THE ELECTRONIC STRUCTURE OF MULTILAYER GRAPHENE

University of Konstanz

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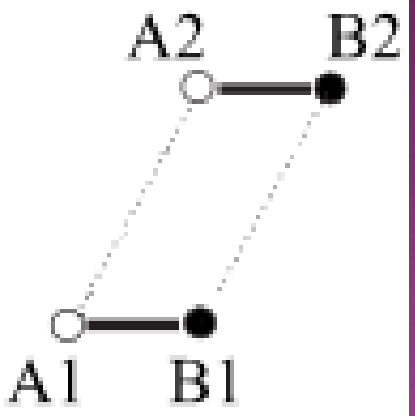
ORGANIZATION OF THE LECTURE

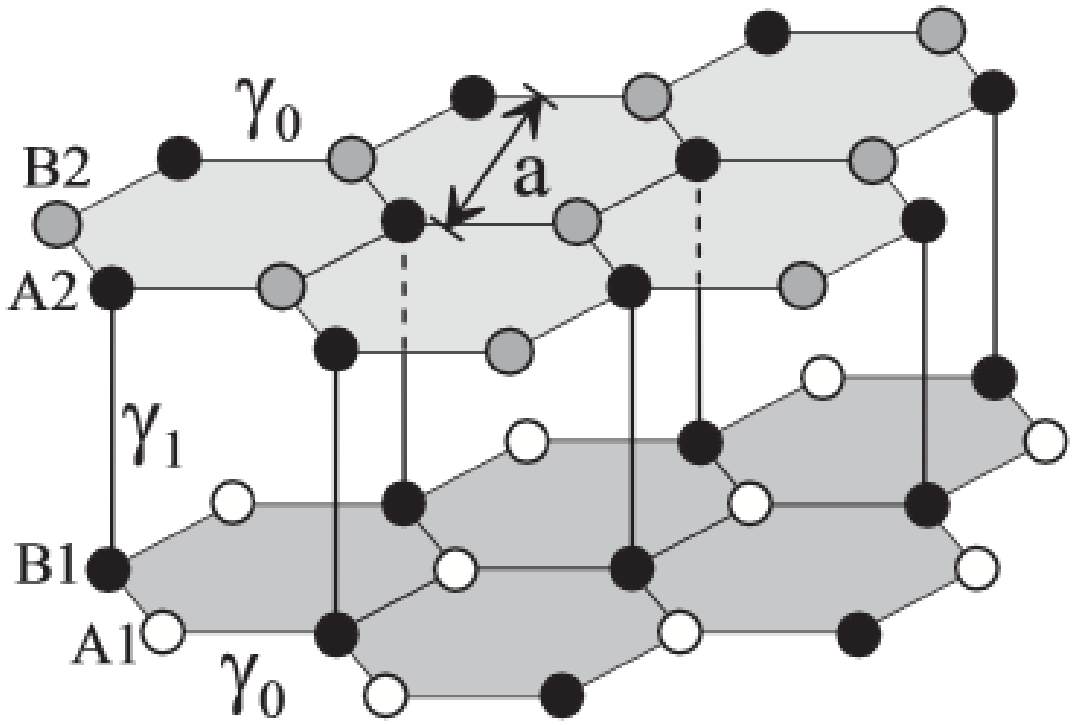
- Electronic structure of bilayer graphene
- Electronic structure of trilayer graphene
- Electronic structure of multilayer graphene
- References for further reading

UNIT CELL OF AB STACKED BILAYER GRAPHENE

- Four atoms in a unit cell
- Second carbon layer is rotated by 60^o
- Interlayer spacing $a \approx 3.35x10^{-10}$
- Interlayer asymmetry opens an energy gap

