Understanding Bilayer Graphene Moiré hopping

Bistritzer & Macdonald

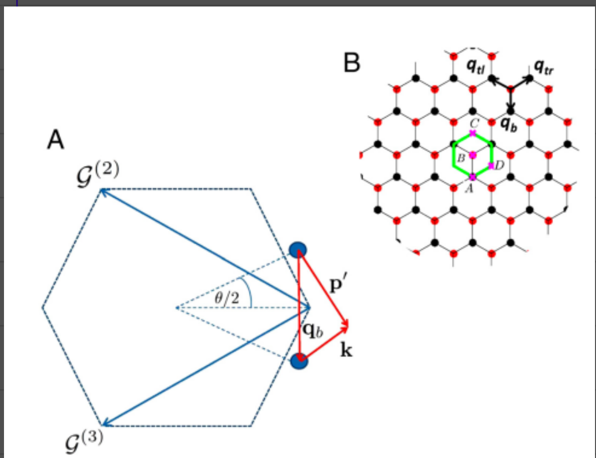


Fig. 1. Momentum-space geometry of a twisted bilayer. (*A*) Dashed line marks the first Brillouin zone of an unrotated layer. The three equivalent Dirac points are connected by $\mathcal{G}^{(2)}$ and $\mathcal{G}^{(3)}$. The circles represent Dirac points of the rotated graphene layers, separated by $k_\theta = 2k_D \sin(\theta/2)$, where k_D is the magnitude of the Brillouin-zone corner wave vector for a single layer. Conservation of crystal momentum implies that $\mathbf{p}' = \mathbf{k} + \mathbf{q}_b$ for a tunneling process in the vicinity of the plotted Dirac points. (*B*) The three equivalent Dirac points in the first Brillouin zone result in three distinct hopping processes. Interference between hopping processes with different wave vectors captures the spatial variation of interlayer coordination that defines the moiré pattern. For all the three processes $|\mathbf{q}_j| = k_\theta$; however, the hopping directions are $(0,-1)$ for $j=1$, $(\sqrt{3}/2, 1/2)$ for $j=2$, and $(-\sqrt{3}/2, 1/2)$ for $j=3$. We interchangeably use 1, 2, 3, *b*, *tr*, and *tl* as subscripts for the three momentum transfers $\mathbf{q}_j$. Repeated hopping generates a *k*-space honeycomb lattice. The green solid line marks the moiré band Wigner–Seitz cell. In a repeated zone scheme the red and black circles mark the Dirac points of the two layers.

Notation:

θ - twist angle

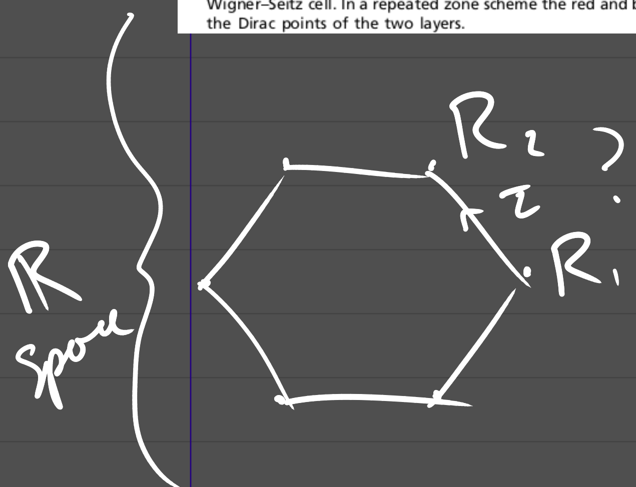
$\bar{d}$ - displacement vector

Position vectors of carbon atoms in misaligned layers

$$R' = M(\theta)(R-\tau)+d$$

↑ rotation

↑ connects two atoms in unit cell



Hamiltonian will have:

- 2 × single layer H (isolated)
- tunneling (hopping)

