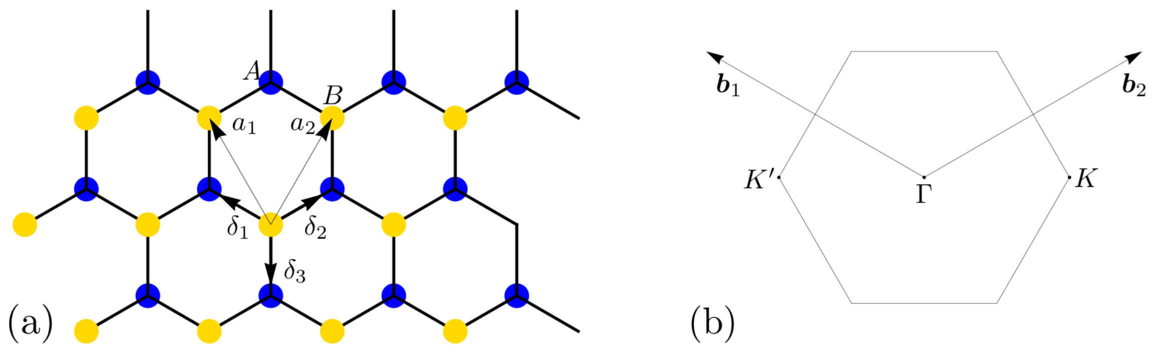
Single-layer graphene

1. Graphene's band structure



$$\vec{a}_1 = a\left(-\frac{\sqrt{3}}{2}, \frac{3}{2}\right), \quad \vec{a}_2 = a\left(\frac{\sqrt{3}}{2}, \frac{3}{2}\right), \quad a = 1.42\,\text{Å}$$

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

$$\vec{b}_1 = \frac{2\pi}{3a}(-\sqrt{3}, 1), \quad \vec{b}_2 = \frac{2\pi}{3a}(\sqrt{3}, 1)$$

$$\vec{a}_1 \cdot \vec{b}_1 = \frac{2\pi}{3}\left(\frac{3}{2} + \frac{3}{2}\right) = 2\pi, \quad \vec{a}_2 \cdot \vec{b}_2 = \frac{2\pi}{3}\left(\frac{3}{2} + \frac{3}{2}\right) = 2\pi$$

$$K_\tau = \left(\tau \frac{4\pi}{3\sqrt{3}a}, 0\right), \quad \tau = \pm 1$$

A minimum tight-binding model can be written as

$$H = -t \sum_{\langle i,j \rangle} a_i^\dagger b_j + h.c.,$$

where $a_j^\dagger, b_j^\dagger$ creates an electron on the j-th lattice site in the A and B sublattice, respectively. The symbol $\langle i,j \rangle$ indicates that summations over i, j are limited to NN only.

We introduce the Fourier transformation

$$\begin{cases} a_i = \dfrac{1}{\sqrt{N}} \displaystyle\sum_{\vec{k}} e^{i\vec{k}\cdot\vec{R}_i} a_{\vec{k}} \\ b_j = \dfrac{1}{\sqrt{N}} \displaystyle\sum_{\vec{p}} e^{i\vec{p}\cdot\vec{R}_j} b_{\vec{p}} \end{cases}$$

and the orthogonal relation $\frac{1}{N}\sum_i e^{i(\vec{k}-\vec{p})\cdot\vec{R}_i} = \delta_{\vec{k},\vec{p}}$.

$$\Rightarrow H = -\frac{t}{N} \sum_{\langle i,j \rangle} \sum_{\vec{k},\vec{p}} e^{-i\vec{k}\cdot\vec{R}_i} e^{i\vec{p}\cdot\vec{R}_j} a_{\vec{k}}^\dagger b_{\vec{p}} + h.c.$$

$$= -\frac{t}{N} \sum_j \sum_{\vec{k},\vec{p}} \left[a_{\vec{k}}^\dagger b_{\vec{p}} e^{i(\vec{p}-\vec{k})\cdot\vec{R}_j} \left(e^{-i\vec{k}\cdot\vec{\delta}_1} + e^{-i\vec{k}\cdot\vec{\delta}_2} + e^{-i\vec{k}\cdot\vec{\delta}_3}\right) + h.c. \right]$$

$$= -t \sum_{\vec{k}} \left[a^{+}_{\vec{k}} b_{\vec{k}} f(\vec{k}) + h.c. \right]$$

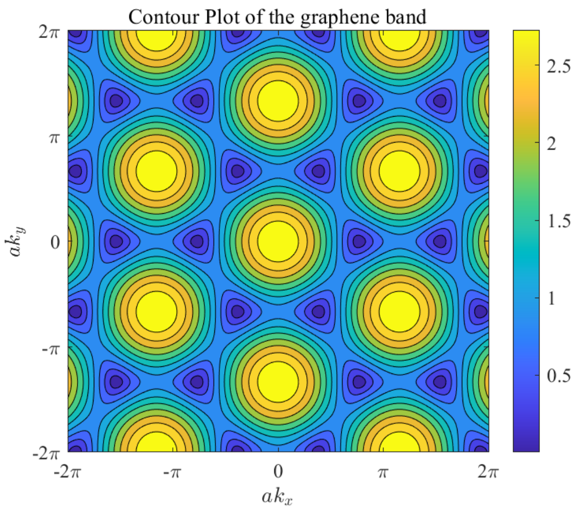
where $\quad f(\vec{k}) = e^{-i\vec{k}\cdot\vec{\delta}_1} + e^{-i\vec{k}\cdot\vec{\delta}_2} + e^{-i\vec{k}\cdot\vec{\delta}_3}$.