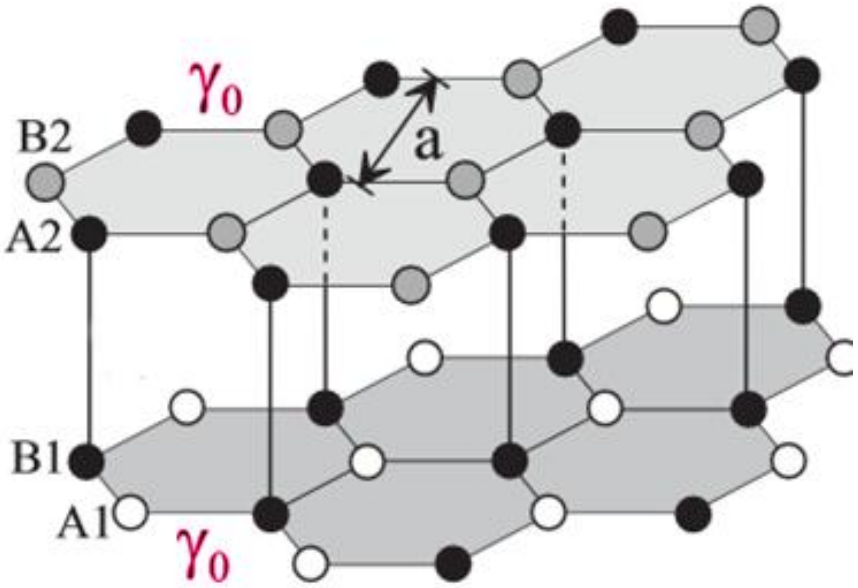


- Spatial arrangement of AB stacked bilayer graphene



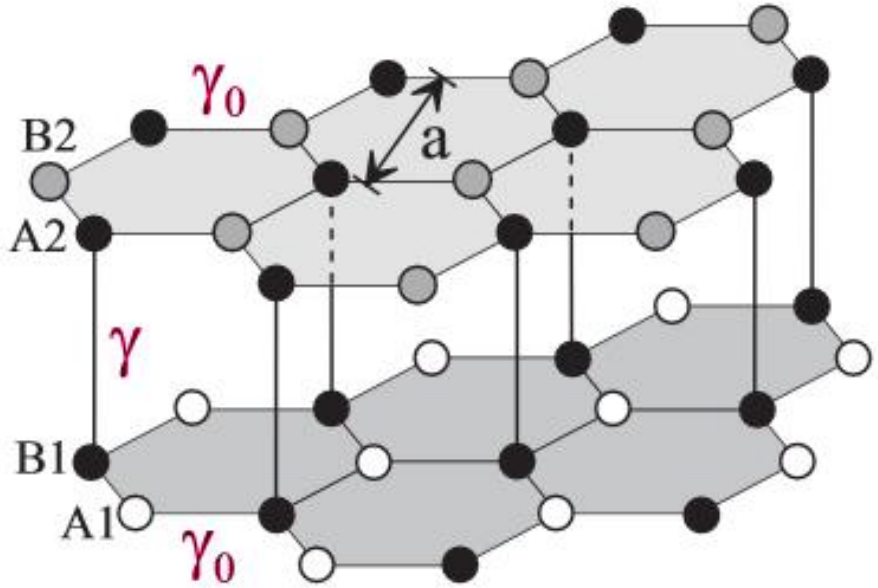
THE HAMILTONIAN

- $H = \begin{bmatrix} 0 & tS(\vec{k}) & ? & 0 \\ tS^*(\vec{k}) & 0 & 0 & 0 \\ ? & 0 & 0 & tS^*(\vec{k}) \\ 0 & 0 & tS(\vec{k}) & 0 \end{bmatrix}$



THE HAMILTONIAN

- $H = \begin{bmatrix} 0 & tS(\vec{k}) & t_\perp & 0 \\ tS^*(\vec{k}) & 0 & 0 & 0 \\ t_\perp & 0 & 0 & tS^*(\vec{k}) \\ 0 & 0 & tS(\vec{k}) & 0 \end{bmatrix}$



- Where $S(\vec{k})$ is as same as in the case of single layer graphene:

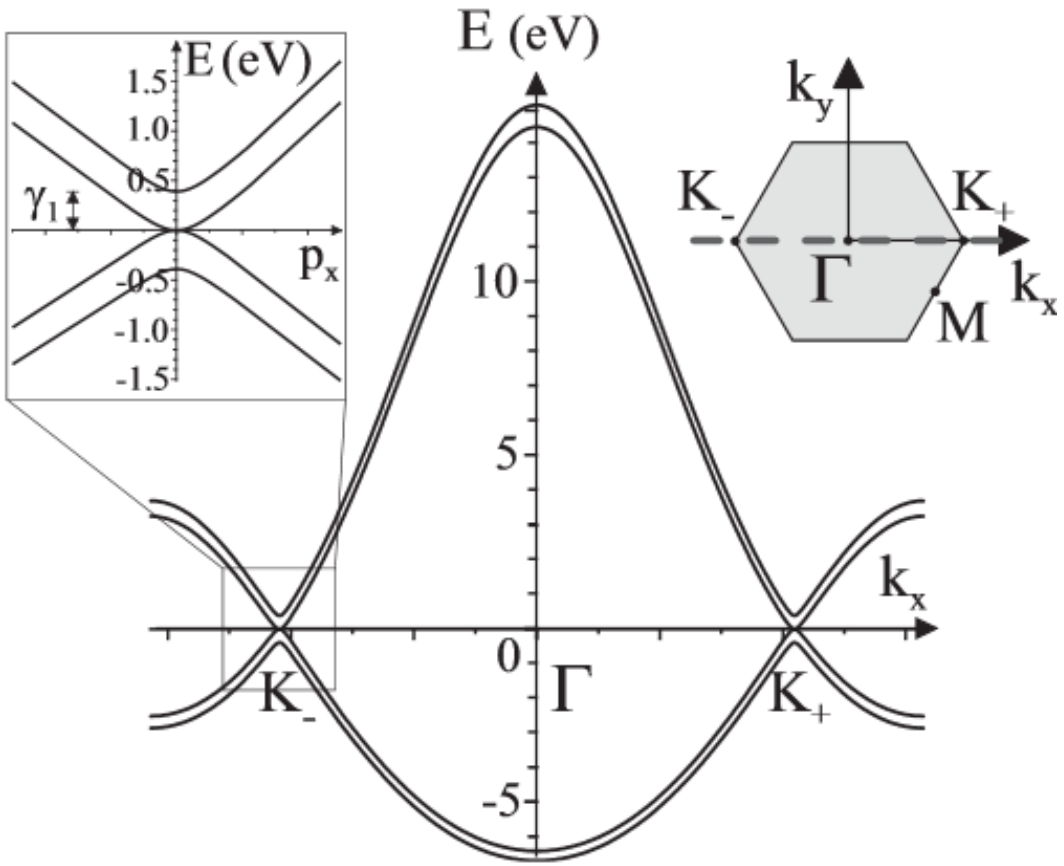
$$S(\vec{k}) = \sum_{\vec{\delta}} e^{i\vec{k}\cdot\vec{\delta}}$$

$$= 2\exp\left(\frac{ik_x a}{2}\right)\cos\left(\frac{k_y a\sqrt{3}}{2}\right)$$

$$+ \exp(-ik_x a\Big)$$

THE DIAGONALIZATION OF HAMILTONIAN

- After the diagonalization we obtain four possible eigenvalues:
- $E\ \ (\vec{k}) = \pm\frac{1}{2}t_{\perp} \pm \sqrt{\frac{1}{4}t_{\perp}^2 + t^2|S(\vec{k})|^2}$
- Near the K, K' points, there are two low energy branches:
- $E\ \ (\vec{k}) \approx \pm\frac{t^2|S(\vec{k})|^2}{t_{\perp}} \approx \frac{\hbar^2 q^2}{2m^*}$, where $\vec{q} = \vec{k} - \vec{K}$ or $\vec{q} = \vec{k} - \vec{K}'$



- $\gamma_0 = 3.033eV$, $\gamma_1 = 0.39eV$

Comparison of Single Layer and Bilayer Dispersion Relations

- Singlelayer
- $E(\vec{k}) = \pm t|S(\vec{k})| \approx v_F q$, where v_F is the Fermi velocity. We easily observe that the dispersion relation is linear in q
- Bilayer
- $E_{1,2}(\vec{k}) \approx \pm \frac{t^2|S(\vec{k})|^2}{t_\perp} \approx \frac{\hbar^2 q^2}{2m^*}$, we easily observe that the dispersion relation is quadratic in q

LOW ENERGY EFFECTIVE HAMILTONIAN

- The low energy Hamiltonian can be obtained by applying a Schrieffer-Wolff transformation.
- The Schrödinger equation can be written as:

$$E_{c_{A1}} - tS(\vec{k})c_{A2} = 0$$

$$-tS^*(\vec{k})c_{B2} + E_{C_{B1}} - t_\perp c_{A_2} = 0$$

$$-t_\perp c_{B1} + E_{c_{A2}} - tS(\vec{k})c_{A1} = 0$$

$$-tS^*(\vec{k})c_{B1} + E_{c_{B2}} = 0$$

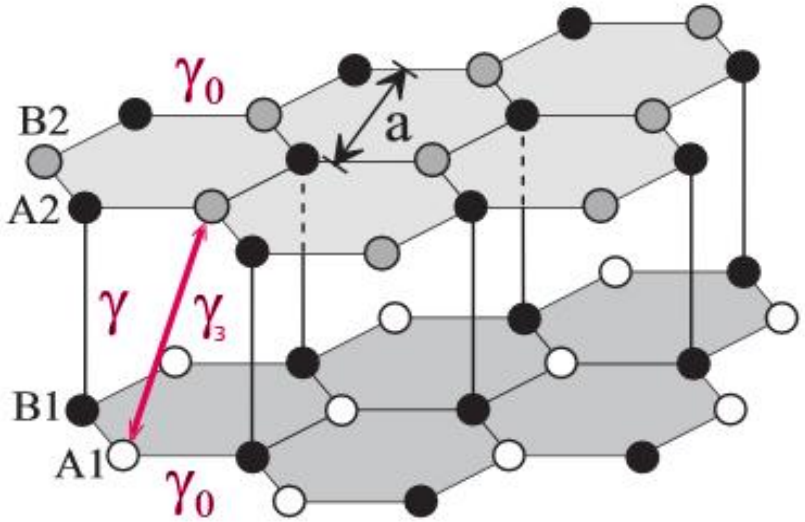
- Expressing c_{A1} and c_{B2} in the terms of the other two c_i and assuming $|E| \ll |t_\perp|$ and $|tS(\vec{k})| \ll t_\perp$ and keeping terms up to $1/t_\perp$ we obtain:

$$E_{c_{A1}} + \frac{|tS(\vec{k})|^2}{t_\perp} c_{B2} = 0$$

$$\frac{|tS^*(\vec{k})|^2}{t_\perp} c_{A1} + E_{c_{B2}} = 0$$

- It is possible to express these two equations as a single Schrodinger equation with a two component Hamiltonian:
- $\widehat{H}_K = \frac{1}{2m^*} \begin{bmatrix} 0 & (\hat{p}_x - i\hat{p}_y)^2 \\ (\hat{p}_x + i\hat{p}_y)^2 & 0 \end{bmatrix}$, where we have used $S(\vec{k}) \approx v\left(\xi p_x + i p_y\right)^2$ valid for $p\,a/\hbar \ll 1$ and $m^* = \gamma_1/(2v^2)$

TAKING INTO ACCOUNT MORE REMOTE HOPPINGS

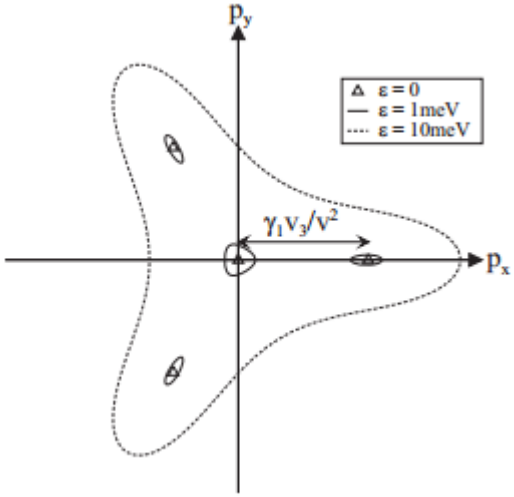


- $\hat{H}_K =$

$$\begin{bmatrix} 0 & \frac{(\hat{p}_x - i\hat{p}_y)^2}{2m^*} + \frac{3\gamma_3 a}{\hbar}(\hat{p}_x - i\hat{p}_y) \\ \frac{(\hat{p}_x + i\hat{p}_y)^2}{2m^*} + \frac{3\gamma_3 a}{\hbar}(\hat{p}_x - i\hat{p}_y) & 0 \end{bmatrix}$$

LIFTSHITZ TRANSITIONS

- γ_3 deforms the isoenergy lines producing so called trigonal warping.
- At very low energies $E \approx 1meV$ this leads to a **Lifshitz transition.** The isoenergy line is broken into four pockets, one central and three leg parts.



- Further ref: *European Physical Journal Special Topics, **148** (1). pp. 91-103.*

APPLYING A VOLTAGE

- We apply a voltage perpendicular to the carbon planes. The process is described by the Hamiltonian:

$$H = \begin{bmatrix} V/2 & tS(\vec{k}) & t_{\perp} & 0 \\ tS^{*}(\vec{k}) & V/2 & 0 & 0 \\ t_{\perp} & 0 & -V/2 & tS^{*}(\vec{k}) \\ 0 & 0 & tS(\vec{k}) & -V/2 \end{bmatrix}$$

- By diagonalizing the Hamiltonian we obtain following energy levels:
- $E_i^2(\vec{k}) = t^2|S(\vec{k})|^2 + \frac{t_\perp^2}{2} + \frac{V^2}{4} \pm \sqrt{\frac{t_\perp^2}{4} + (t_\perp^2 + V^2)t^2|S(\vec{k})|^2}$
- Near K, K'
- $E(\vec{k}) \approx \pm\left(\frac{V}{2} - \frac{V\hbar^2 v^2}{t_\perp^2}k^2 + \frac{\hbar^4 v^4}{t_\perp^2 V}k^4\right)$
- We conclude that adding an external bias can open a bandgap.