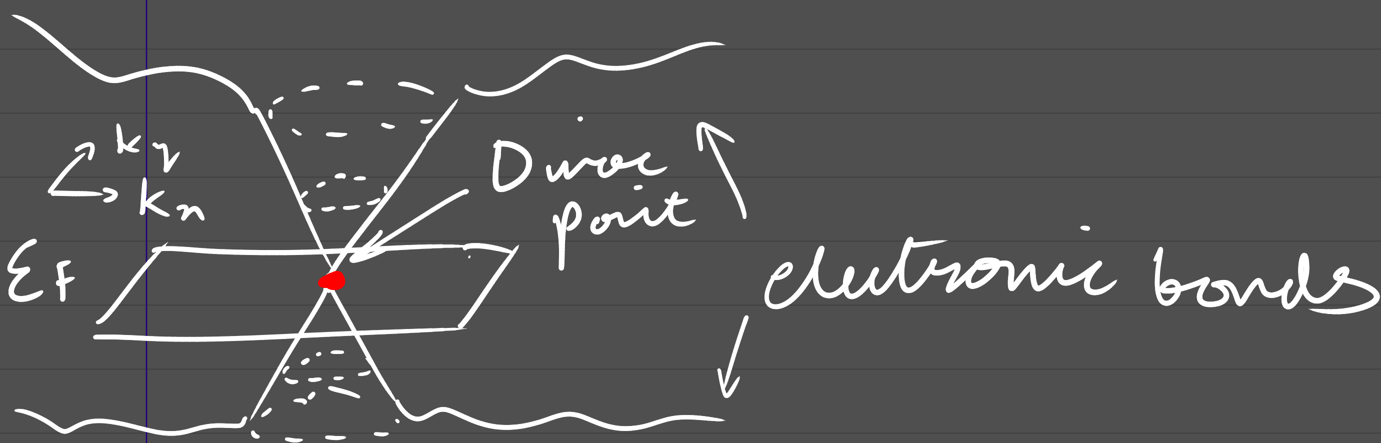
Single layer w/ rotation θ to a fixed coordinate system has hamiltonian

$$h_k = -vk \begin{bmatrix} 0 & e^{i(\theta_k - \theta)} \\ e^{-i(\theta_k - \theta)} & 0 \end{bmatrix}$$

v - Dirac Velocity,

k - momentum measured from Dirac - point

Dirac point : 'two cones that meet at/near fermi level



Dirac - Velocity v_0 : 'E-k dispersion at large momenta k'

$$E(k) = \hbar v_0 |k|$$

Important!

Classical: $E = \frac{1}{2} m |v|^2 = \frac{|k|^2}{2m}$

free Dirac particle: (relativistic)

$$E = \pm \sqrt{\hbar^2 v_0^2 k^2 + \underbrace{m^2 c^4}_{\text{rest mass } E}}$$

$\Rightarrow$

$$E(k) = \hbar v_0 |k|$$ ($\vec{k}$ measured from Dirac-point)

$\underbrace{E \propto k}_{\text{Dirac}}$, not $\underbrace{E \propto k^2}_{\text{Classical}}$

Decoupled bilayer hamiltonian is

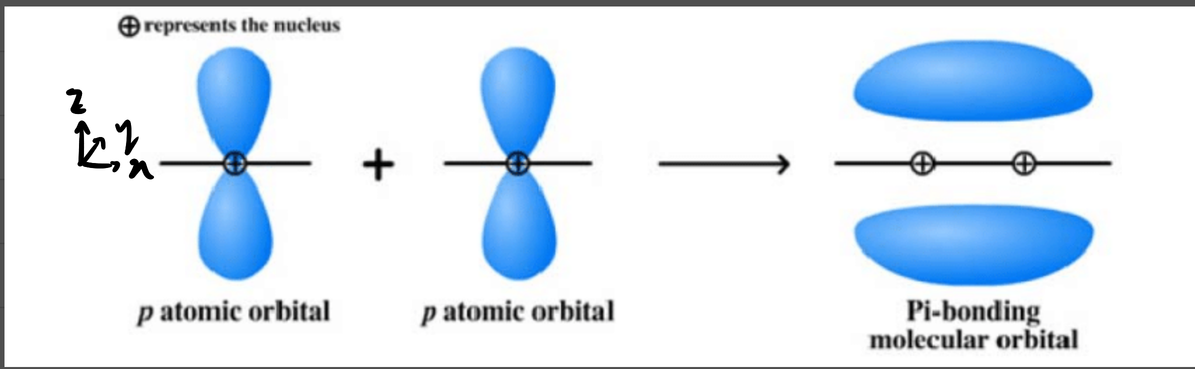
$$|1\rangle h(\theta/2) \langle 1| + |2\rangle h(-\theta/2) \langle 2|$$