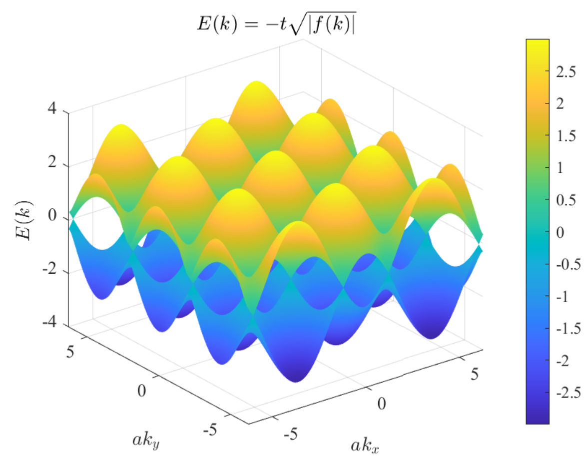
$$H = -t \sum_{\vec{k}} (a^{+}_{\vec{k}}, b^{+}_{\vec{k}}) \begin{pmatrix} 0 & f(\vec{k}) \\ f^{*}(\vec{k}) & 0 \end{pmatrix} \begin{pmatrix} a_{\vec{k}} \\ b_{\vec{k}} \end{pmatrix}$$

$$\equiv \sum_{\vec{k}} (a^{+}_{\vec{k}}, b^{+}_{\vec{k}})\, h(\vec{k}) \begin{pmatrix} a_{\vec{k}} \\ b_{\vec{k}} \end{pmatrix}, \quad \text{where} \quad h(\vec{k}) = -t \begin{pmatrix} 0 & f(\vec{k}) \\ f^{*}(\vec{k}) & 0 \end{pmatrix}.$$

$$E(\vec{k}) = \pm t\, |f(\vec{k})|$$

$$= \pm t \left[3 + 2\cos(\sqrt{3}\, a k_x) + 4\cos\left(\tfrac{\sqrt{3}}{2} a k_x\right) \cos\left(\tfrac{3}{2} a k_y\right) \right]^{\frac{1}{2}}$$





A linear dispersion at low energies

We expand $f(\vec{k})$ near the valleys as follows:

$$f(\vec{K}_\tau + \vec{k}) = e^{-i\vec{k}\cdot\vec{\delta}_1} e^{-i\vec{K}_\tau\cdot\vec{\delta}_1} + e^{-i\vec{k}\cdot\vec{\delta}_2} e^{-i\vec{K}_\tau\cdot\vec{\delta}_2} + e^{-i\vec{k}\cdot\vec{\delta}_3} e^{-i\vec{K}_\tau\cdot\vec{\delta}_3}$$

$$= e^{-i\vec{k}\cdot\vec{\delta}_1} e^{i2\pi\tau/3} + e^{-i\vec{k}\cdot\vec{\delta}_2} e^{-i2\pi\tau/3} + e^{-i\vec{k}\cdot\vec{\delta}_3},$$

where both ak_x, ak_y are assumed to be small. Thus we have

$$f(\vec{K}_\tau + \vec{k}) \cong (1 + e^{i2\pi\tau/3} + e^{-i2\pi\tau/3}) + (-i\vec{k})\cdot(\vec{\delta}_1 e^{i2\pi\tau/3} + \vec{\delta}_2 e^{-i2\pi\tau/3} + \vec{\delta}_3)$$

$$= 0 - i\vec{k}\cdot\left[-\tfrac{3a}{2}(i\tau, 1)\right] = -\tfrac{3a}{2}(\tau k_x - i k_y)$$

We define a Fermi velocity v_F s.t. $\hbar v_F = \frac{3at}{2}$.

The low-energy Hamiltonian is then

$$h(\vec{K}_\tau + \vec{k}) = -t\begin{pmatrix} 0 & f(\vec{K}_\tau + \vec{k}) \\ f^*(\vec{K}_\tau + \vec{k}) & 0 \end{pmatrix} \simeq \hbar v_F \begin{pmatrix} 0 & \tau k_x - ik_y \\ \tau k_x + ik_y & 0 \end{pmatrix}$$

2. Haldane's graphene model

$$H_{Haldane} = H_1 + H_2 + H_M, \text{ where}$$

$$H_1 = -t_1 \sum_{\langle i,j \rangle} (a_i^\dagger b_j + h.c.)$$

$$H_2 = -t_2 \sum_{\langle\langle i,j \rangle\rangle} \left[e^{i\phi \nu_{ij}} (a_i^\dagger a_j + b_i^\dagger b_j) + h.c. \right]$$

$$H_M = M \sum_i (a_i^\dagger a_i - b_i^\dagger b_i), \quad M > 0 \text{ WLOG}.$$

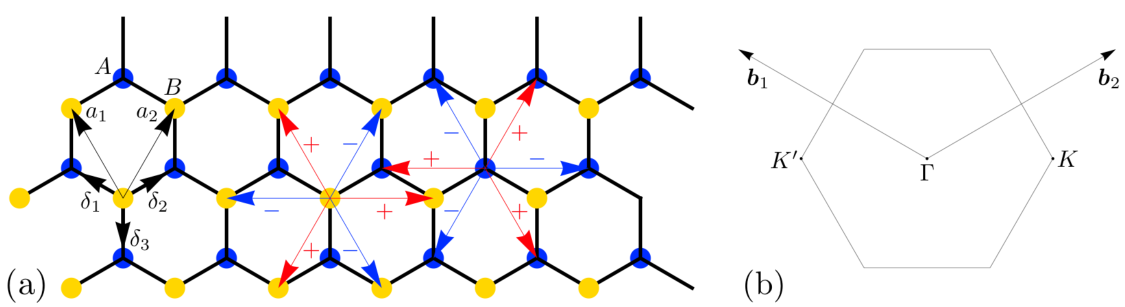
Again, we take the Fourier transformation $\begin{cases} a_i = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{R}_i} a_{\vec{k}} \\ b_i = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{R}_i} b_{\vec{k}} \end{cases}$

$$H_1 = \sum_{\vec{k}} (a_{\vec{k}}^\dagger \quad b_{\vec{k}}^\dagger) \begin{pmatrix} 0 & f(\vec{k}) \\ f^*(\vec{k}) & 0 \end{pmatrix} \begin{pmatrix} a_{\vec{k}} \\ b_{\vec{k}} \end{pmatrix}$$

$\hookrightarrow f(\vec{k}) = -t_1 \left(e^{-i\vec{k}\cdot\vec{\delta}_1} + e^{-i\vec{k}\cdot\vec{\delta}_2} + e^{-i\vec{k}\cdot\vec{\delta}_3} \right)$

$\nu_{ij} = 1$: $\vec{R}_i + \vec{a}_1$, $\vec{R}_i - \vec{a}_2$, $\vec{R}_i - \vec{a}_1 + \vec{a}_2$

$\nu_{ij} = -1$: $\vec{R}_i - \vec{a}_1$, $\vec{R}_i + \vec{a}_2$, $\vec{R}_i + \vec{a}_1 - \vec{a}_2$



