Tight-binding model for graphene bilayer

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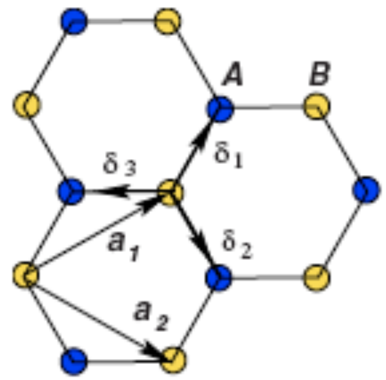
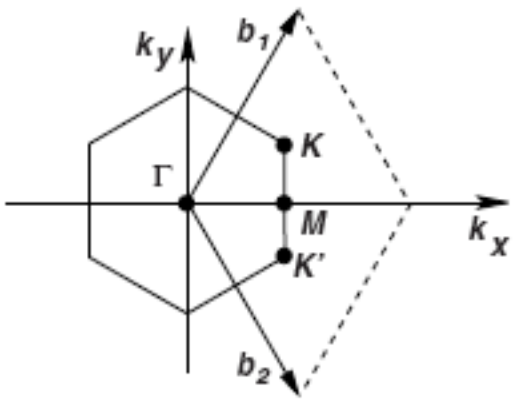
Bilayer Stacking

$$\mathbf{a}_1 = \frac{a}{2}(\sqrt{3}, \sqrt{3}) \qquad \mathbf{a}_2 = \frac{a}{2}(\sqrt{3}, -\sqrt{3})$$

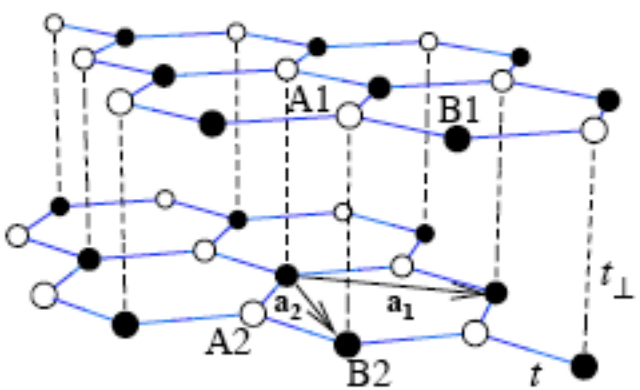
$$\boldsymbol{\delta}_1 = \frac{a}{2}(1, \sqrt{3}) \quad \boldsymbol{\delta}_2 = \frac{a}{2}(1, -\sqrt{3}) \quad \boldsymbol{\delta}_3 = -a(1, 0)$$