'rotate both layers w.r.t same coordinate system'

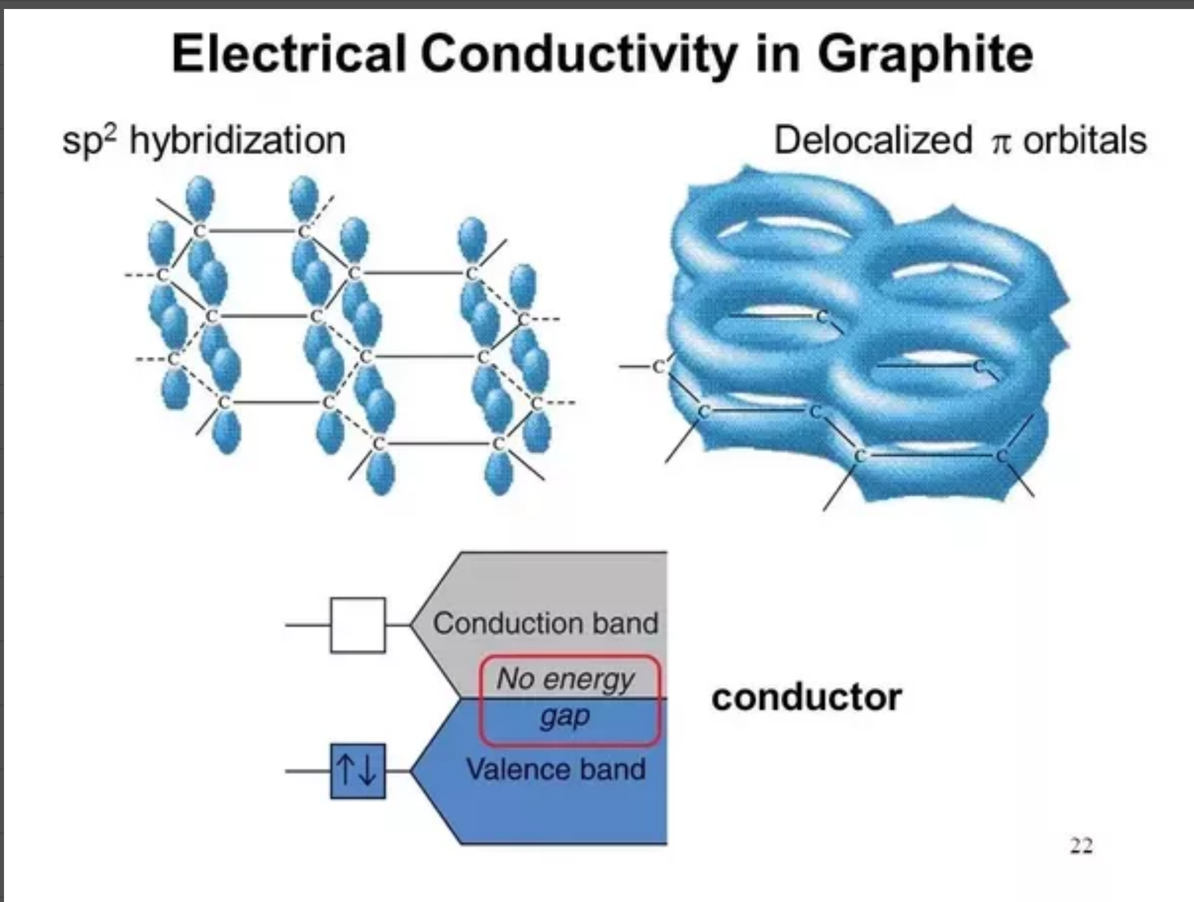
note! $|i\rangle\langle i|$ projects onto layer!