TWISTED BILAYER GRAPHENE

- A-B stacked bilayer graphene is an ideal case obtained when interlayer rotations are $\frac{\pi}{3}$

- In nature there are imperfections which more or less differ from the A-B stacked case.

- Our next goal is to briefly discuss the theory of twisted bilayer graphene with a small twist angle.

- Twisting the layers by a small angle with respect to each other significantly increases the number of atoms in a unit cell (for example twisting the layers for $\theta = 2.1^{o}$ causes the unit cell to contain 2884 atoms)

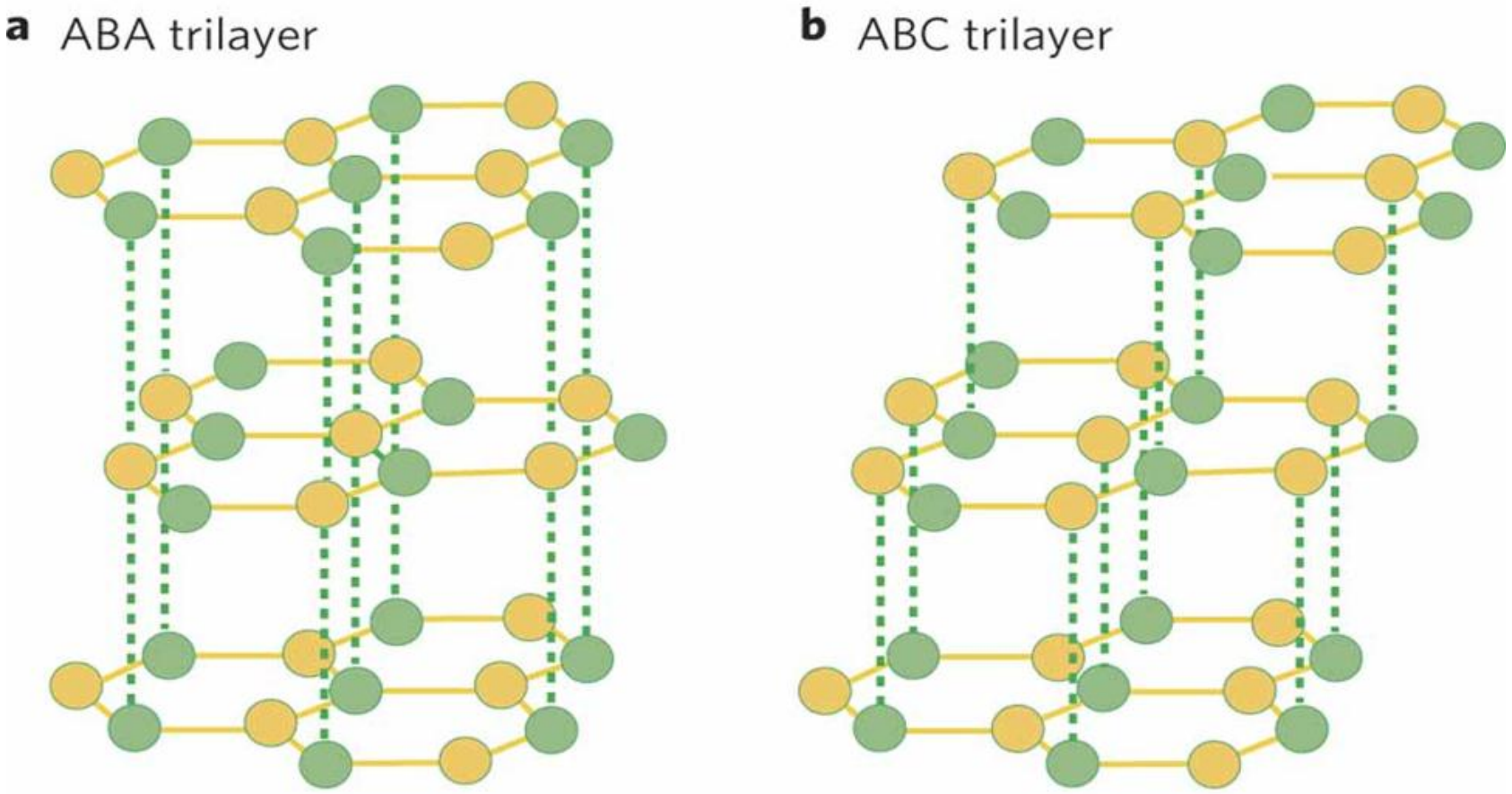
- Due to the large number of atoms per unit cell the nearest neighbor approach is not mathematically easily applicable and a perturbative approach can be used instead