Explicitly, we have

$$H_2 = -t_2 \sum_i \Big[e^{i\phi} \left(b^\dagger_{i-\vec{a}_1+\vec{a}_2} b_i + b^\dagger_{i-\vec{a}_2} b_i + b^\dagger_{i+\vec{a}_1} b_i \right) + e^{-i\phi} \left(b^\dagger_{i+\vec{a}_1-\vec{a}_2} b_i + b^\dagger_{i+\vec{a}_2} b_i + b^\dagger_{i-\vec{a}_1} b_i \right) \Big]$$

$$- t_2 \sum_i \Big[e^{i\phi} \left(a^\dagger_{i+\vec{a}_1-\vec{a}_2} a_i + a^\dagger_{i+\vec{a}_2} a_i + a^\dagger_{i-\vec{a}_1} a_i \right) + e^{-i\phi} \left(a^\dagger_{i-\vec{a}_1+\vec{a}_2} a_i + a^\dagger_{i-\vec{a}_2} a_i + a^\dagger_{i+\vec{a}_1} a_i \right) \Big]$$

$$H_2 = \sum_k \begin{pmatrix} a^\dagger_{\vec{k}} & b^\dagger_{\vec{k}} \end{pmatrix} \begin{pmatrix} \epsilon_A(\vec{k}) & 0 \\ 0 & \epsilon_B(\vec{k}) \end{pmatrix} \begin{pmatrix} a_{\vec{k}} \\ b_{\vec{k}} \end{pmatrix}$$

where
$$\begin{cases} \epsilon_A(\vec{k}) = -2t_2 \left[\cos[\vec{k}\cdot(\vec{a}_1-\vec{a}_2) - \phi] + \cos(\vec{k}\cdot\vec{a}_2 - \phi) + \cos(\vec{k}\cdot\vec{a}_1 + \phi) \right] \\ \epsilon_B(\vec{k}) = -2t_2 \left[\cos[\vec{k}\cdot(\vec{a}_1-\vec{a}_2) + \phi] + \cos(\vec{k}\cdot\vec{a}_2 + \phi) + \cos(\vec{k}\cdot\vec{a}_1 - \phi) \right] \end{cases}$$

$$H_{Haldane} = \sum_{\vec{k}} \begin{pmatrix} a^\dagger_{\vec{k}} & b^\dagger_{\vec{k}} \end{pmatrix} \mathcal{H}_{Haldane}(\vec{k}) \begin{pmatrix} a_{\vec{k}} \\ b_{\vec{k}} \end{pmatrix}$$, where

$$\mathcal{H}_{Haldane}(\vec{k}) = \begin{pmatrix} \epsilon_A(\vec{k}) + M & f(\vec{k}) \\ f^*(\vec{k}) & \epsilon_B(\vec{k}) - M \end{pmatrix}$$

$$= h_0(\vec{k})\,\mathbb{1} + h_x(\vec{k})\,\sigma_x + h_y(\vec{k})\,\sigma_y + h_z(\vec{k})\,\sigma_z$$, where

$$h_x(\vec{k}) = -t_1 \left[\cos(\vec{k}\cdot\vec{\delta}_1) + \cos(\vec{k}\cdot\vec{\delta}_2) + \cos(\vec{k}\cdot\vec{\delta}_3) \right]$$

$$h_y(\vec{k}) = -t_1 \left[\sin(\vec{k}\cdot\vec{\delta}_1) + \sin(\vec{k}\cdot\vec{\delta}_2) + \sin(\vec{k}\cdot\vec{\delta}_3) \right]$$

$$h_0(\vec{k}) = \frac{\epsilon_A(\vec{k}) + \epsilon_B(\vec{k})}{2}$$

$$= -2t_2 \cos(\phi) \left[\cos[\vec{k}\cdot(\vec{a}_1-\vec{a}_2)] + \cos(\vec{k}\cdot\vec{a}_2) + \cos(\vec{k}\cdot\vec{a}_1) \right]$$

$$h_z(\vec{k}) = \frac{\epsilon_A(\vec{k}) - \epsilon_B(\vec{k})}{2} + M$$

$$= M - 2t_2 \sin(\phi) \left[\sin[\vec{k}\cdot(\vec{a}_1-\vec{a}_2)] + \sin(\vec{k}\cdot\vec{a}_2) - \sin(\vec{k}\cdot\vec{a}_1) \right]$$

Symmetry analysis

1. Always respects the C_3 rotational symmetry.

$$\vec{\delta}_1 \longrightarrow \vec{\delta}_2 \longrightarrow \vec{\delta}_3 \longrightarrow \vec{\delta}_1$$

2. The system has no time-reversal symmetry unless $\phi = 0, \pi$.
3. Respects inversion symmetry only when $M = 0$

Low energy Hamiltonian near valleys

$$H_{eff} = 3t_2 \cos\phi + \hbar v (\tau k_x \sigma_x + k_y \sigma_y) + \Delta_z^\tau \sigma_z$$

where $\Delta_z^\tau = M - 3\sqrt{3}\, t_2 \tau \sin\phi$

$$\Longrightarrow E_{gap}^\tau = 2\,|\Delta_z^\tau| = 2\,\left|M - 3\sqrt{3}\, t_2 \tau \sin\phi\right|$$

3. Berry curvature, Chern number

$$\sigma_{xy} = \frac{e^2}{h} \int \frac{d^2\vec{k}}{2\pi} F_{xy}(\vec{k})$$

$$\hookrightarrow = \frac{\partial \vec{A}_y(\vec{k})}{\partial k_x} - \frac{\partial \vec{A}_x(\vec{k})}{\partial k_y} \quad \text{Berry curvature}$$

$$\vec{A}_\alpha(\vec{k}) = \sum_{n \in \text{filled bands}} \langle n\vec{k} | \, i \frac{\partial}{\partial k_\alpha} | n\vec{k} \rangle \, , \quad \alpha = x, y \quad \text{Berry connection}$$

$$C = \int_{BZ} \frac{d^2\vec{k}}{2\pi} F_{xy}(\vec{k}) \quad \text{Chern number}$$

Twisted bilayer graphene

We start with a Bernal stacking, then rotate the second layer by θ and finally translate it by $\vec{\tau}$. This way, each layer is described by the lattice

$$\vec{R}^{(1)}_{n_1,n_2} = n_1 \vec{a}_1 + n_2 \vec{a}_2$$

$$\vec{R}^{(2)}_{n_1,n_2} = R_\theta (n_1 \vec{a}_1 + n_2 \vec{a}_2 - \vec{\delta}) + \vec{\tau}$$

$$\hookrightarrow \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

$$\Rightarrow \vec{R}^{(2)}_{n_1,n_2} = R_\theta (\vec{R}^{(1)}_{n_1,n_2} - \vec{\delta}) + \vec{\tau}$$

Moiré pattern

$$\vec{G}^m : \quad \vec{b}_1^m = \vec{b}_1 - \vec{b}_1^\theta , \quad \vec{b}_2^m = \vec{b}_2 - \vec{b}_2^\theta$$

$$\vec{R}^m : \quad \vec{a}_i^m \cdot \vec{b}_j^m = 2\pi \delta_{ij}$$

Rotated Dirac Hamiltonian

$$H^{\pm K}_{SLG} (\vec{q},\theta) = \pm \hbar v_F |\vec{q}| \begin{pmatrix} 0 & e^{\mp i(\theta_{\vec{q}} + \theta)} \\ e^{\pm i(\theta_{\vec{q}} + \theta)} & 0 \end{pmatrix}$$

Interlayer hopping term

$$T^{\alpha,\beta}_{\vec{k},\vec{k}'} = \langle \psi^{(1)}_{\vec{k},\alpha} | H_\perp | \psi^{(2)}_{\vec{k}',\beta} \rangle$$

describes a process where an electron with momentum $\vec{k}'$ in layer 2, sublattice β, hops to a momentum state $\vec{k}$ in layer 1, sublattice α.