π-orbitals:

π-orbital is a hybrid orbital of 2× p orbitals ~ 'covalent bond'



Note similarity to d_{z^2} orbital!
→ projects in z direction (have p_z)



in Graphene:

Inter-layer tunnelling between π-orbitals is a smooth function $t(r)$ of spatial separation projected onto the graphene plane

$$T^{\alpha\beta}_{kp'} = \langle \psi^{(1)}_{k\alpha} | H_T | \psi^{(2)}_{p'\beta} \rangle$$

is the matrix element of the tunnelling hamiltonian H_T which describes the process of electron with momentum

$$p' = M(\theta)\,p \quad \text{on lattice } \beta$$

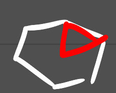
hopping to state with momentum k on lattice α

in a π-band TBM the projection of the wave-functions of the two layers to a given lattice one

$$|\psi^{(1)}_{k\alpha}\rangle = \frac{1}{\sqrt{N}} \sum_{R} e^{ik(R+\tau_\alpha)} |R+\tau_\alpha\rangle$$

&

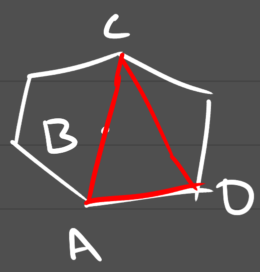
$$|\psi^{(2)}_{p'\beta}\rangle = \frac{1}{\sqrt{N}} \sum_{R'} e^{ip(R'+\tau'_\beta)} |R'+\tau'_\beta\rangle \quad ?$$



R is summed over the triangular Bravais lattice ask!?

two-centre approx $\Longrightarrow$

↕ ?



$$\langle R+\tau_\alpha | H_T | R'+\tau'_\beta \rangle$$

$$= t(R+\tau_\alpha - R' - \tau'_\beta)$$

$A \to B \to C \to D \to A$

for the inter-layer hopping amplitude we find

$$T^{\alpha\beta}_{kp'} = \sum_{G_1, G_2} \frac{t_{\bar{k}+G_1}}{\Omega} e^{i[G_1 \tau_\alpha - G_2(\tau_\beta - \tau) - G_2' d]} \delta_{\bar{k}+G_1, \bar{p}'+G_2'}$$

