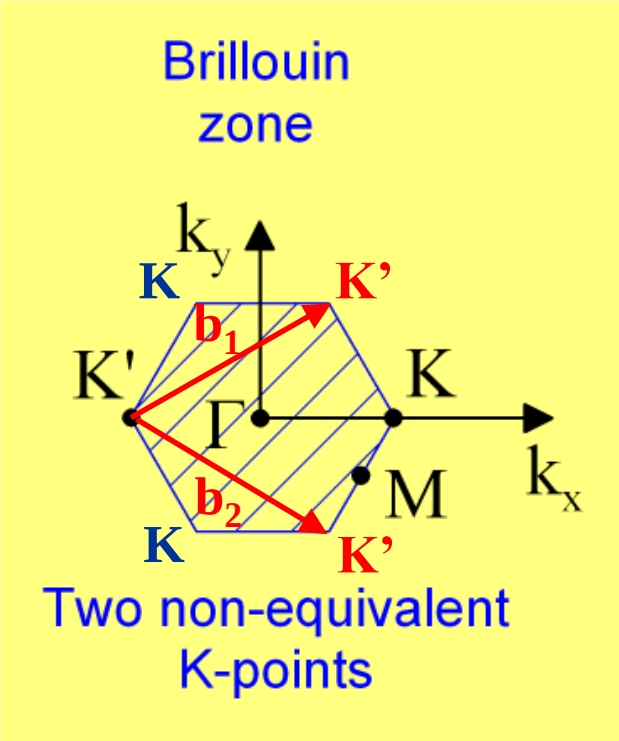
K points also referred to as "valleys"

Show 3d band structure

2 Expansion near the K points

2.1 Exactly at the K point

6 corners of the Brillouin zone (K points), but only two are non-equivalent

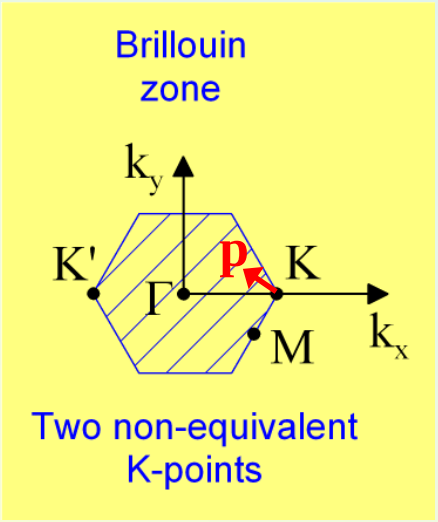


We consider two K points with the following wave vectors:

$$\vec{K} = \left(\frac{4\pi}{3a}, 0\right); \quad \vec{K}' = \left(-\frac{4\pi}{3a}, 0\right)$$

2 Expansion near the K points

2.2 Linear expansion



Consider two non-equivalent K points:

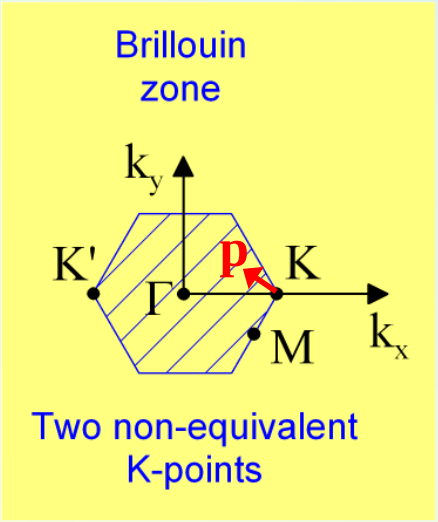
$$\vec{K}, \vec{K}' = \xi\left(\frac{4\pi}{3a}, 0\right); \qquad \xi = \pm 1$$

and small momentum near them:

$$\vec{k} = \xi\left(\frac{4\pi}{3a}, 0\right) + \frac{\vec{p}}{\hbar}$$

2 Expansion near the K points

2.2 Linear expansion



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and small momentum near them:

$$\vec{k} = \xi\left(\frac{4\pi}{3a},0\right) + \frac{\vec{p}}{\hbar}$$

Linear expansion in small momentum: $f\left(\vec{k}\right) = -\frac{\sqrt{3}a}{2\hbar}\left(\xi p_x - i p_y\right) + O\left(pa/\hbar\right)^2$

$$H = \begin{pmatrix} 0 & -\gamma_0 f\left(\vec{k}\right) \\ -\gamma_0 f^*\left(\vec{k}\right) & 0 \end{pmatrix} \approx v \begin{pmatrix} 0 & \xi p_x - i p_y \\ \xi p_x + i p_y & 0 \end{pmatrix}$$

$$S = \begin{pmatrix} 1 & sf\left(\vec{k}\right) \\ sf^*\left(\vec{k}\right) & 1 \end{pmatrix} \approx \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + O\left(\frac{spa}{\hbar}\right)$$

$$v = \frac{\sqrt{3}a\gamma_0}{2\hbar} \approx 10^6\, m/s$$

2 Expansion near the K points

2.2 Linear expansion

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$$v = \frac{\sqrt{3} a \gamma_0}{2\hbar} \approx 10^6 \, m/s$$

New notation for components on A and B sites

$$C_j = \begin{pmatrix} C_{j1} \\ C_{j2} \end{pmatrix} \quad \Leftrightarrow \quad \psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

$$S^{-1} H C_j = E_j C_j \quad \Rightarrow \quad v \begin{pmatrix} 0 & \xi p_x - i p_y \\ \xi p_x + i p_y & 0 \end{pmatrix} \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = E \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

2 Expansion near the K points

2.3 Dirac-like equation

For one K point (e.g. ξ=+1) we have a 2 component wave function,

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

with the following effective Hamiltonian:

$$H = v\begin{pmatrix} 0 & p_x - ip_y \\ p_x + ip_y & 0 \end{pmatrix} = v\begin{pmatrix} 0 & \pi^+ \\ \pi & 0 \end{pmatrix} = v\left(\sigma_x p_x + \sigma_y p_y\right) = v\vec{\sigma}.\vec{p}$$

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

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

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

2 Expansion near the K points

2.3 Dirac-like equation

To take into account both K points (ξ=+1 and ξ=-1) we can use a 4 component wave function,

$$\psi = \begin{pmatrix} \psi_{AK} \\ \psi_{BK} \\ \psi_{AK'} \\ \psi_{BK'} \end{pmatrix}$$

with the following effective Hamiltonian:

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

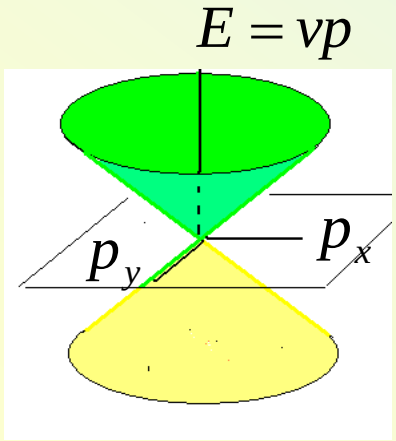
2 Expansion near the K points

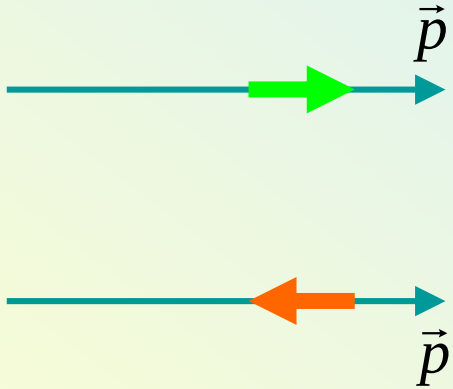
2.3 Dirac-like equation

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

Helical electrons

pseudospin direction is linked to an axis determined by electronic momentum.





for conduction band electrons,

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

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

valence band ('holes')

Show 3D picture

2 Expansion near the K points

2.4 Absence of backscattering

$$H = v\begin{pmatrix} 0 & \pi^{+} \\ \pi & 0 \end{pmatrix} = vp\begin{pmatrix} 0 & e^{-i\varphi} \\ e^{i\varphi} & 0 \end{pmatrix}; \qquad E = vp \quad \Leftrightarrow \quad \psi(\varphi) = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{-i\varphi/2} \\ e^{i\varphi/2} \end{pmatrix}$$

2 Expansion near the K points

2.4 Absence of backscattering

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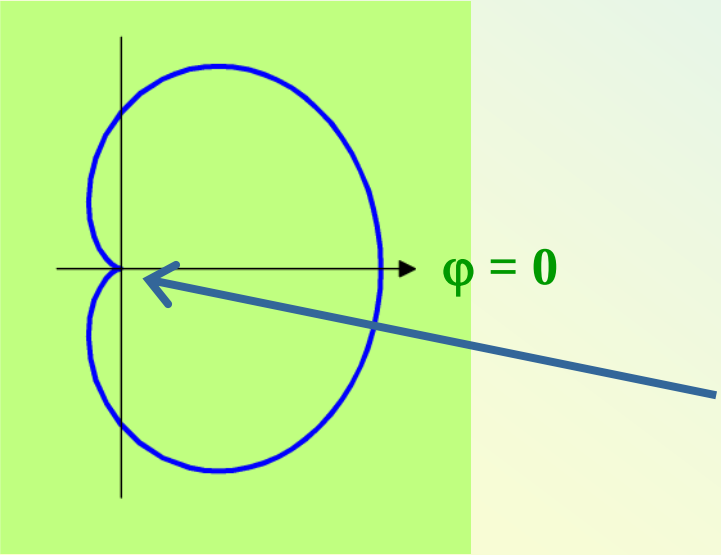
angular scattering probability:



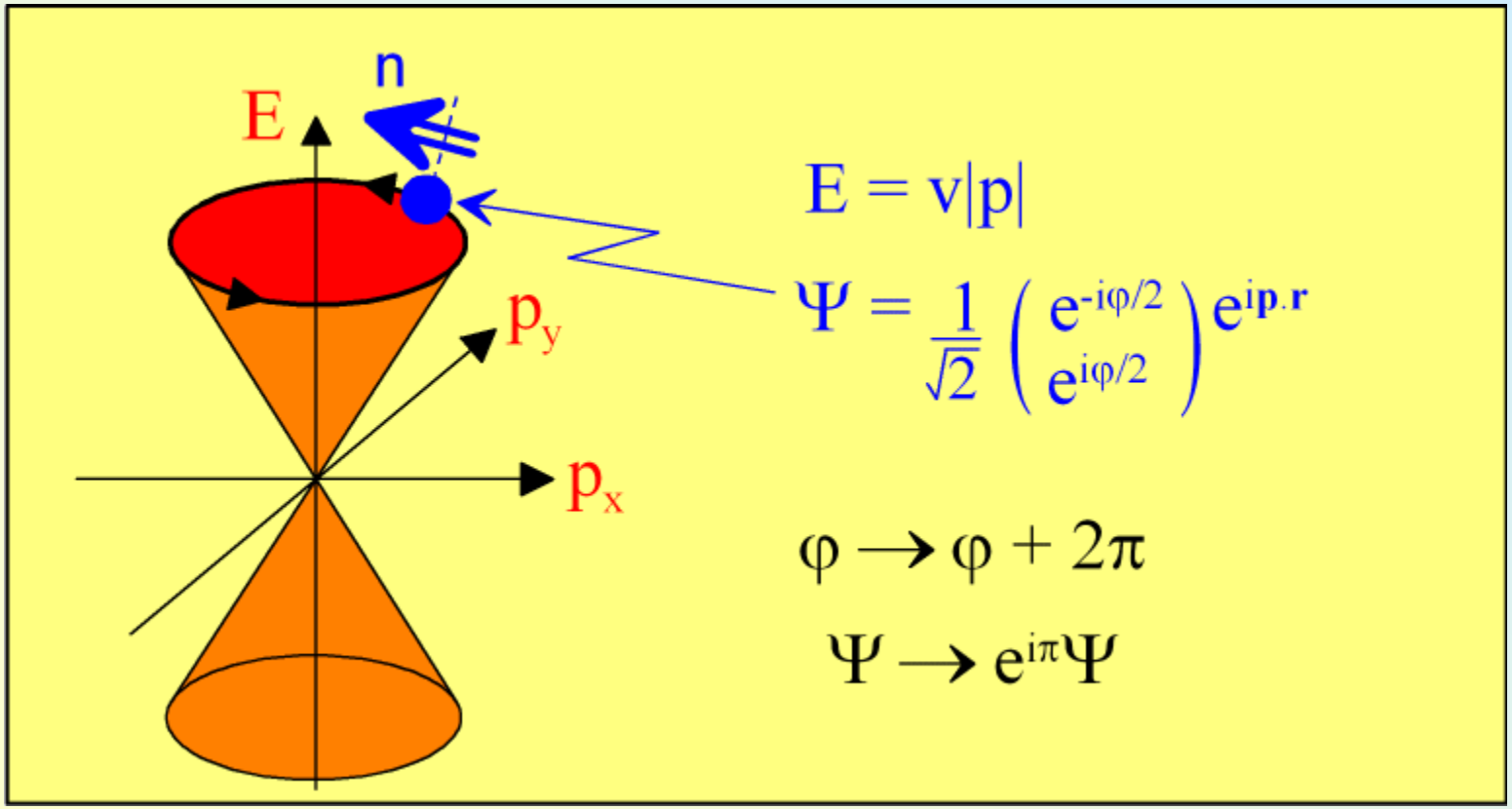
$$\left|\langle\psi(\varphi)|\psi(\varphi=0)\rangle\right|^2 = \cos^2(\varphi/2)$$