In the tight-binding approximation, we have

$$\begin{cases} |\psi^{(1)}_{\vec{k},\alpha}\rangle = \dfrac{1}{\sqrt{N_1 N_2}} \displaystyle\sum_{n_1,n_2} e^{i\vec{k}(\vec{R}^{(1)}_{n_1,n_2} + \vec{\delta}^{(1)}_\alpha)} \; |\vec{R}^{(1)}_{n_1,n_2} + \vec{\delta}^{(1)}_\alpha, \alpha\rangle \\ |\psi^{(2)}_{\vec{k}',\beta}\rangle = \dfrac{1}{\sqrt{N_1 N_2}} \displaystyle\sum_{n_1,n_2} e^{i\vec{k}'\cdot(\vec{R}^{(2)}_{n_1,n_2} + \vec{\delta}^{(2)}_\beta)} \; |\vec{R}^{(2)}_{n_1,n_2} + \vec{\delta}^{(2)}_\beta, \beta\rangle \end{cases}$$

where $\vec{\delta}^{(1)}_\alpha = \vec{\delta}_\alpha$, $\vec{\delta}^{(2)}_\beta = \vec{\delta}^\theta_\beta$.

$$T^{\alpha,\beta}_{\vec{k}+\vec{q}_1,\, \vec{k}^\theta+\vec{q}_2^\theta} = \frac{1}{N_1 N_2} \sum_{n_1,n_2} \sum_{n_1',n_2'} e^{-i(\vec{k}+\vec{q}_1)\cdot(\vec{R}^{(1)}_{n_1,n_2} + \vec{\delta}^{(1)}_\alpha)} e^{i(\vec{k}^\theta + \vec{q}_2^\theta)\cdot(\vec{R}^{(2)}_{n_1',n_2'} + \vec{\delta}^{(2)}_\beta)}$$

$$\times \langle \vec{R}^{(1)}_{n_1,n_2} + \vec{\delta}^{(1)}_\alpha, \alpha | H_\perp | \vec{R}^{(2)}_{n_1',n_2'} + \vec{\delta}^{(2)}_\beta, \beta\rangle$$

$$= \frac{1}{N_1 N_2} \sum_{n_1,n_2} \sum_{n_1',n_2'} e^{-i(\vec{k}+\vec{q}_1)\cdot(\vec{R}_{n_1,n_2} + \vec{\delta}_\alpha)} e^{i(\vec{k}^\theta + \vec{q}_2^\theta)\cdot(\vec{R}^\theta_{n_1',n_2'} - \vec{\delta}^\theta + \vec{\tau} + \vec{\delta}^\theta_\beta)}$$

$$\times t_\perp(\vec{R}_{n_1,n_2} - \vec{R}^\theta_{n_1',n_2'} + \vec{\delta}_\alpha - \vec{\delta}^\theta_\beta + \vec{\delta}^\theta - \vec{\tau})$$

FT to $t_\perp$:

$$t_\perp(\vec{R}_{n_1,n_2} - \vec{R}^\theta_{n_1',n_2'} + \vec{\delta}_\alpha - \vec{\delta}^\theta_\beta + \vec{\delta}^\theta - \vec{\tau}) = \int_{\mathbb{R}^2} \frac{d\vec{k}}{(2\pi)^2} t_\perp(\vec{k}) e^{i\vec{k}\cdot(\vec{R}_{n_1,n_2} - \vec{R}^\theta_{n_1',n_2'} + \vec{\delta}_\alpha - \vec{\delta}^\theta_\beta + \vec{\delta}^\theta - \vec{\tau})}$$

Use $\displaystyle\sum_{\vec{k}} \longrightarrow \frac{A_{total}}{(2\pi)^2} \int_{\mathbb{R}^2} d\vec{k}$

$\Longrightarrow$

$$T^{\alpha,\beta}_{\vec{k}+\vec{q}_1,\, \vec{k}^\theta+\vec{q}_2^\theta} = \frac{1}{(N_1 N_2)^2} \sum_{n_1,n_2} \sum_{n_1',n_2'} \sum_{\vec{k}} e^{i[\vec{k} - (\vec{k}+\vec{q}_1)]\cdot\vec{R}_{n_1,n_2}} e^{i[(\vec{k}^\theta + \vec{q}_2^\theta) - \vec{k}]\cdot\vec{R}^\theta_{n_1',n_2'}}$$

$$\times e^{i[\vec{k} - (\vec{k}+\vec{q}_1)]\cdot\vec{\delta}_\alpha} e^{i[(\vec{k}^\theta + \vec{q}_2^\theta) - \vec{k}]\cdot(\vec{\delta}^\theta_\beta - \vec{\delta}^\theta + \vec{\tau})} \; \frac{t_\perp(\vec{k})}{A_{u.c.}}$$

Now, use the orthogonality relations :

$$\sum_{n_1,n_2} e^{i[\vec{k}-(\vec{K}+\vec{q}_1)]\cdot\vec{R}_{n_1,n_2}} = \begin{cases} N_1 N_2 & \text{if } \vec{k}-(\vec{K}+\vec{q}_1) = G^{(1)}_{k,l} = G_{k,l}, \ \forall k,l \\ 0 & \text{otherwise} \end{cases}$$

$$\sum_{n_1',n_2'} e^{i[(\vec{K}^\theta+\vec{q}_2^{\,\theta})-\vec{k}]\cdot\vec{R}^\theta_{n_1',n_2'}} = \begin{cases} N_1 N_2 & \text{if } \vec{k}-(\vec{K}^\theta+\vec{q}_2^{\,\theta}) = G^{(2)}_{m,n} = G^\theta_{m,n} \ \forall m,n \\ 0 & \text{otherwise} \end{cases}$$