Ω is unit cell area,

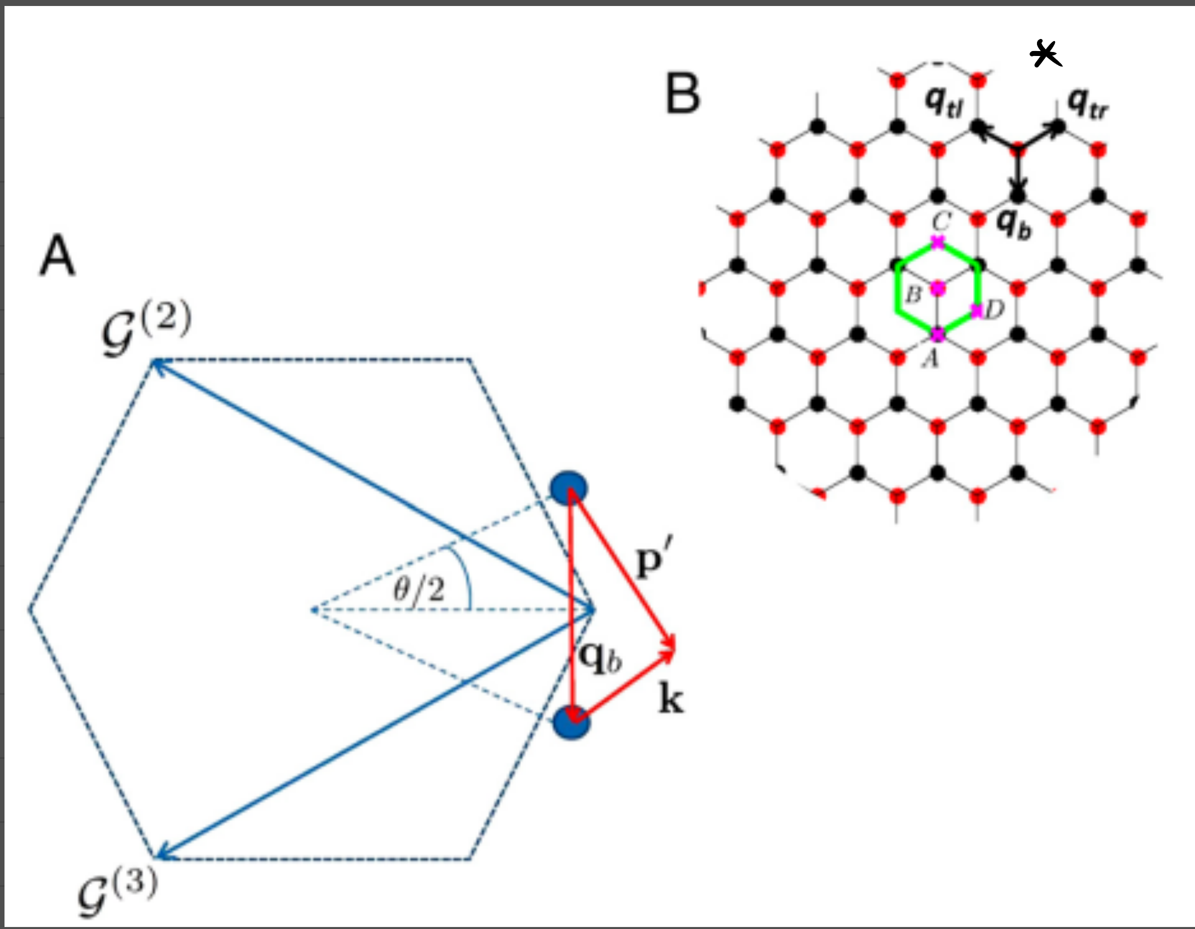
t_q is the fourier transform of the tunnelling amplitude $t(r)$ $(p' = k + q_B)$

G_1, G_2 are summed over reciprocal lattice vectors,

$$G_2' = M(\theta) G_2$$

$\bar{k}$ `bar' notation $\to$ k measured relative to centre of the Brillouin Zone & not relative to the Dirac point

note: Crystal momentum is conserved because $t(r)$ is only dependent on the difference between lattice positions



(*) In total 3 hopping processes with corresponding momentum transfers q_j s.t $|q_j| = k_\theta$ are assumed

Derivation of inter - layer tunnelling elements

Real to reciprocal via fourier

<u>Definition</u>: Fourier (MMK)

in real space:

$$t(\underline{r}) \equiv t(\underline{r}_{2d}, z)$$

<u>Fourier Transform</u>:

$$t(\underline{r}, z) = \frac{A_{uc}}{(2\pi)^2} \int t(\underline{k}, z)\, e^{i\underline{k}\cdot\underline{r}}\, d\underline{k}$$

$$t(\underline{k}, z) = \frac{1}{A_{uc}} \int t(\underline{r}, z)\, e^{-i\underline{k}\cdot\underline{r}}\, d\underline{r}$$

$\underline{r}$, $\underline{k}$ are 2D in lattice plane

A_{uc} = Area of unit cell

t has units of energy

<u>Bloch state</u> notation:

$\underline{k}$ - wavevector

j - sublattice

l - layer

N_l - # of unit cells in a layer l

we have (Bistritzer)

$$|\underline{k}, j, l\rangle = \frac{1}{\sqrt{N_l}} \sum_{\underline{R}} e^{i\underline{k}\cdot(\underline{R}+\underline{\tau}_j)} \phi_j(\underline{r}-\underline{R}-\underline{\tau}_j, z-z_l)$$

where the sum is over primitive lattice vectors $\underline{R}$ (check!?)