under pseudospin conservation, helicity suppresses backscattering in a monolayer

- Klein paradox
- Show angular dependence

2 Expansion near the K points

2.5 Berry's phase π



Show Dirac belt

Show definition of Berry phase

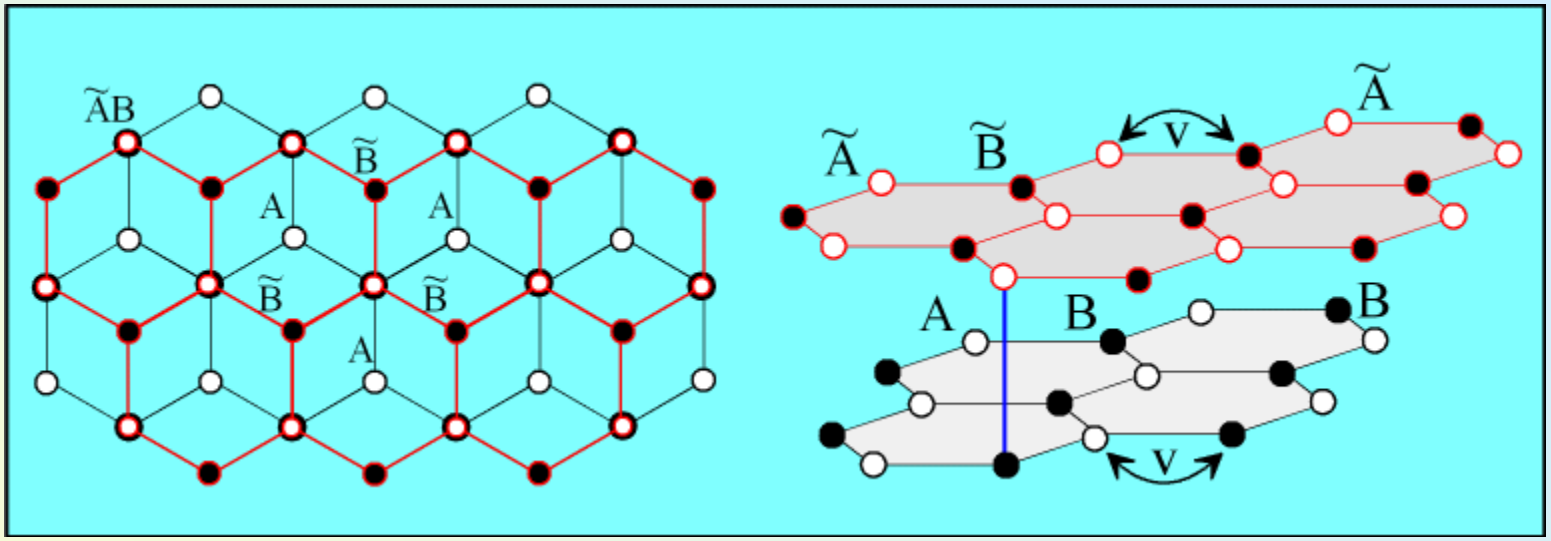
Monolayer graphene

$$H = v\begin{pmatrix} 0 & \pi^{+} \\ \pi & 0 \end{pmatrix} = vp\begin{pmatrix} 0 & e^{-i\varphi} \\ e^{i\varphi} & 0 \end{pmatrix};$$

$$E = vp \quad \Leftrightarrow \quad \psi(\varphi) = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{-i\varphi/2} \\ e^{i\varphi/2} \end{pmatrix}$$

massless Dirac fermions with Berry's phase π

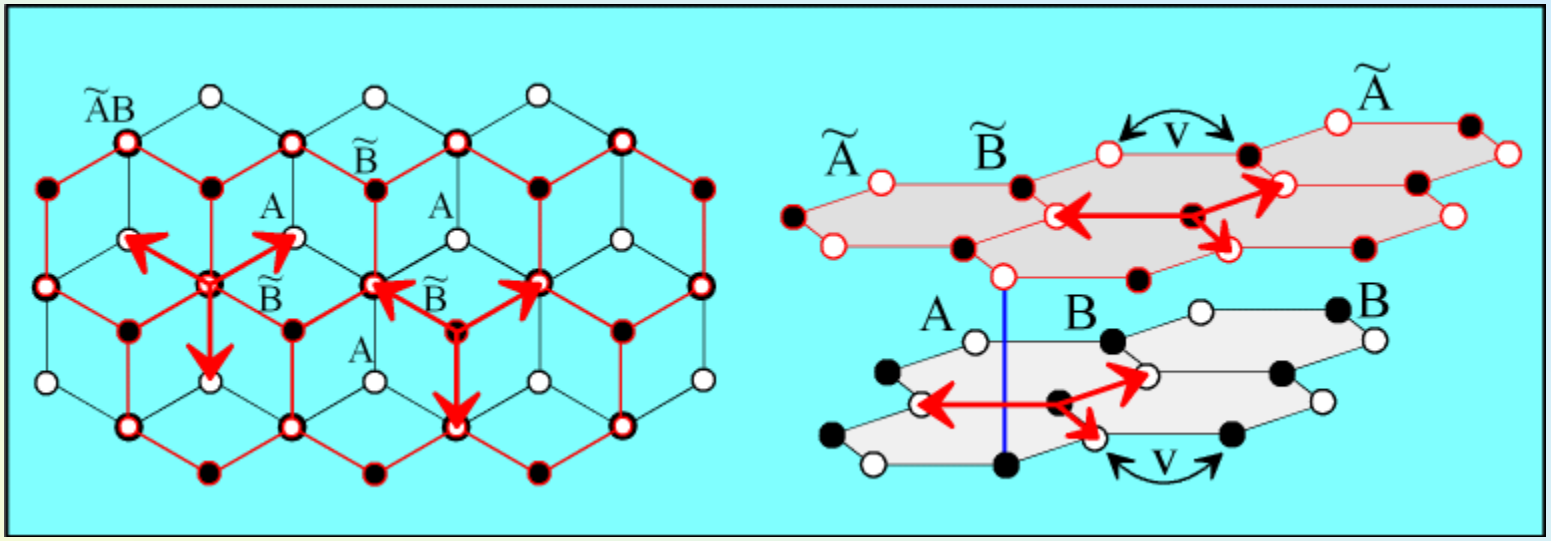
3. Bilayer graphene [Bernal (AB) stacking]