which implies

$$\vec{k} = \vec{K}+\vec{q}_1+\vec{G}_{k,l} = \vec{K}^\theta+\vec{q}_2^{\,\theta}+\vec{G}^\theta_{m,n}$$

$$\Longrightarrow$$

$$T^{\alpha,\beta}_{\vec{K}+\vec{q}_1,\vec{K}^\theta+\vec{q}_2^{\,\theta}} = \sum_{k,l,m,n} \frac{t_\perp(\vec{K}+\vec{q}_1+G_{k,l})}{A_{u.c.}} e^{i[\vec{G}_{k,l}\vec{\delta}_\alpha-\vec{G}_{m,n}(\vec{\delta}_\beta-\vec{\delta})-\vec{G}^\theta_{m,n}\cdot\vec{\tau}]}$$

$$\times\ \delta_{\vec{K}+\vec{q}_1+\vec{G}_{k,l},\ \vec{K}^\theta+\vec{q}_2^{\,\theta}+\vec{G}^\theta_{m,n}}$$

$$\simeq \frac{t_\perp(\vec{K})}{A_{u.c.}}\sum_{m,n}\Big[e^{-i[\vec{G}_{m,n}\cdot(\vec{\delta}_\beta-\vec{\delta})+\vec{G}_{m,n}\cdot\vec{\tau}]}\,\delta_{\vec{K}+\vec{q}_1,\ \vec{K}^\theta+\vec{q}_2^{\,\theta}+\vec{G}^\theta_{m,n}}$$

$\boxed{\vec{G}=0,\vec{b}_2,-\vec{b}_1}$

$$+ e^{i[\vec{b}_2\cdot\vec{\delta}_\alpha-\vec{G}_{m,n}(\vec{\delta}_\beta-\vec{\delta})-\vec{G}^\theta_{m,n}\cdot\vec{\tau}]}\,\delta_{\vec{K}+\vec{q}_1+\vec{b}_2,\ \vec{K}^\theta+\vec{q}_2^{\,\theta}+\vec{G}^\theta_{m,n}}$$

$$+ e^{-i[\vec{b}_1\cdot\vec{\delta}_\alpha+\vec{G}_{m,n}(\vec{\delta}_\beta-\vec{\delta})+\vec{G}^\theta_{m,n}\cdot\vec{\tau}]}\,\delta_{\vec{K}+\vec{q}_1-\vec{b}_1,\ \vec{K}^\theta+\vec{q}_2^{\,\theta}+\vec{G}^\theta_{m,n}}\Big]$$

$$= \frac{t_\perp(\vec{K})}{A_{u.c.}}\Big[\delta_{\vec{K}+\vec{q}_1,\ \vec{K}^\theta+\vec{q}_2^{\,\theta}} + e^{i[\vec{b}_2\cdot(\vec{\delta}_\alpha-\vec{\delta}_\beta+\vec{\delta})-\vec{b}_2^\theta\cdot\tau]}\,\delta_{\vec{K}+\vec{q}_1+\vec{b}_2,\ \vec{K}^\theta+\vec{q}_2^{\,\theta}+\vec{b}_2^\theta}$$

$$+ e^{-i[\vec{b}_1\cdot(\vec{\delta}_\alpha-\vec{\delta}_\beta+\vec{\delta})-\vec{b}_1^\theta\cdot\tau]}\,\delta_{\vec{K}+\vec{q}_1-\vec{b}_1,\ \vec{K}^\theta+\vec{q}_2^{\,\theta}-\vec{b}_1^\theta}\Big]$$

In a matrix notation $T = \begin{pmatrix} T^{A,A} & T^{A,B} \\ T^{B,A} & T^{B,B} \end{pmatrix}$, we rewrite the last expression as

$$T_{\vec{K}+\vec{q}_1, \vec{K}^\theta+\vec{q}_2^\theta} = \frac{t_\perp(\vec{K})}{A_{u.c.}} \Big[T_1 \delta_{\vec{q}_2^\theta - \vec{q}_1, \vec{K}-\vec{K}^\theta} + T_2 \delta_{\vec{q}_2^\theta - \vec{q}_1, (\vec{K}+\vec{b}_2)-(\vec{K}^\theta+\vec{b}_2^\theta)}$$

$$+ T_3 \delta_{\vec{q}_2^\theta - \vec{q}_1, (\vec{K}-\vec{b}_1)-(\vec{K}^\theta-\vec{b}_1^\theta)} \Big]$$

$$= T_{\vec{q}_b} \delta_{\vec{q}_2^\theta - \vec{q}_1, \vec{q}_b} + T_{\vec{q}_{tr}} \delta_{\vec{q}_2^\theta - \vec{q}_1, \vec{q}_{tr}} + T_{\vec{q}_{tl}} \delta_{\vec{q}_2^\theta - \vec{q}_1, \vec{q}_{tl}}$$

where $T_{\vec{q}_b} = \frac{t_\perp(\vec{K})}{A_{u.c.}} T_1$, $T_{\vec{q}_{tr}} = \frac{t_\perp(\vec{K})}{A_{u.c.}} T_2$, $T_{\vec{q}_{tl}} = \frac{t_\perp(\vec{K})}{A_{u.c.}} T_3$

$$T_1 = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad T_2 = e^{-i\vec{b}_2^\theta\cdot\vec{\tau}} \begin{pmatrix} e^{i\phi} & 1 \\ e^{-i\phi} & e^{i\phi} \end{pmatrix}, \quad T_3 = e^{i\vec{b}_1^\theta\cdot\vec{\tau}} \begin{pmatrix} e^{-i\phi} & 1 \\ e^{i\phi} & e^{-i\phi} \end{pmatrix}$$

$$\phi = \frac{2\pi}{3}$$

$$\vec{q}_b = \vec{K} - \vec{K}^\theta, \quad \vec{q}_{tr} = (\vec{K}+\vec{b}_2)-(\vec{K}^\theta+\vec{b}_2^\theta), \quad \vec{q}_{tl} = (\vec{K}-\vec{b}_1)-(\vec{K}^\theta-\vec{b}_1^\theta)$$