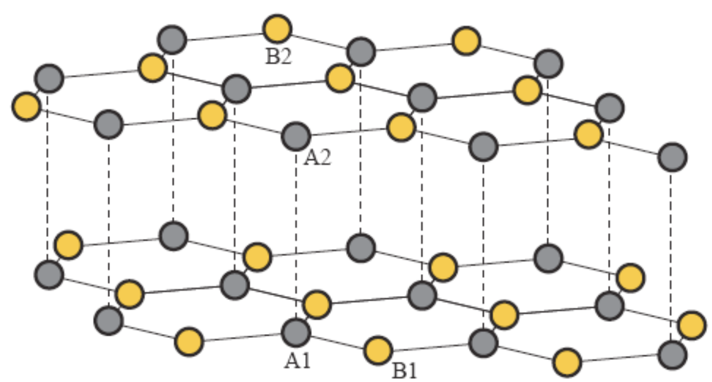
$$a = 2.46 \text{ Å}$$





Bernal stacking





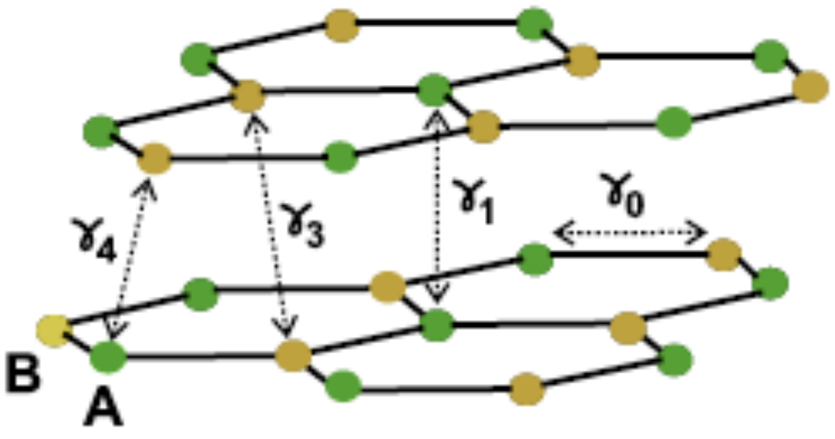
Tight-binding in Bernal stacking

$\gamma_0 = t$ in-plane hopping

$\gamma_1 = t_\perp \approx 0.4$ eV hopping energy between A1 and A2

$\gamma_3 \approx 0.3$ eV hopping energy between B1 and B2

$\gamma_4 \approx 0.04$ eV hopping energy between A1(A2) and B2(B1)



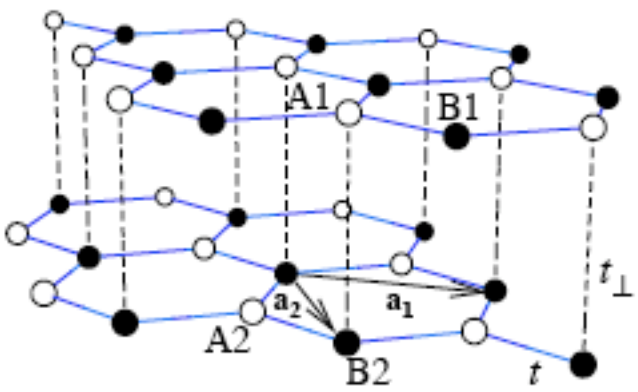
$a_{m,i,\sigma} \quad (b_{m,i,\sigma})$ annihilates an electron with spin s, on sublattice A(B), in plane m=1,2, at site i

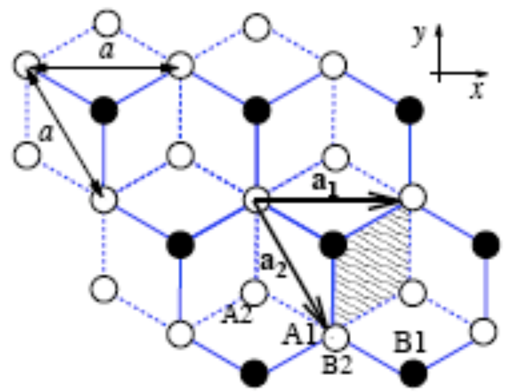
$$\begin{aligned}\mathcal{H} &= -\gamma_0 \sum_{\langle i,j \rangle, m, \sigma} (a^\dagger_{m,i,\sigma} b_{m,j,\sigma} + h.c.) - \gamma_1 \sum_{j,\sigma} (a^\dagger_{1,j,\sigma} a_{2,j,\sigma} + h.c.) \\ &- \gamma_3 \sum_{j,\sigma} (b^\dagger_{1,j,\sigma} b_{2,j,\sigma} + h.c.) - \gamma_4 \sum_{j,\sigma} (a^\dagger_{1,j,\sigma} b_{2,j,\sigma} + a^\dagger_{2,j,\sigma} b_{1,j,\sigma} + h.c.)\end{aligned}$$

Minimal tight-binding model

Neglect contributions coming from γ_3, γ_4 $\mathbf{a}_1 = (a, 0)$ $\mathbf{a}_2(\frac{a}{2}, -\frac{a\sqrt{3}}{2})$