4 atoms per unit cell

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

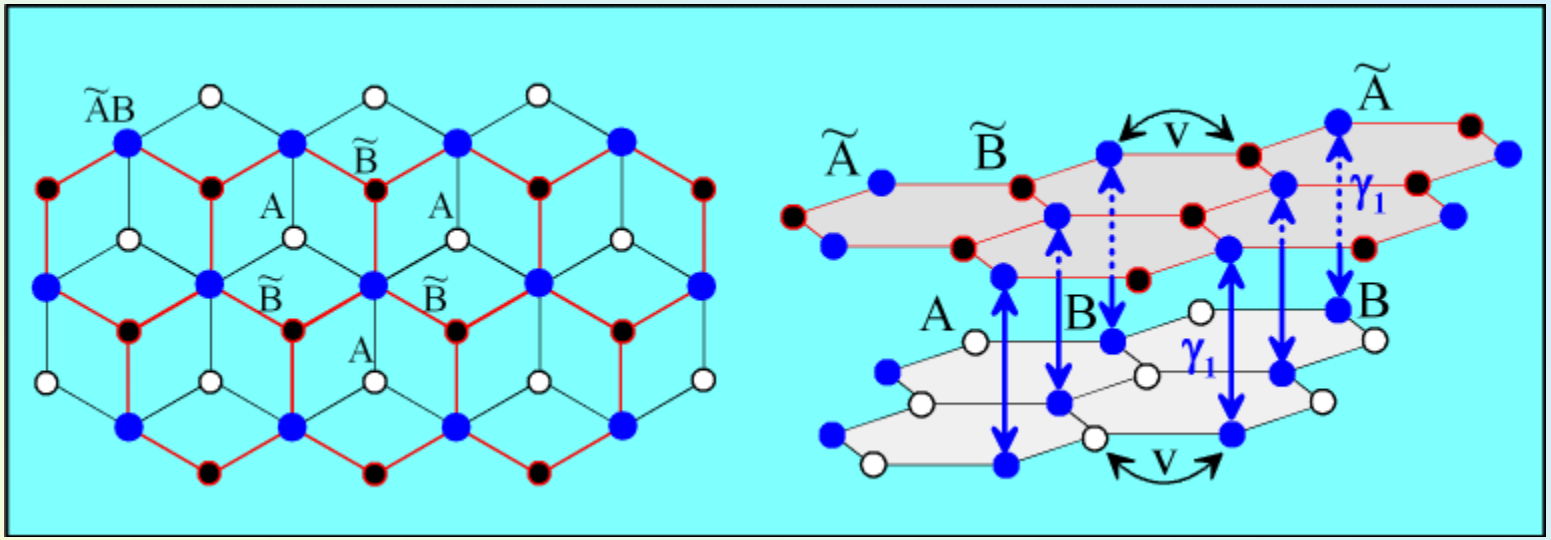
3. Bilayer graphene [Bernal (AB) stacking]



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

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

3. Bilayer graphene [Bernal (AB) stacking]



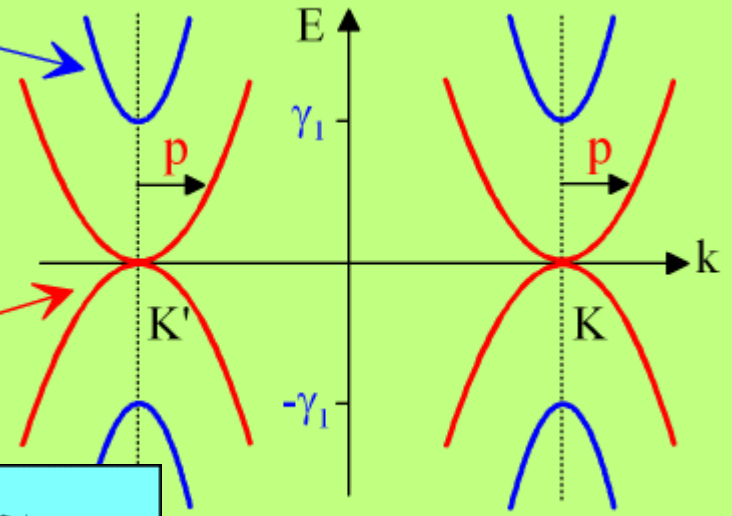
Bilayer Hamiltonian

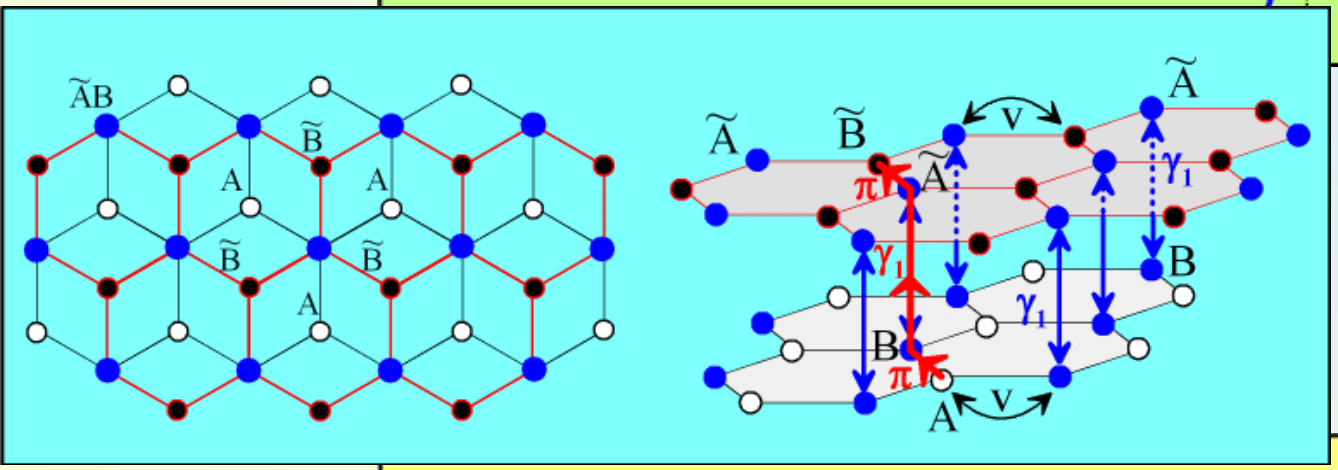
$$H = \begin{array}{c} \begin{matrix} A & \tilde{B} & \tilde{A} & B \end{matrix} \\ \begin{pmatrix} 0 & 0 & 0 & v\pi^+ \\ 0 & 0 & v\pi & 0 \\ 0 & v\pi^+ & 0 & \gamma_1 \\ v\pi & 0 & \gamma_1 & 0 \end{pmatrix} \end{array} \begin{matrix} A \\ \tilde{B} \\ \tilde{A} \\ B \end{matrix}$$

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

Quadratic dispersion at low energy:

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





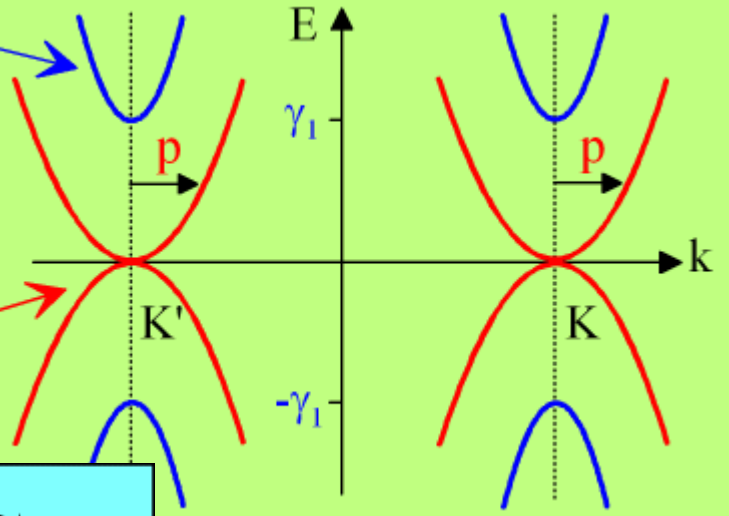
Bilayer Hamiltonian

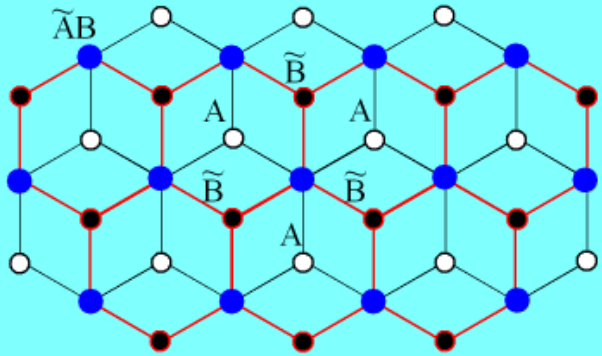
$$H = \begin{array}{c} \begin{matrix} A & \tilde{B} & \tilde{A} & B \end{matrix} \\ \begin{pmatrix} 0 & 0 & 0 & v\pi^+ \\ 0 & 0 & v\pi & 0 \\ 0 & v\pi^+ & 0 & \gamma_1 \\ v\pi & 0 & \gamma_1 & 0 \end{pmatrix} \end{array} \begin{matrix} A \\ \tilde{B} \\ \tilde{A} \\ B \end{matrix}$$

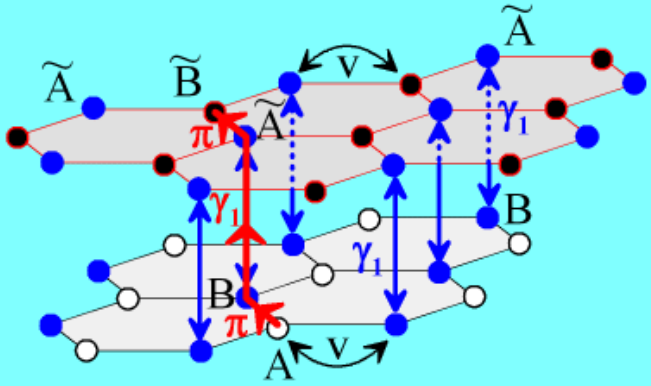
$\tilde{A}B$ orbitals form dimers with energy $|E| \gtrsim \gamma_1$

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

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

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)

$$\pi = p_x + ip_y$$

3 Bilayer graphene

Berry phase 2π quasiparticles

$$H = -\frac{1}{2m}\begin{pmatrix} 0 & (\pi^{+})^{2} \\ \pi^{2} & 0 \end{pmatrix} = -\frac{p^{2}}{2m}\begin{pmatrix} 0 & e^{-2i\varphi} \\ e^{2i\varphi} & 0 \end{pmatrix}; \qquad E = \frac{p^{2}}{2m} \quad \Leftrightarrow \quad \psi(\varphi) = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{-i\varphi} \\ e^{i\varphi} \end{pmatrix}$$

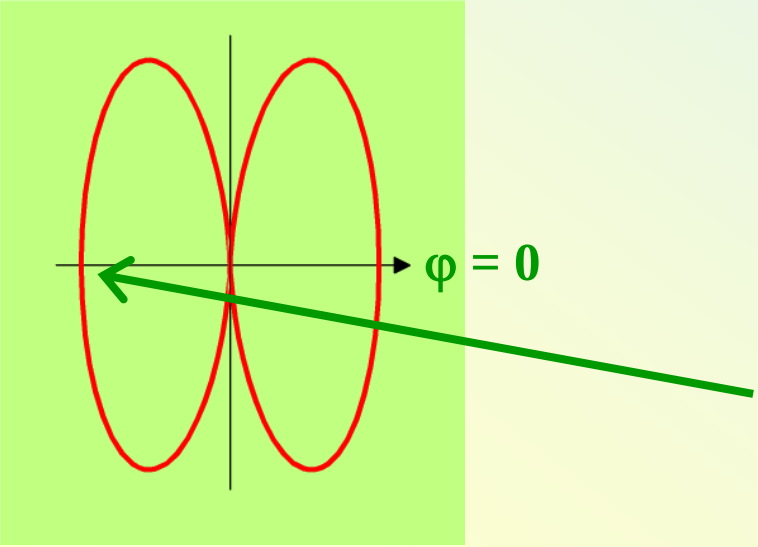
3 Bilayer graphene

Berry phase 2π quasiparticles

$$H = -\frac{1}{2m}\begin{pmatrix} 0 & (\pi^+)^2 \\ \pi^2 & 0 \end{pmatrix} = -\frac{p^2}{2m}\begin{pmatrix} 0 & e^{-2i\varphi} \\ e^{2i\varphi} & 0 \end{pmatrix}; \qquad E = \frac{p^2}{2m} \quad \Leftrightarrow \quad \psi(\varphi) = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{-i\varphi} \\ e^{i\varphi} \end{pmatrix}$$

No absence of backscattering

angular scattering probability:



$$\left|\langle \psi(\varphi) | \psi(\varphi = 0) \rangle\right|^2 = \cos^2(\varphi)$$

no suppression of backscattering in a bilayer

Some topics in graphene physics

1) Integer Quantum Hall effect

unusual sequencing of Hall conductivity plateaus

2) Minimal conductivity

see talks this afternoon: Jakub Tworzdlo; Jozsef Cserti

3) Tunnelling of chiral quasiparticles

MI Katsnelson, KS Novoselov, and AK Geim, cond-mat/0604343;
VV Cheianov and VI Falko, PRB 74, 041403