MAIN RESULTS OF THE PERTURBATIVE APPROACH

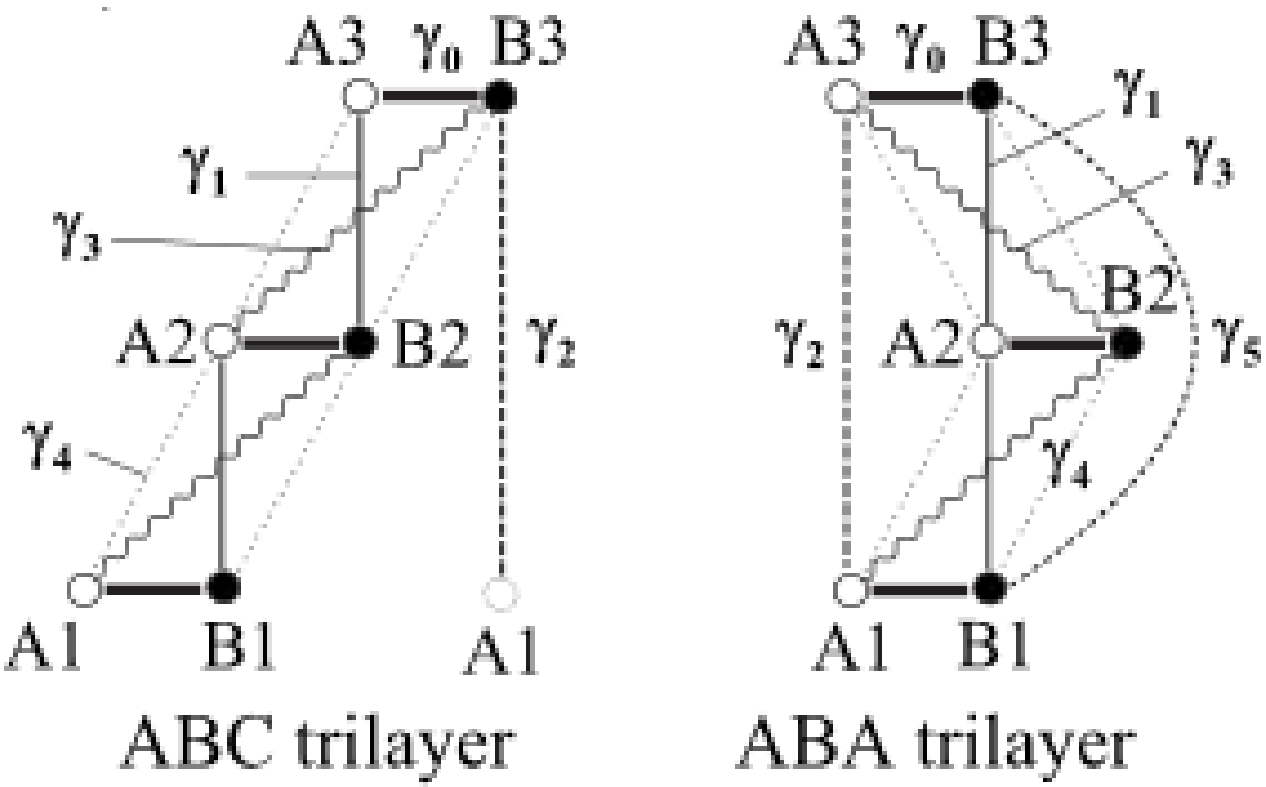
- The low energy dispersion is linear as in the case of single layer
- In contrast to bilayer graphene a perpendicular electric field does not open a gap
- Further ref: *Phys Rev Lett* ***99***, *256802 (2007)*

- For few layer graphene different stacking orders are possible.
- We will shortly discuss the possible stacking orders of trilayer graphene.