Bernal stacking





$t \approx 3.1$ eV in-plane hopping

$t_\perp \approx 0.4$ eV hopping energy between A1 and B2

$$\mathcal{H} = -t \sum_{i,\mathbf{R},\sigma} \left[a^\dagger_{i,\sigma}(\mathbf{R}) b_{i,\sigma}(\mathbf{R}) + a^\dagger_{i,\sigma}(\mathbf{R}) b_{i,\sigma}(\mathbf{R} - \mathbf{a}_1) + a^\dagger_{i,\sigma}(\mathbf{R}) b_{i,\sigma}(\mathbf{R} - \mathbf{a}_2) + h.c. \right]$$

$$- t_\perp \sum_{\mathbf{R},\sigma} \left(a^\dagger_{1,\sigma}(\mathbf{R}) b_{2,\sigma}(\mathbf{R}) + h.c. \right)$$

Perpendicular electric and magnetic field

External E field: electrostatic energy difference between the two layers

External B field: affects only the in-plane hopping $t \longrightarrow t e^{ie \int_{\mathbf{R}}^{\mathbf{R}+\boldsymbol{\delta}} \mathbf{A} \cdot d\mathbf{r}}$

$$\begin{aligned}
\mathcal{H} &= -t \sum_{i,\mathbf{R},\sigma} \left[a^{\dagger}_{i,\sigma}(\mathbf{R}) b_{i,\sigma}(\mathbf{R}) + a^{\dagger}_{i,\sigma}(\mathbf{R}) b_{i,\sigma}(\mathbf{R} - \mathbf{a}_1) + a^{\dagger}_{i,\sigma}(\mathbf{R}) b_{i,\sigma}(\mathbf{R} - \mathbf{a}_2) + h.c. \right] \\
&- t_{\perp} \sum_{\mathbf{R},\sigma} \left(a^{\dagger}_{1,\sigma}(\mathbf{R}) b_{2,\sigma}(\mathbf{R}) + h.c. \right) + \frac{V}{2} \sum_{\mathbf{R},\sigma} \left[n_{A1,\sigma}(\mathbf{R}) + n_{B1,\sigma}(\mathbf{R}) - n_{A2,\sigma}(\mathbf{R}) - n_{B2,\sigma}(\mathbf{R}) \right]
\end{aligned}$$

Bulk electronic properties

impose periodic boundary condition

apply a Fourier transform

$$a_{i,\sigma}(\mathbf{R}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}} a_{i,\sigma,\mathbf{k}}$$

$$b_{i,\sigma}(\mathbf{R}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}} b_{i,\sigma,\mathbf{k}}$$

$$\mathcal{H} = \sum_{\sigma,\mathbf{k}} \psi^{\dagger}_{\sigma,\mathbf{k}} \mathcal{H}_{\mathbf{k}} \psi_{\sigma,\mathbf{k}}$$

$$\mathcal{H}_{\mathbf{k}} = \begin{pmatrix} V/2 & -t\ s_{\mathbf{k}} & 0 & -t_{\perp} \\ -t\ s^*_{\mathbf{k}} & V/2 & 0 & 0 \\ 0 & 0 & -V/2 & -t\ s_{\mathbf{k}} \\ -t_{\perp} & 0 & -t\ s^*_{\mathbf{k}} & -V/2 \end{pmatrix} \qquad \psi_{\sigma,\mathbf{k}} = \begin{pmatrix} a_{1,\sigma,\mathbf{k}} \\ b_{1,\sigma,\mathbf{k}} \\ a_{2,\sigma,\mathbf{k}} \\ b_{2,\sigma,\mathbf{k}} \end{pmatrix}$$