So $\phi_j(\underbrace{\underline{r}-\underline{R}-\underline{\tau}_j}_{2D}, \underbrace{z-z_l}_{\text{inter-layer}})$

is a wavefunction of the real gap

$$\Rightarrow \langle \underline{k}', j', l' | \delta\hat{H} | \underline{k}, j, l\rangle$$

$$= \frac{1}{\sqrt{N_l N_{l'}}} \sum_{\underline{R}\underline{R}'} e^{i\underline{k}\cdot(\underline{R}+\underline{\tau}_j)} \cdot e^{-i\underline{k}'\cdot(\underline{R}'+\underline{\tau}_{j'})}$$

$$\cdot \underbrace{\langle \phi_{j'} | \delta\hat{H} | \phi_j\rangle}$$

$$= t(\underline{R}'-\underline{R}+\underline{\tau}_{j'}-\underline{\tau}_j, z_{l'}-z)$$

(two-centre approx)

Two centre approx: hopping depends only on distance $\checkmark$,

we also assume $t(\underline{r}, z) = t(r, z)$

i.e direction of $\underline{r}$ doesn't effect t

Now: take fourier transform to get $t(q, z)$

$$\Rightarrow \langle \underline{k}', j', l' | \delta \hat{H} | k, j, l \rangle$$

$$= \frac{A_{uc}}{(2\pi)^2 \sqrt{N_l N_{l'}}} \sum_{\underline{R} R'} e^{i\underline{k}\cdot(\underline{R}+\underline{\tau}_j)} \cdot e^{-i\underline{k}'\cdot(\underline{R}'+\underline{\tau}_{j'})}$$

$$\cdot \int t(q, z)\, e^{iq\cdot(R'-R+\tau_{j'}-\tau_j)}$$

$$= \frac{A_{uc}}{(2\pi)^2 \sqrt{N_l N_{l'}}} \int t(q, z) \sum_{\underline{R}\underline{R}'} e^{i(\underline{k}-q)\cdot(\underline{R}+\underline{\tau}_j)}$$

$$\cdot e^{-i(\underline{k}'-q)\cdot(\underline{R}'-\underline{\tau}_j)}\, dq$$

Taking the sum over (primitive) lattice vectors $\underline{R}$

$$\sum_{\underline{R}} e^{i(\underline{k}-q)\cdot\underline{R}} = N \sum_{\underline{G}} \delta_{\underline{k}-q, G}$$

for $\underline{G}$ reciprocal lattice vectors

$\Rightarrow \langle \underline{k}', j', l' | \delta\hat{H} | \underline{k}, j, l \rangle$

$$= \frac{A_{uc}\sqrt{N_l N_{l'}}}{(2\pi)^2} \int \sum_{\underline{G}\,\underline{G}'} t(\underline{q}, z)\, \delta_{\underline{k}-\underline{q},\underline{G}}\, \delta_{\underline{q}-\underline{k}',\underline{G}'} \cdot e^{i\underline{G}\cdot\underline{\tau}_j} e^{i\underline{G}'\cdot\underline{\tau}_{j'}}\, d\underline{q}$$

convert integral to a sum over $\underline{q}$

$$\int d\underline{q} = \frac{(2\pi)^2}{\sqrt{S_l S_{l'}}} \sum_{\underline{q}}$$

for S_l area of layer l

using the kronecker-δ, we can remove the sum over $\underline{q}$ ($\delta_{\underline{q}-\underline{k}',\underline{G}}$) $\Rightarrow \underline{q} = \underline{k}' + \underline{G}'$