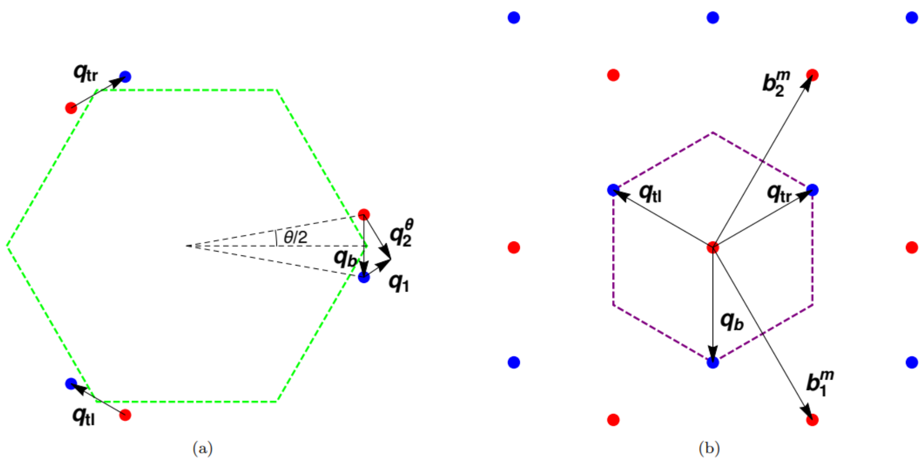


Figure 2.10: Momentum-space geometrical picture for the interlayer hopping on a tBLG. (a) The green dashed line marks the first BZ for an unrotated SLG; the red (blue) circles mark the three equivalent Dirac points K for layer 1 (2). Crystal momentum conservation is attained when $\boldsymbol{q}_2^\theta - \boldsymbol{q}_1 = \boldsymbol{q}_b, \boldsymbol{q}_{tr}, \boldsymbol{q}_{tl}$; in this reference frame, the three momentum transfers have modulus $|\boldsymbol{q}_j| = 2|\boldsymbol{K}|\sin(\theta/2)$ and directions $(0,-1)$ for $j = b$ (bottom), $(\sqrt{3}/2, 1/2)$ for $j = tr$ (top right), and $(-\sqrt{3}/2, 1/2)$ for $j = tl$ (top left). (b) The three equivalent Dirac points in the first BZ result in three distinct hopping processes in reciprocal space (matrix elements); when we capture all "orders" of hopping (possible hopping processes after previous ones), we obtain this $\boldsymbol{k}$-space honeycomb structure, which captures the periodicity of the moiré pattern. The purple dashed line marks a moiré unit cell in reciprocal space.

We move to the reference frame shown in Fig. 2.10 : $\pm \frac{\theta}{2}$ rotation .

We have

$$\vec{q}_b = \frac{8\pi \sin(\frac{\theta}{2})}{3\sqrt{3}\, d}(0,-1) \, , \quad \vec{q}_{tr} = \frac{8\pi \sin(\frac{\theta}{2})}{3\sqrt{3}\, d}\left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right)$$

$$\vec{q}_{tl} = \frac{8\pi \sin(\frac{\theta}{2})}{3\sqrt{3}\, d}\left(-\frac{\sqrt{3}}{2}, \frac{1}{2}\right)$$

$$\vec{b}_1^m = \vec{q}_b - \vec{q}_{tl} = \frac{8\pi \sin(\frac{\theta}{2})}{3d}\left(\frac{1}{2}, -\frac{\sqrt{3}}{2}\right)$$

$$\vec{b}_2^m = \vec{q}_{tr} - \vec{q}_b = \frac{8\pi \sin(\frac{\theta}{2})}{3d}\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$$

$$\vec{a}_1^m = \frac{\sqrt{3}\, d}{2\sin(\frac{\theta}{2})}\left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right), \quad \vec{a}_2^m = \frac{\sqrt{3}\, d}{2\sin(\frac{\theta}{2})}\left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right)$$

$$A_{m.u.c.} = \left|\vec{a}_1^m \times \vec{a}_2^m\right| = \frac{3\sqrt{3}\, d^2}{8\sin^2(\frac{\theta}{2})}$$

Hamiltonian matrix construction

$$H = H_1 + H_2 + H_\perp$$

In the TB-approximation, the wavefunctions read $|\psi_{\vec{k}}\rangle = \sum_{\alpha, i} C_\alpha^{(i)}(\vec{k}) |\psi_{\vec{k},\alpha}^{(i)}\rangle$

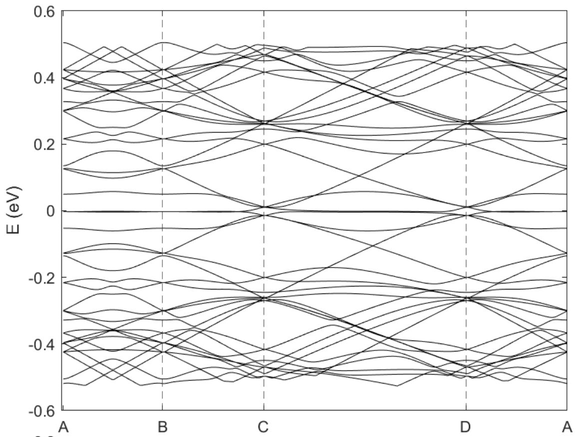
In the continuum low-energy model within a K expansion, we have

$$\langle \psi^{(1)}_{\vec{K}+\vec{q}_1, \alpha} | H_\perp | \psi^{(2)}_{\vec{K}^\theta + \vec{q}_2^\theta, \beta}\rangle = T^{\alpha,\beta}_{\vec{K}+\vec{q}_1,\, \vec{K}^\theta + \vec{q}_2^\theta}$$

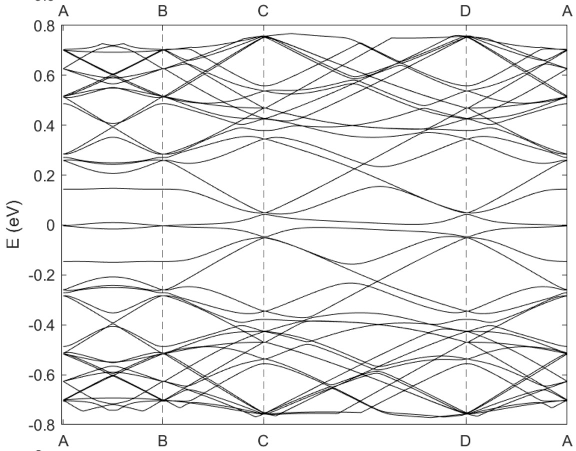
$$\langle \psi^{(1)}_{\vec{K}+\vec{q}_1, \alpha} | H_1 | \psi^{(1)}_{\vec{K}+\vec{p}_1, \beta}\rangle = H^{\alpha,\beta}_{SLG,\vec{K}}\left(\vec{q}_1, -\frac{\theta}{2}\right) \delta_{\vec{q}_1, \vec{p}_1}$$

$$\langle \psi^{(2)}_{\vec{K}+\vec{q}_1, \alpha} | H_2 | \psi^{(2)}_{\vec{K}+\vec{p}_2, \beta}\rangle = H^{\alpha,\beta}_{SLG,\vec{K}}\left(\vec{q}_2, \frac{\theta}{2}\right) \delta_{\vec{q}_2, \vec{p}_2}$$