4-component spinor

$$s_{\mathbf{k}} = 1 + e^{i\mathbf{k}\cdot\mathbf{a}_1} + e^{i\mathbf{k}\cdot\mathbf{a}_2} \qquad \epsilon_{\mathbf{k}} = \pm t|s_{\mathbf{k}}|$$

single layer graphene dispersion

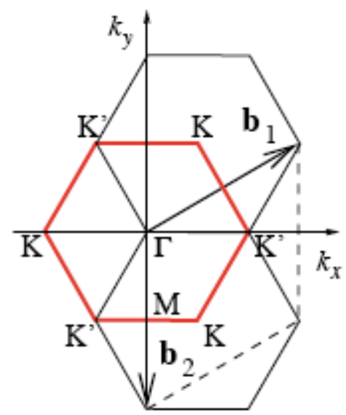
$$E^{\pm\pm}_{\mathbf{k}}(V) = \pm\sqrt{\epsilon^2_{\mathbf{k}} + \frac{t^2_{\perp}}{2} + \frac{V^2}{4} \pm \sqrt{\frac{t^4_{\perp}}{4} + (t^2_{\perp} + V^2)\epsilon^2_{\mathbf{k}}}}$$

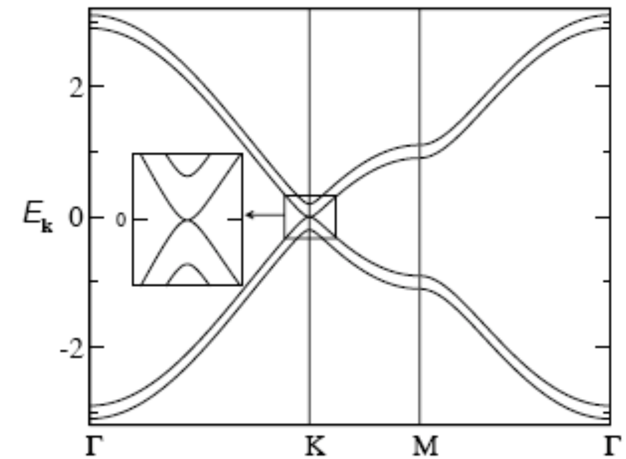
4 bands

Energy disperison for V=0

$$E_{\mathbf{k}}^{\pm\pm} = \pm\frac{t_\perp}{2} \pm \sqrt{\epsilon_{\mathbf{k}}^2 + \frac{t_\perp^2}{4}}$$

Conduction (+) and valence (-) bands touch at the corners of the BZ, the K and K' points





Undoped Bilayer graphene has one electron per p-orbital

Fermi energy crosses at the K and K' points

Gapless semiconductor

Fermi see: K and K' inequivalent points

$$p = \hbar k$$

parabolic dispersion

$$E^{\pm\pm} \approx \pm\frac{t_\perp}{2} \pm \left(\frac{v_F^2 p^2}{t_\perp} + \frac{t_\perp}{2}\right)$$