$\Rightarrow \langle \underline{k}', j', l' | \delta\hat{H} | \underline{k}, j, l \rangle$

$$= \sum_{\underline{G},\underline{G}'} t(\underline{k}' + \underline{G}', z)\, e^{i(\underline{G}\cdot\underline{\tau}_j)} e^{i(\underline{G}'\cdot\underline{\tau}_{j'})}\, \delta_{\underline{k}-\underline{G},\underline{k}'+\underline{G}'}$$

equivalent to the main result of Koshino

$\Rightarrow$ at most only one set of $\underline{G}, \underline{G}'$ connects the given initial & final wave-vectors $\underline{k}, \underline{k}'$

$\Rightarrow$ we have determined the sets of $\underline{k}, \underline{k}'$ coupled by moiré

$\Rightarrow$ interlayer coupling block in hamiltonian is either 0 or one of these allowed.

So, for some given K,

$$K' = K + G - G'$$

$$= K + m_1 G_1 + m_2 G_2 + m_1' G_1' + m_2' G_2'$$

Trivial if $G = G' = 0$

our system: if R_1, R_2 are PLV

$$G_1 = \frac{4\pi}{\sqrt{3}\, a^2} R_1$$

$$G_2 = -\frac{4\pi}{\sqrt{3}\, a^2} R_2$$

rotation in Reciprocal = -ve of rotation in real

So $R_1' = R(\theta) R_1$

$\Rightarrow$ $G_1' = R(-\theta) G_1$

$$R_1 = \begin{pmatrix} \frac{\sqrt{3}a}{2} \\ a/2 \end{pmatrix}, \quad R_2 = \begin{pmatrix} -\frac{\sqrt{3}a}{2} \\ \frac{a}{2} \end{pmatrix}$$

$$G_1 = \begin{pmatrix} 2\pi/a \\ 2\pi/\sqrt{3}a \end{pmatrix}, \quad G_2 = \begin{pmatrix} 2\pi/a \\ -2\pi/\sqrt{3}a \end{pmatrix}$$

$$R(-\theta) = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$$

$$\Rightarrow \underline{K}' = \begin{pmatrix} K_1' \\ K_2' \end{pmatrix} = \begin{pmatrix} K_1 \\ K_2 \end{pmatrix} + \frac{2\pi m_1}{a} \begin{pmatrix} 1 \\ 1/\sqrt{3} \end{pmatrix}$$

$$+ \frac{2\pi m_2}{a} \begin{pmatrix} 1 \\ -1/\sqrt{3} \end{pmatrix} + \frac{2\pi m_1'}{a} \begin{pmatrix} \cos\theta + 1/\sqrt{3}\sin\theta \\ -\sin\theta + 1/\sqrt{3}\cos\theta \end{pmatrix}$$

$$+ \frac{2\pi}{a} m_2' \begin{pmatrix} \cos\theta - 1/\sqrt{3}\sin\theta \\ -\sin\theta - 1/\sqrt{3}\cos\theta \end{pmatrix}$$

So

$$k_1' = k_1 + \frac{2\pi}{a}\Big(m_1 + m_2 + m_1'\left(\cos\theta + \tfrac{1}{\sqrt{3}}\sin\theta\right)$$
$$+ m_2'\left(\cos\theta - \tfrac{1}{\sqrt{3}}\sin\theta\right)\Big)$$

$$k_2' = k_2 + \frac{2\pi}{a}\Big(\frac{m_1}{\sqrt{3}} - \frac{m_2}{\sqrt{3}} + m_1'\left(-\sin\theta + \tfrac{1}{\sqrt{3}}\cos\theta\right)$$
$$+ m_2'\left(-\sin\theta - \tfrac{1}{\sqrt{3}}\cos\theta\right)\Big)$$