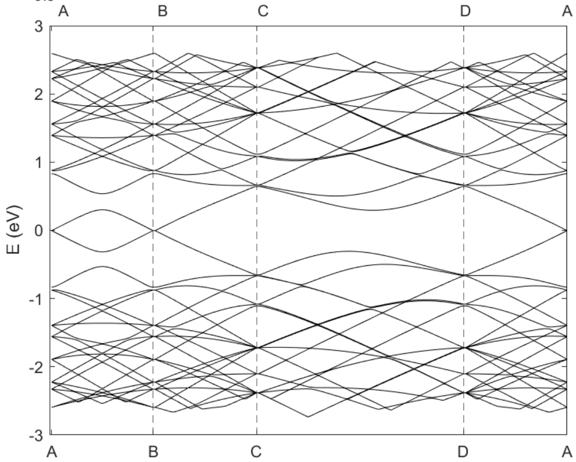
$$
\begin{array}{cccc|c}
|K+\boldsymbol{q},1\rangle & |K^{\theta}+\boldsymbol{q}+\boldsymbol{q}_b,2\rangle & |K^{\theta}+\boldsymbol{q}+\boldsymbol{q}_{tr},2\rangle & |K^{\theta}+\boldsymbol{q}+\boldsymbol{q}_{tl},2\rangle & \\
\hline
H^{K}_{SLG}(\boldsymbol{q},-\theta/2) & T_{\boldsymbol{q}_b} & T_{\boldsymbol{q}_{tr}} & T_{\boldsymbol{q}_{tl}} & \langle K+\boldsymbol{q},1| \\
T^{\dagger}_{\boldsymbol{q}_b} & H^{K}_{SLG}(\boldsymbol{q}+\boldsymbol{q}_b,\theta/2) & 0 & 0 & \langle K^{\theta}+\boldsymbol{q}+\boldsymbol{q}_b,2| \\
T^{\dagger}_{\boldsymbol{q}_{tr}} & 0 & H^{K}_{SLG}(\boldsymbol{q}+\boldsymbol{q}_{tr},\theta/2) & 0 & \langle K^{\theta}+\boldsymbol{q}+\boldsymbol{q}_{tr},2| \\
T^{\dagger}_{\boldsymbol{q}_{tl}} & 0 & 0 & H^{K}_{SLG}(\boldsymbol{q}+\boldsymbol{q}_{tl},\theta/2) & \langle K^{\theta}+\boldsymbol{q}+\boldsymbol{q}_{tl},2|
\end{array}
$$



$\theta = 1.05°$



$\theta = 1.5°$



$\theta = 5°$

Twisted $MoTe_2$ ($tMoTe_2$)

$$H_\tau = \begin{bmatrix} \dfrac{-\hbar^2(\vec{k}-\tau K_+)^2}{2m^*} + \Delta_+(\vec{r}) & \Delta_{T,\tau}(\vec{r}) \\ \Delta^\dagger_{T,\tau}(\vec{r}) & \dfrac{-\hbar^2(\vec{k}-\tau K_-)^2}{2m^*} + \Delta_-(\vec{r}) \end{bmatrix}$$

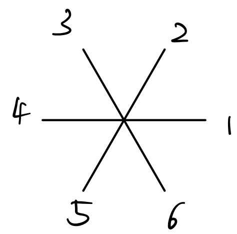
\# arXiv: 2305.01006

$$\Delta_\pm(\vec{r}) = 2V \sum_{j=1,3,5} \cos(\vec{g}_j \cdot \vec{r} \pm \psi)$$

$$\Delta_{T,\tau}(\vec{r}) = w\left(1 + e^{-i\tau \vec{g}_2\cdot\vec{r}} + e^{-i\tau\vec{g}_3\cdot\vec{r}}\right)$$

$$\vec{K}_\pm = \frac{4\pi}{3a_m}\left[-\frac{\sqrt{3}}{2}, \mp\frac{1}{2}\right], \quad \vec{g}_j = \frac{4\pi}{\sqrt{3}a_m}\left[\cos\frac{(j-1)\pi}{3}, \sin\frac{(j-1)\pi}{3}\right], j=1,\cdots,6$$

$$a_m \sim a_0/2\sin\tfrac{\theta}{2} \sim a_0/\theta$$



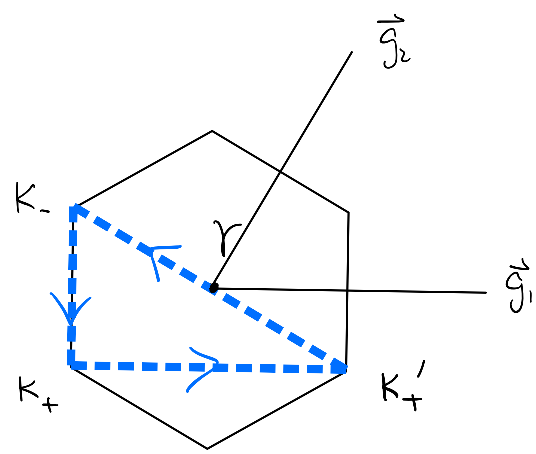
$a_0 = 3.472\,Å$, $m^* = 0.62\, m_e$

$V = 8\,meV$, $\psi = -89.6°$, $w = -8.5\,meV$

$$\Delta_\pm(\vec{r}) = V\sum_{j=1,3,5}\left(e^{i\vec{g}_j\cdot\vec{r}\pm\psi} + e^{-i\vec{g}_j\cdot\vec{r}\pm\psi}\right)$$

$$= Ve^{\pm\psi}\sum_{j=1,3,5} e^{i\vec{g}_j\cdot\vec{r}} + Ve^{\mp\psi}\sum_{j=2,4,6} e^{i\vec{g}_j\cdot\vec{r}}$$

$$\Delta_{T,\tau}(\vec{r}) = w\left(1 + e^{i\tau\vec{g}_5\cdot\vec{r}} + e^{i\tau\vec{g}_6\cdot\vec{r}}\right)$$