TRILAYER GRAPHENE



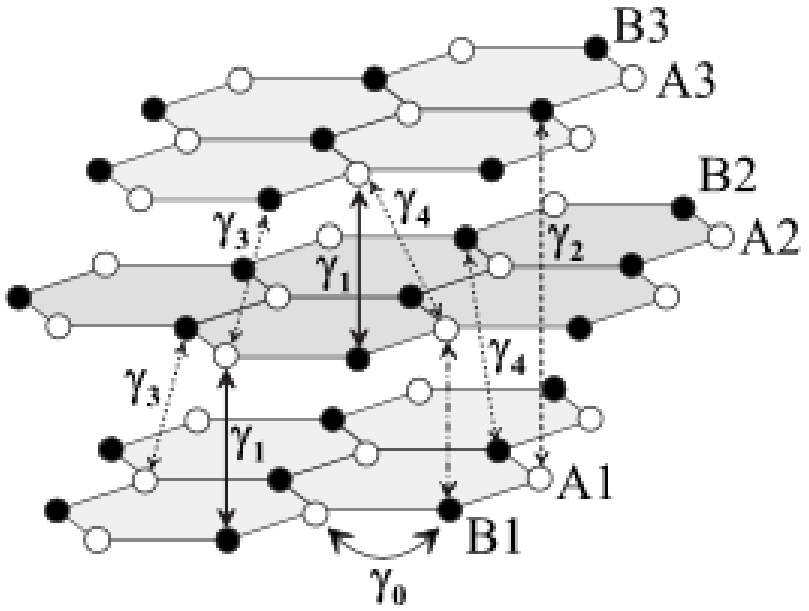
UNIT CELL OF TRILAYER GRAPHENE



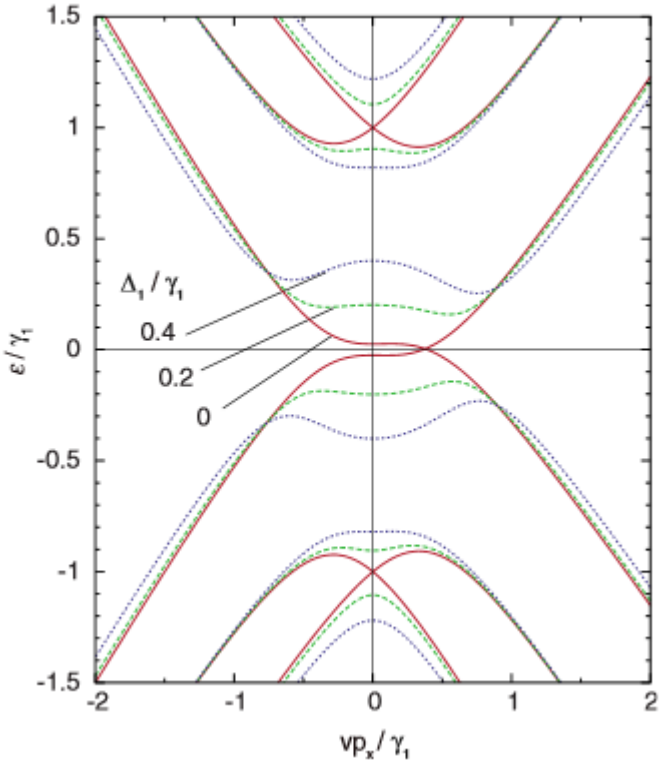
TIGHT BINDING MODEL OF ABC TRILAYER GRAPHENE

- $\hat{H} = \begin{bmatrix} D_1 & V & W \\ V^\dagger & D_2 & V \\ W^\dagger & V^\dagger & D_3 \end{bmatrix}$
- $D_i = \begin{bmatrix} U_i & v_0\pi^\dagger \\ v_0\pi & U_i \end{bmatrix}$, *i=1,2,3*
- $V = \begin{bmatrix} -v_4\pi^\dagger & v_3\pi \\ \gamma_1 & -v_4\pi^\dagger \end{bmatrix}$
- $W = \begin{bmatrix} 0 & \gamma_2/2 \\ 0 & 0 \end{bmatrix}$, $v_i = (\sqrt{3}/2)a\,\gamma_i/\hbar$,

  $\pi = \xi p_x + ip_y$, $\pi^\dagger = \xi p_x - ip_y$



SPECTRUM OF THE HAMILTONIAN



- Band *dispersion in the vicinity of* K_+ *along* p_x
- $\gamma_0 = 3.16eV, \gamma_1 = 0.39eV, \gamma_2 = -0.020eV,$
- $\gamma_3 = 0.315eV, \gamma_4 = 0.044eV$

EFFECTIVE TWO LEVEL HAMILTONIAN (LOW ENERGY LIMIT)

- Using Löwdin partitioning we obtain :

- $\hat{H}_{ABC}^{(eff)} = \hat{H}_3 + \hat{H}_{3w} + \hat{H}_{3c} + \hat{H}_{\Delta 1} + \hat{H}_{\Delta 2}$
- $H_3 = \frac{v^3}{\gamma_1^2}\begin{bmatrix} 0 & (\pi^\dagger)^3 \\ \pi^3 & 0 \end{bmatrix}$
- $\hat{H}_{3w} = \left(-\frac{2vv_3p^2}{\gamma_1} + \frac{\gamma_2}{2}\right)\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
- $\hat{H}_{3c} = \left(\frac{2vv_4p^2}{\gamma_1}\right)\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
- $\hat{H}_{\Delta 1} = \Delta_1\left(1 - \frac{v^2p^2}{{\gamma_1}^2}\right)\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
- $\hat{H}_{\Delta 2} = \Delta_2\left(1 - \frac{3v^2p^2}{\gamma_1^2}\right)\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