expanding at

$$a\mathbf{K}' = (4\pi/3, 0) = -a\mathbf{K}$$

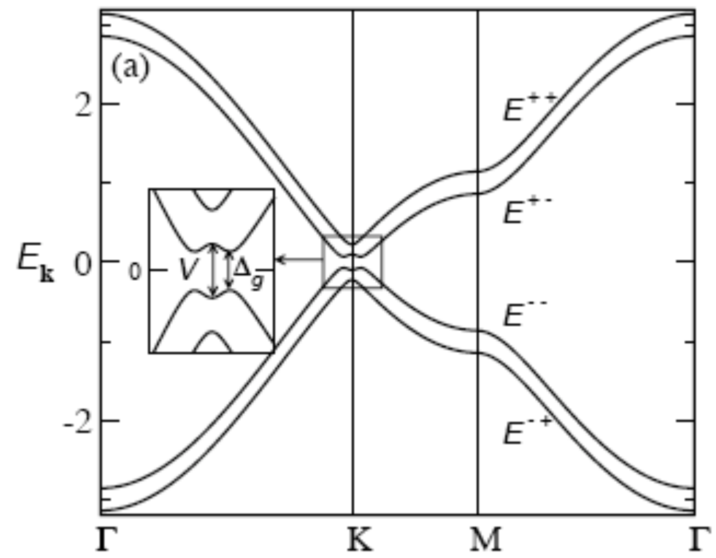
effective mass

$$m^* = \frac{t_\perp}{2v_F^2} \approx 0.03 m_e$$

Energy disperison for V

Gap: semiconductor

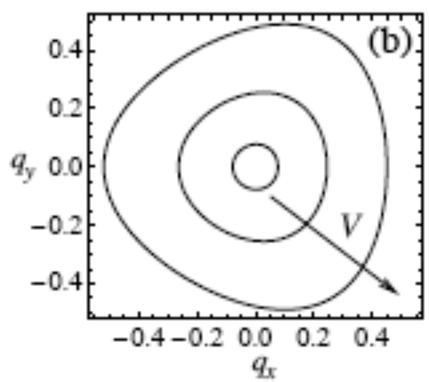
$$E_{\mathbf{k}}^{\pm\pm}(V) = \pm\sqrt{\epsilon_{\mathbf{k}}^2 + \frac{t_\perp^2}{2} + \frac{V^2}{4} \pm \sqrt{\frac{t_\perp^4}{4} + (t_\perp^2 + V^2)\epsilon_{\mathbf{k}}^2}}$$



A **tunable** gap opens between the conduction and valence band

Fermi see no longer a point

for $V < t_\perp$ Fermi see a ring



Trigonal distortion originating from single layer dispersiojn

$v_F p \ll V \ll t_\perp$ $$E^{\pm-}(V) \approx \pm\frac{V}{2} \mp \frac{V v_F^2}{t_\perp^2} p^2 \pm \frac{v_F^4}{t_\perp^2 V} p^4$$ Mexican hat: Fermi ring

$V \ll v_F p \ll t_\perp$ $$E^{\pm-}(V) \approx \pm\sqrt{\frac{V^2}{4} + \frac{v_F^4}{t_\perp^2} p^4}$$ Eigenvalues effective two-band Hamiltonian

Low energy physics

Near the K point linear expansion of $\epsilon_{\mathbf{k}} \approx v_F \hbar (k_x - i k_y) \equiv v_F p e^{-i\varphi_{\mathbf{p}}}$

$$\mathcal{H}_K = \begin{pmatrix} V/2 & v_F p e^{-i\varphi_{\mathbf{p}}} & 0 & -t_\perp \\ v_F p e^{i\varphi_{\mathbf{p}}} & V/2 & 0 & 0 \\ 0 & 0 & -V/2 & v_F p e^{-i\varphi_{\mathbf{p}}} \\ -t_\perp & 0 & v_F p e^{i\varphi_{\mathbf{p}}} & -V/2 \end{pmatrix} \qquad \mathcal{H}_{K'} = \mathcal{H}_K^*$$

Bloch's Theorem: $E_n(-i\nabla)\psi_{n,\mathbf{k}}(\mathbf{r}) = E_{n,\mathbf{k}}\psi_{n,\mathbf{k}}(\mathbf{r})$

$$\pi = p_x + i p_y$$
$$p = -i\hbar\nabla - e\mathbf{A}$$
$$B = \mathrm{rot}\mathbf{A}$$
$$[\pi, \pi^\dagger] = 2\hbar e B$$

$$\mathcal{H} = \xi \begin{pmatrix} V/2 & 0 & 0 & v_F \pi^\dagger \\ 0 & -V/2 & v_F \pi & 0 \\ 0 & v_F \pi^\dagger & -V/2 & \xi t_\perp \\ v_F \pi & 0 & \xi t_\perp & V/2 \end{pmatrix}$$