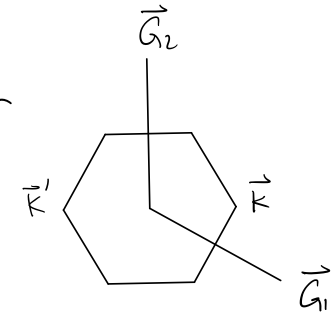


Rhombohedral Pentalayer graphene / hBN

$$H_s = \sum_s \sum_{\vec{k}\in BZ} \psi^\dagger_{\vec{k},\sigma} \left[H_{PLG}(\vec{k}) + \kappa V_{moiré}(0) \right] \psi_{\vec{k},\sigma}$$
$$+ \kappa \sum_\sigma \sum_j \sum_{\vec{k}\in BZ} \psi^\dagger_{\vec{k}+\vec{g}_j,\sigma} V_{moiré}(\vec{g}_j) \psi_{\vec{k},\sigma}$$

$$V_{moiré}(\vec{r}) = V_{moiré}(0) + \sum_j V_{moiré}(\vec{g}_j) e^{i\vec{r}\cdot\vec{g}_j}$$

$$\vec{R}_1 = a_G [1, 0]^T, \quad \vec{R}_2 = a_G \left[\tfrac{1}{2}, \tfrac{\sqrt{3}}{2}\right]^T$$
$$\vec{G}_1 = \frac{2\pi}{a_G}\left[1, -\tfrac{1}{\sqrt{3}}\right]^T, \quad \vec{G}_2 = \frac{2\pi}{a_G}\left[0, \tfrac{2}{\sqrt{3}}\right]^T$$
$$\vec{K} = -\vec{K}' = \tfrac{2}{3}\vec{G}_1 + \tfrac{1}{3}\vec{G}_2 = \frac{2\pi}{a_G}\left[\tfrac{2}{3}, 0\right]^T$$



The Hamiltonian of the pristine RnG in a perpendicular displacement field is

$$H_{RnG}(\vec{k}) = H_0(\vec{k}) + V_d$$
$$[V_d]_{\ell\ell'} = \delta_{\ell\ell'}\left[\ell - (n_\ell - 1)/2\right] u_d$$

n_ℓ → # layers

ℓ → $0 \to n_\ell - 1$

top ↦ bottom

$$H_0(\vec{k}) = \begin{bmatrix} h^{(0)} & h^{(1)} & h^{(2)} & & & \\ h^{(1)\dagger} & h^{(0)} & \ddots & & & \\ h^{(2)\dagger} & \ddots & \ddots & & & \\ & \ddots & & & h^{(1)} & h^{(2)} \\ & & & h^{(1)\dagger} & h^{(0)} & h^{(1)} \\ & & & h^{(2)\dagger} & h^{(1)\dagger} & h^{(0)} \end{bmatrix}$$

where

$$h^{(0)} = -t_0 \begin{bmatrix} 0 & f_{\vec{k}} \\ f^*_{\vec{k}} & 0 \end{bmatrix}$$
$$h^{(1)} = \begin{bmatrix} t_4 f_{\vec{k}} & t_3 f^*_{\vec{k}} \\ t_1 & t_4 f_{\vec{k}} \end{bmatrix}$$
$$h^{(2)} = \begin{bmatrix} 0 & \frac{t_2}{2} \\ 0 & 0 \end{bmatrix}$$
$$f_{\vec{k}} = \sum_j \exp(i\vec{k}\cdot\vec{\delta}_j)$$

$$\vec{\delta}_n = R_{2\pi n/3}\left[0,\ a_G/\sqrt{3}\right]^T, \quad n = 0,1,2, \quad a_G = 2.46\,\text{Å}$$

$$(t_0, t_1, t_2, t_3, t_4) = (3100, 380, -21, 290, 141)\ \text{meV}$$

The reciprocal vector for hBN $\quad \vec{G}_i' = \dfrac{a_G}{a_{hBN}} R_\theta \vec{G}_i, \quad \dfrac{a_G}{a_{hBN}} \sim 1.018$

moiré vector $\quad \vec{g}_1 = \vec{G}_1 - \vec{G}_1', \quad \vec{g}_n = R_{2\pi(n-1)/3}\,\vec{g}_1, \quad n = 2,3$

$$\vec{g}_n = -\vec{g}_{n-3} \quad n = 4,5,6$$

$$\Longrightarrow V^{top}_{moiré}(\vec{r}) = V^{top}_{moiré}(0) + \sum_{j=1}^{6} V^{top}_{moiré}(\vec{g}_j)\, e^{i\vec{r}\cdot\vec{g}_j}$$

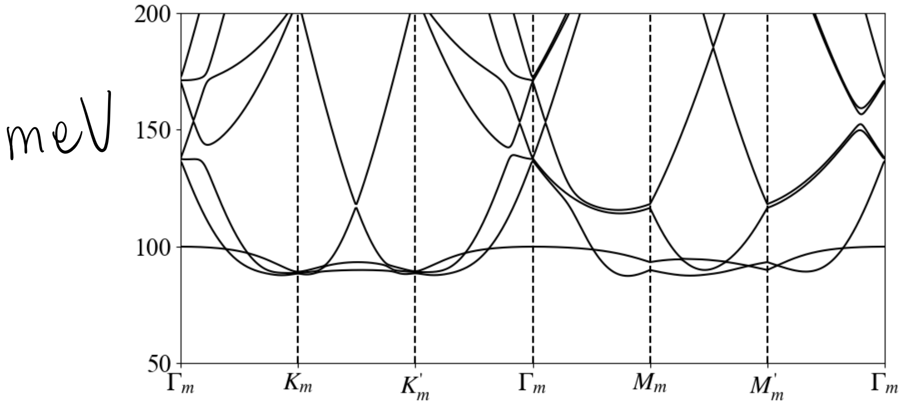
Hermicity, $C_3 \Longrightarrow$

$$\begin{cases} V^{top}_{moiré}(0) = V^{top\,\dagger}_{moiré}(0) \\ V^{top}_{moiré}(\vec{g}_j) = V^{top\,\dagger}_{moiré}(-\vec{g}_j) \\ V^{top}_{moiré}(0) = U_3\, V^{top}_{moiré}(0)\, U_3^\dagger \\ V^{top}_{moiré}(R_{2\pi/3}\vec{g}_j) = U_3\, V^{top}_{moiré}(g_j)\, U_3^\dagger \end{cases}$$

$$U_3 = \begin{bmatrix} 1 & \\ & w \end{bmatrix}, \quad w = e^{2\pi i/3} \sim C_3$$

We take $\quad V^{top}_{moiré}(0) = V_0\,\mathbb{1}, \quad V^{top}_{moiré}(\vec{g}_1) = V_1 e^{-i\psi}\begin{bmatrix} 1 & 1 \\ w & w \end{bmatrix}$

$$(V_0, V_1, \psi) = (28.9\ \text{meV},\ 21\ \text{meV},\ -0.29)$$



C_3 symmetry of some bands :)