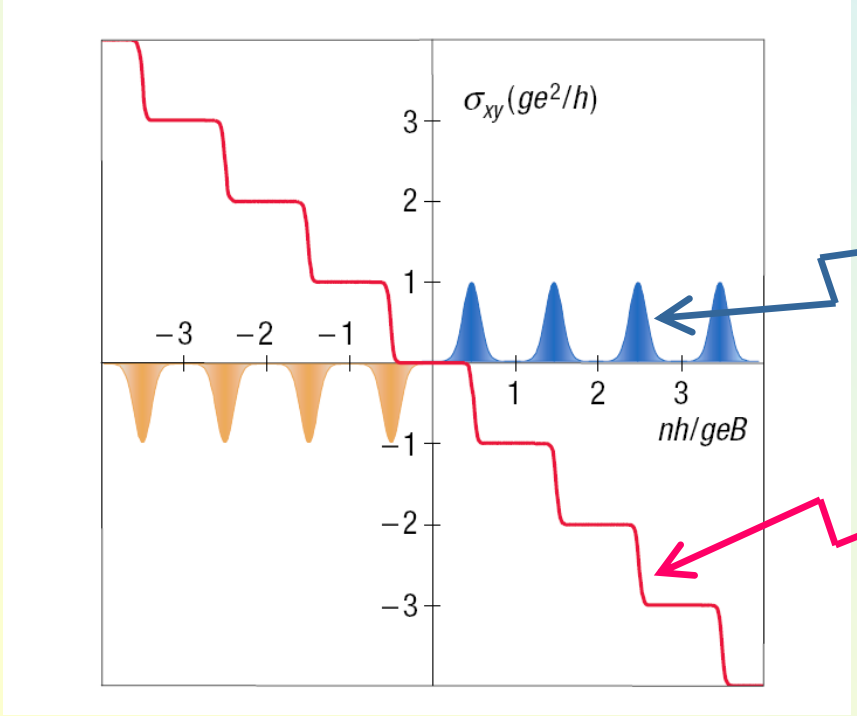
4) Weak localisation (?)

H Suzuura and T Ando, PRL 89, 266603 (2002); SV Morozov *et al*, PRL 97, 016801 (2006); DV Khveshchenko; AF Morpurgo and F Guinea; E McCann *et al* [all cond-mat 2006]

5) Andreev reflection

see talk this afternoon: Carlo Beenakker

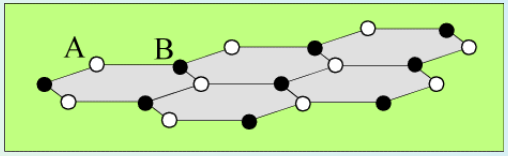
Integer Quantum Hall effect in a 2d semiconductor

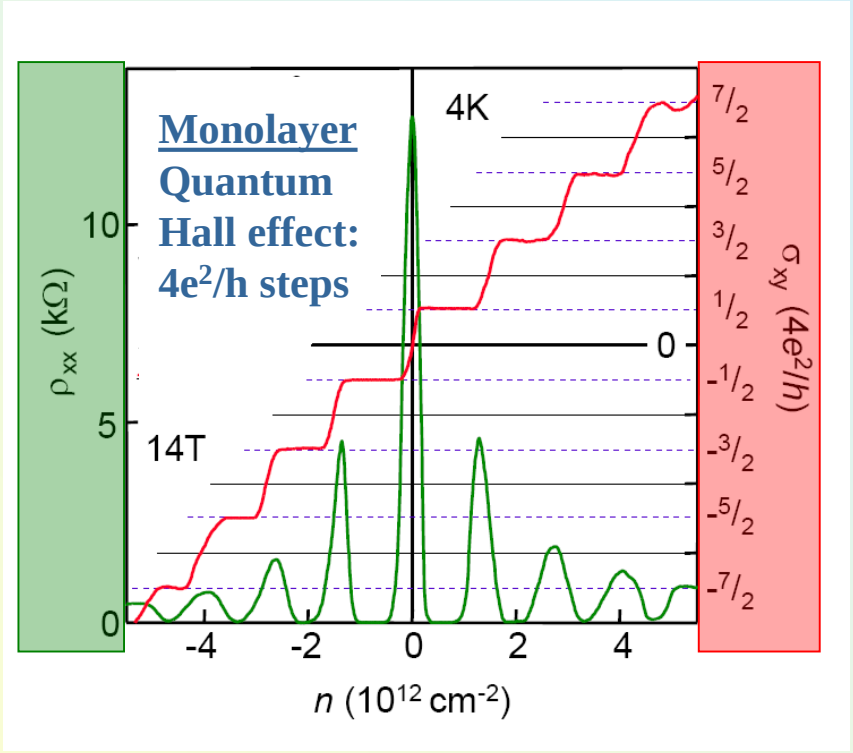


Each filled Landau level with additional degeneracy g contributes conductance quantum ge^2/h towards the Hall conductivity

3 Integer quantum Hall effect

Graphene monolayer





Novoselov *et al*, Nature 438, 197 (2005);
Zhang *et al*, Nature 438, 201 (2005).

Landau levels and QHE

Monolayer:

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

Bilayer:

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

In a perpendicular magnetic field B:

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

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

$\pi \rightarrow$ lowering operator

$\pi^+ \rightarrow$ raising operator

} of magnetic oscillator eigenstates ϕ_n

We are able to determine the spectrum of discrete Landau levels

States at zero energy are determined by

monolayer: $\pi\phi_0 = 0$

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

Show super-symmetry

Get HO and take sqrt.

Check Ezawa

Check McLure

2D Landau levels of chiral electrons

J=1 monolayer

J=2 bilayer

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

$$\pi^J \varphi_0 = \ldots = \pi^J \varphi_{J-1} = 0$$

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

valley index

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

also, two-fold real spin degeneracy

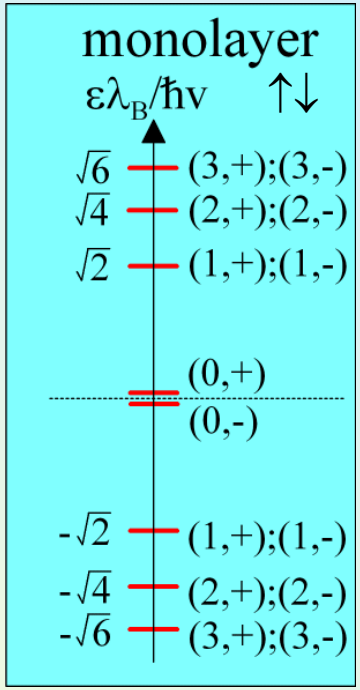
monolayer:

energy scale $\hbar v/\lambda_B$

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

state at zero energy:

$$\pi\phi_0 = 0$$



4-fold degenerate zero-energy Landau level for electrons with Berry's phase π

J.McClure, Phys. Rev. 104, 666 (1956)
F.Haldane, PRL 61, 2015 (1988)
Y.Zheng and T.Ando, Phys. Rev. B 65, 245420 (2002)
V.P. Gusynin and S.G. Sharapov, Phys. Rev. Lett 95, 146801 (2005)
N.M.R. Peres, F. Guinea and A.H. Castro Neto, PRB 73, 125411 (2006)

bilayer:

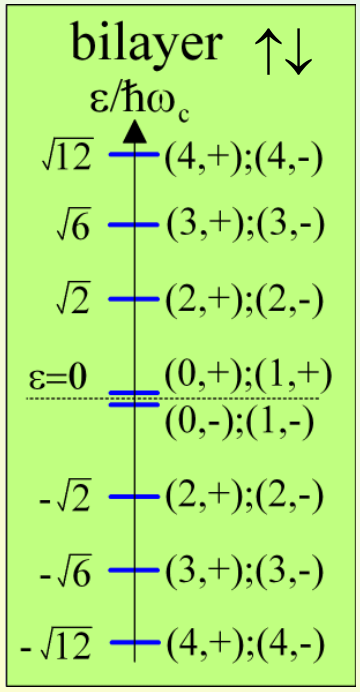
energy scale $\hbar\omega_c$

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

states at zero energy:

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

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

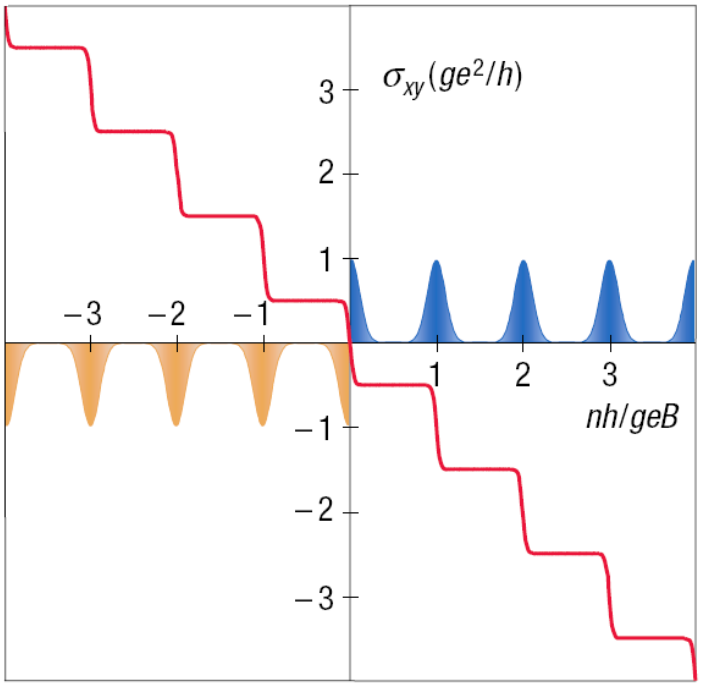


8-fold degenerate zero-energy Landau level for electrons with Berry's phase 2π

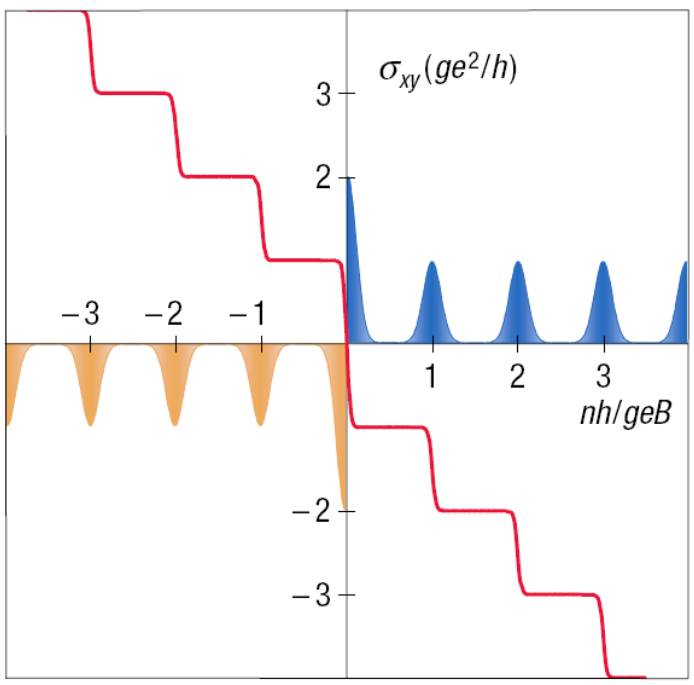
E.McCann and V.I. Fal'ko, Phys. Rev. Lett. 96, 086805 (2006)