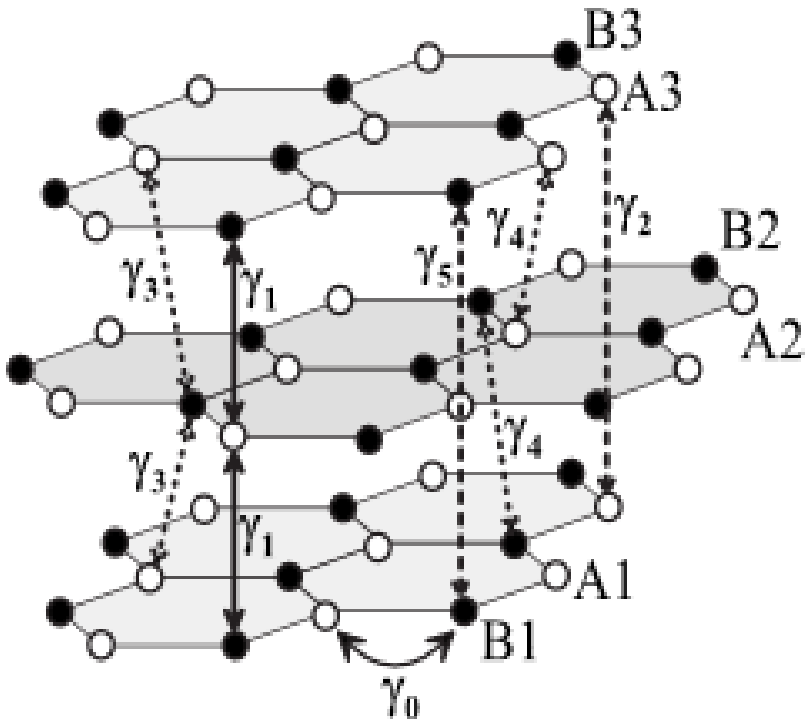
DISPERSION RELATION

- Near the K,K' points the dispersion relation is: $E(\vec{k}) \approx \frac{t^3 |S(\vec{k})|^3}{{t_\perp}^2} \propto \pm q^3$

- So we conclude that ABC stacked graphene has cubic touching of the conduction and valence bands.

ABA STACKED THREE LAYER GRAPHENE

- $\hat{H} = \begin{bmatrix} D_1 & V & W \\ V^\dagger & D_2 & V \\ W^\dagger & V^\dagger & D_1 \end{bmatrix}$
- $D_i = \begin{bmatrix} U_i & v_0\pi^\dagger \\ v_0\pi^\dagger & U_i \end{bmatrix}$
- $V = \begin{bmatrix} -v_4\pi^\dagger & v_3\pi \\ \gamma_1 & -v_4\pi^\dagger \end{bmatrix}$
- $W = \begin{bmatrix} \gamma_2/2 & 0 \\ 0 & \gamma_5/2 \end{bmatrix}$



THE LOW ENERGY HAMILTONIAN

- Considering only the largest inter layer hopping term, and following the same procedure as in ABC stacked graphene we obtain the low energy Hamiltonian:
- $\widehat{H} = \begin{bmatrix} 0 & v\pi^{\dagger} & 0 & 0 \\ v\pi & 0 & 0 & 0 \\ 0 & 0 & 0 & x \\ 0 & 0 & x^{\dagger} & 0 \end{bmatrix}$
- Where $x = \frac{v^2\pi\pi^{\dagger}}{\gamma_1\sqrt{2}\sqrt{\pi\pi^{\dagger}}}$

DISPERSION RELATION NEAR THE E = 0

- There are four low energy bands. Two disperse lineary and two disperse quadraticly (as in bilayer).

- $E_k = \pm v_F |\vec{k}|$

- $E = \pm \frac{t_\perp \sqrt{2}}{2} \pm \sqrt{\frac{t_\perp^2}{2} + v_F^2 |\vec{k}|^2}$

- Comparing ABA and ABC we see that the dispersion depends on the order of stacking.

FURTHER READING

Bilayer graphene (and warping)
PRL 96, 086805 (2006)

Trilayer graphene:
Phys. Rev. B 80, 165409 (2009) (ABC and warping)
Phys. Rev. B 82, 035409 (2010)
Phys. Rev. B 79, 125443 (2009) (ABA stack + gate)

Twisted bilayer graphene
Phys Rev Lett 99, 256802
Phys Rev B 81, 161405

Electronic transport in Bilayer graphene
New J. Phys. **11** 095010