ξ valley

at K point $\xi = 1$ $\begin{bmatrix} A1 \\ B2 \\ A2 \\ B1 \end{bmatrix}$

at K' point $\xi = -1$ $\begin{bmatrix} B2 \\ A1 \\ B1 \\ A2 \end{bmatrix}$

Effective two-band Hamiltonian

$$\mathcal{H} = \begin{pmatrix} H_{11} & H_{22} \\ H_{21} & H_{22} \end{pmatrix}$$

$$H_{11} = \xi \frac{V}{2} \sigma_z$$

$$H_{22} = -\xi \frac{V}{2} \sigma_z + t_\perp \sigma_x$$

$$H_{12} = H_{21} = \xi v_F (p_x \sigma_x + p_y \sigma_y)$$

$$v_F p, V \ll t_\perp$$

$$||H_{22}|| \gg ||H_{11}||, ||H_{12}||$$

we want to find an effective description of the dynamics of the subspace of H_{11}

Introduce the Green function $G = (\mathcal{H} - E)^{-1}$

$$G = \begin{pmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{pmatrix} = \begin{pmatrix} G_{11}^{(0)-1} & H_{12} \\ H_{21} & G_{22}^{(0)-1} \end{pmatrix}^{-1} \qquad G_{ii}^{(0)} = (H_{ii} - E)^{-1}$$

Asking that $GG^{-1} = G(\mathcal{H} - E) = 1$

we obtain $G_{11}^{-1} + E = H_{11} - H_{12} G_{22}^{(0)} H_{21}$

for $|E| \ll t_\perp \quad G_{22}^{(0)} \approx H_{22}^{-1}$

$$\mathcal{H}_{\text{eff}} = H_{11} - H_{12} H_{22}^{-1} H_{21}$$

Effective Hamiltonian

$$\mathcal{H}_{\text{eff}} = -\frac{1}{2m}\begin{pmatrix} 0 & (\pi^\dagger)^2 \\ \pi^2 & 0 \end{pmatrix} + \xi V\left[\frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - \frac{v_F^2}{t_\perp^2}\begin{pmatrix} \pi^\dagger\pi & 0 \\ 0 & -\pi\pi^\dagger \end{pmatrix}\right]$$

$\xi = 1$ involves $\begin{bmatrix} A1 \\ B2 \end{bmatrix}$

$\xi = -1$ involves $\begin{bmatrix} B2 \\ A1 \end{bmatrix}$

$$\pi = p_x + ip_y$$

$$\mathbf{p} = -i\hbar\nabla - e\mathbf{A}$$

$$m = \frac{t_\perp}{2v_F^2}$$

$V = 0$ $\quad E^\pm(p) = \pm\frac{p^2}{2m}$ $\quad \psi_\pm = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{-i\varphi} \\ \pm e^{i\varphi} \end{pmatrix}$

$V \neq 0$ $\quad E^\pm(p) = \pm\sqrt{\left(\frac{p^2}{2m}\right)^2 + \frac{V^2}{4}\left(\frac{p^2}{mt_\perp} - 1\right)^2}$

Chirality and Berry phase

$$H_1 = \xi v_F \begin{pmatrix} 0 & \pi^\dagger \\ \pi & 0 \end{pmatrix} \qquad H_2 = -\frac{1}{2m} \begin{pmatrix} 0 & (\pi^\dagger)^2 \\ \pi^2 & 0 \end{pmatrix}$$

Family of Hamiltonians which are chiral in the sublattice space

$$H_J = \xi^J f(|p|)\boldsymbol{\sigma} \cdot \mathbf{n}$$

$$\mathbf{n} = \mathbf{e}_x \cos(J\varphi) + \mathbf{e}_y \sin(J\varphi)$$
$$\mathbf{p}/p = (\cos(\varphi), \sin(\varphi))$$
$$\pi = pe^{i\varphi}$$

degree of chirality:
J=1 monolayer
J=2 bilayer

$$\Sigma = \frac{1}{2}\boldsymbol{\sigma} \cdot \frac{\mathbf{p}}{|\mathbf{p}|}$$

Chirality operator (elicity)

Berry phase: propagation along a closed orbit $J\pi$

monolayer π

bilayer 2π

Due to inverted definition of sublattice component → Quasiparticle in different valley have opposite chirality $\xi = \pm 1$