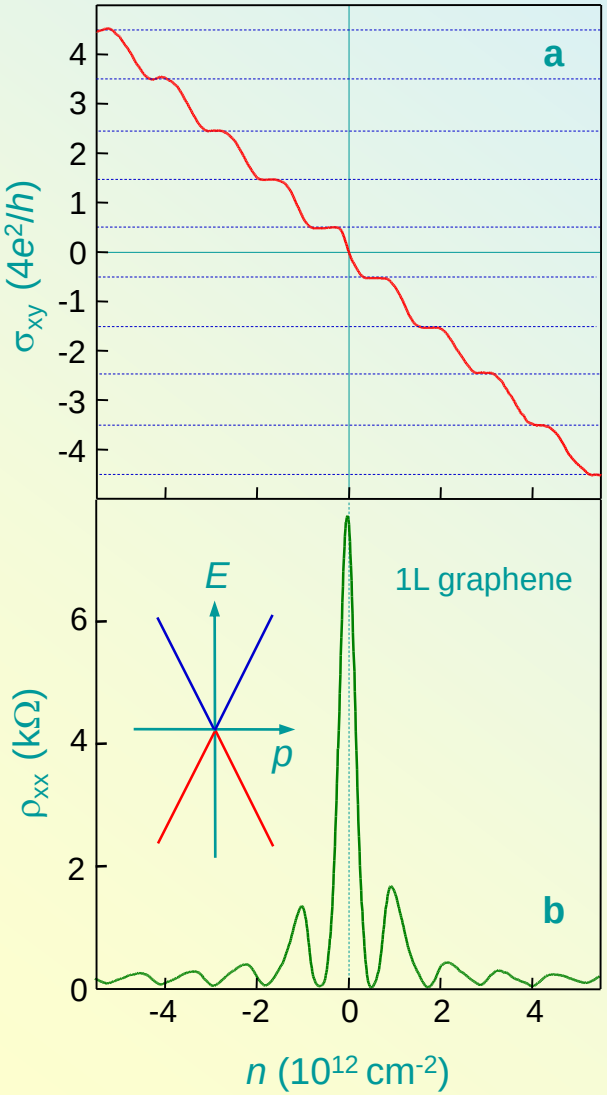
QHE in graphene

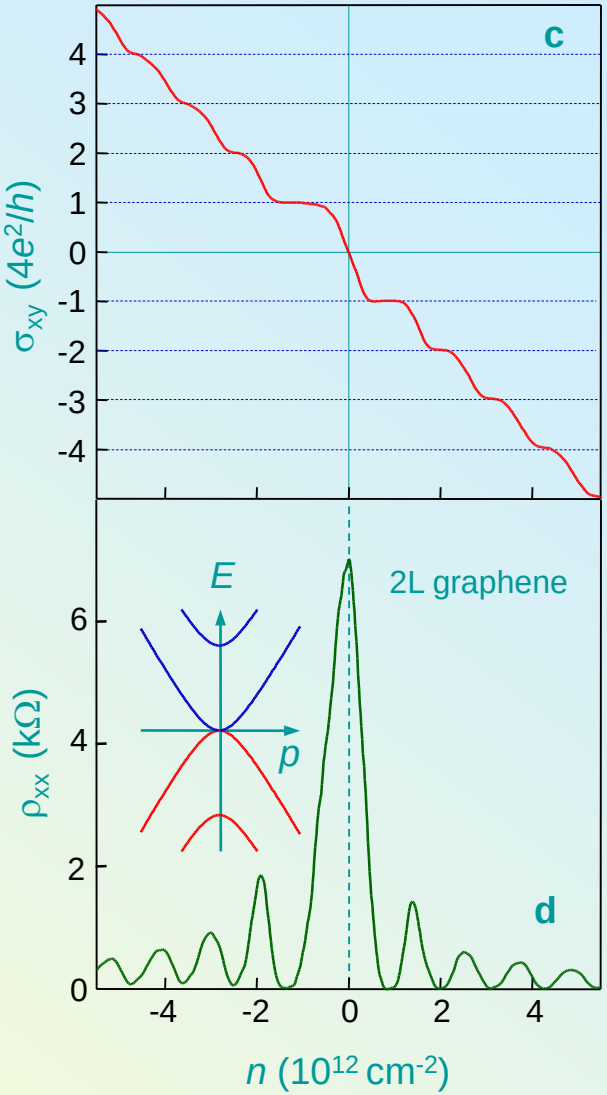
monolayer



bilayer







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

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

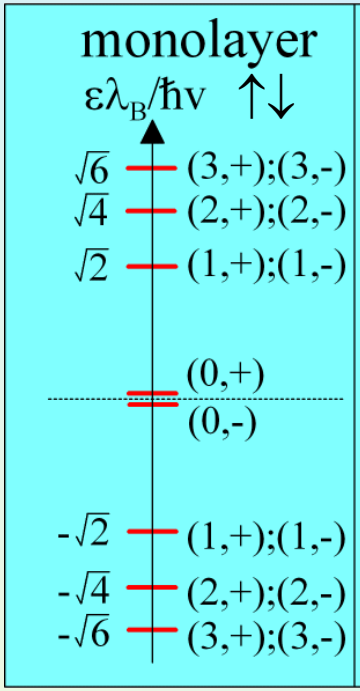
Nature Physics 2, 177-180 (2006)

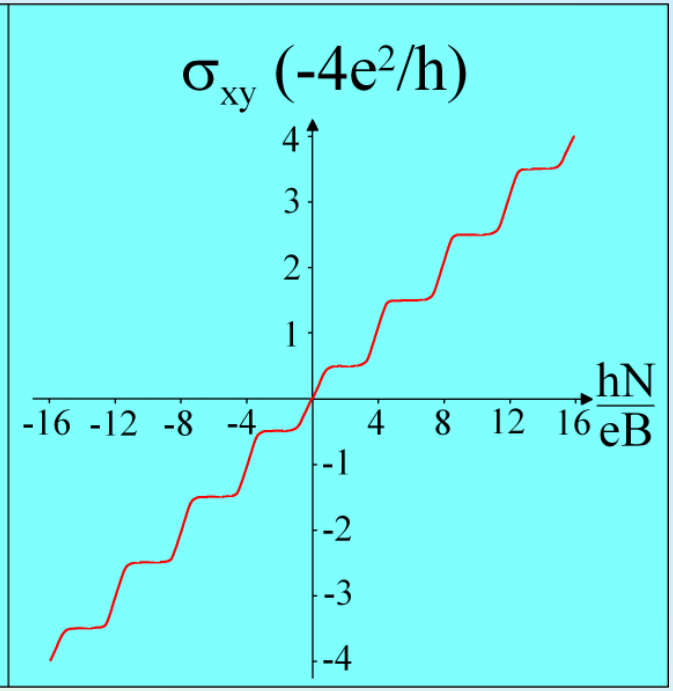
monolayer:

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

state at zero energy:

$$\pi\phi_0 = 0$$





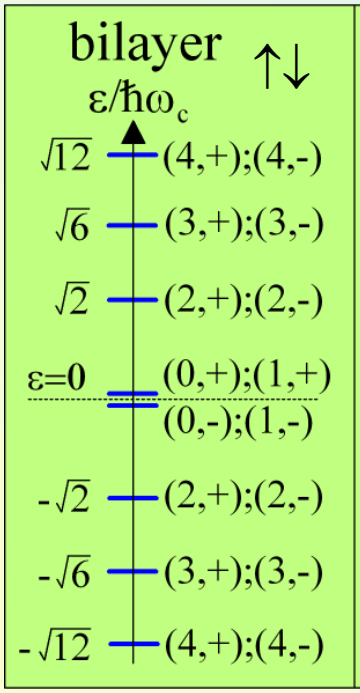
bilayer:

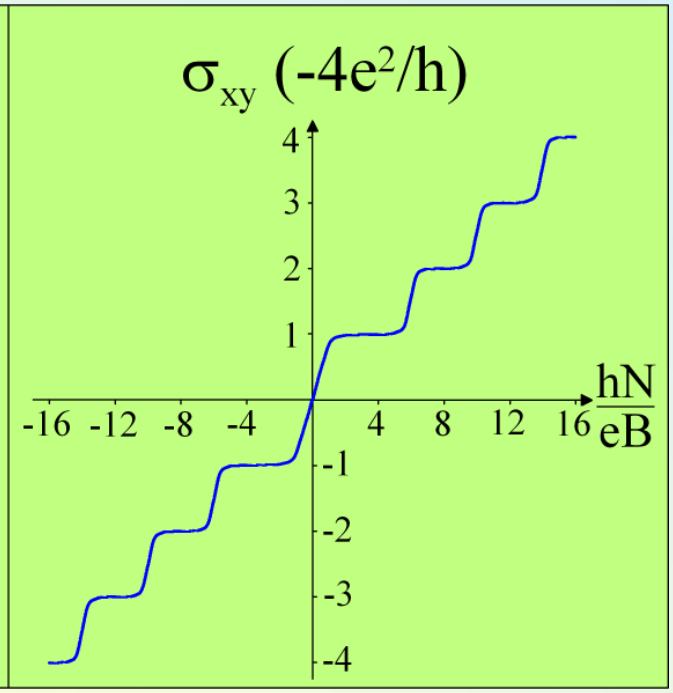
$$H = \frac{-1}{2m} \begin{pmatrix} 0 & (\pi^+)^2 \\ \pi^2 & 0 \end{pmatrix}$$

states at zero energy:

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

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





Summary

Graphene monolayer – 2D electron system
with Berry phase π quasiparticles and 4 times degenerate
zero-energy Landau levels manifested in the quantum Hall effect.

Graphene bilayer – 2D electron system
with Berry phase 2π quasiparticles and 8 times degenerate
zero-energy Landau levels manifested in the quantum Hall effect.

The End