Lets consider $|G| = |G'|$

ignore i.e G' is just rotated G by $-\theta$

$\Rightarrow m_1 = m_1'$, $m_2 = m_2'$

i.e
$$\underbrace{R(-\theta)\left(\begin{pmatrix} m_1 \\ m_2 \end{pmatrix} \cdot \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}\right)}_{=G} = \underbrace{\begin{pmatrix} m_1' \\ m_2' \end{pmatrix} \cdot \begin{pmatrix} a_1' \\ a_2' \end{pmatrix}}_{=G'}$$

$$= \begin{pmatrix} m_1' \\ m_2' \end{pmatrix} \cdot \left(R(-\theta)\begin{pmatrix} a_1 \\ a_2 \end{pmatrix}\right)$$

check this!

$$\Longleftrightarrow \begin{pmatrix} m_1 \\ m_2 \end{pmatrix} = \begin{pmatrix} m_1' \\ m_2' \end{pmatrix}$$

$$\Rightarrow K_1' - K_1 = \frac{2\pi}{a} \begin{pmatrix} 1 + \cos\theta + 1/\sqrt{3} \sin\theta \\ 1 + \cos\theta - 1/\sqrt{3} \sin\theta \end{pmatrix} \cdot \begin{pmatrix} m_1 \\ m_2 \end{pmatrix}$$

$$\& \quad K_2' - K_2 = \frac{2\pi}{a} \begin{pmatrix} 1/\sqrt{3} - \sin\theta + 1/\sqrt{3}\cos\theta \\ 1/\sqrt{3} - \sin\theta - 1/\sqrt{3}\cos\theta \end{pmatrix} \cdot \begin{pmatrix} m_1 \\ m_2 \end{pmatrix}$$

for small θ :

$$q_1 := K_1' - K_1 \sim \frac{2\pi}{a} \begin{pmatrix} 2 \\ 2 \end{pmatrix} \cdot \begin{pmatrix} m_1 \\ m_2 \end{pmatrix}$$

$$q_2 := K_2' - K_2 \sim \frac{2\pi}{a} \begin{pmatrix} 2/\sqrt{3} \\ 0 \end{pmatrix} \cdot \begin{pmatrix} m_1 \\ m_2 \end{pmatrix}$$

$$\Rightarrow q = \begin{pmatrix} q_1 \\ q_2 \end{pmatrix} \approx \frac{4\pi}{a} \begin{pmatrix} m_1 + m_2 \\ m_1/\sqrt{3} \end{pmatrix}$$

SAN!!! read this

Good (?)

small θ

$$G_i^m = G_i - G_i' = (1-R) G_i \overset{\Sigma}{=} (1-R)(m_1 G_1 + m_2 G_2)$$

$$\Rightarrow K' = K + G^m \overset{\Sigma}{=} K + m_1 G_1^m + m_2 G_2^m$$

$$= K + (1-R)(m_1 G_1 + m_2 G_2)$$

$$\xRightarrow[(5)]{\text{Koshino}} U_{X'X}(K', K)$$

(5)
$$= -\sum_{G G'} t_{x'x}(k+G)\, e^{-i(G\cdot\tau_n)+i(G'\cdot\tau_{n'})}$$

$\underbrace{\delta_{k+G,\,k'+G'}}$

$\Rightarrow k+G = k'+G'$

after $\sum_{G'}$ $\Rightarrow k' = k+G^m$

$(G_i' = G_i - G_i^m)$

$\Sigma_{G'}$

$$\Rightarrow U_{x'x}(k+G^m, k)$$

$$= -\sum_{G} t_{n'n}(k+G^m, k)\, e^{-i(G\cdot\tau_n)+i(G-G^m\cdot\tau_{n'})}$$

$\sum_G \Rightarrow G = m_1G_1 + m_2G_2$

$$= -t_{n'n}(k+m_1G_1+m_2G_2)$$

$$\cdot e^{-i(m_1G_1+m_2G_2)\cdot\tau_n + i\underbrace{(m_1G_1+m_2G_2-m_1G_1^m-m_2G_2^m)}\cdot\tau_{n'}}$$

$$= m_1(G_1 - G_1^m) + m_2(G_2 - G_2^m)$$

$$= m_1G_1' + m_2G_2'$$

$$\Rightarrow U_{n'n}(k', k)$$

$$= -t_{n'n}(k + m_1G_1 + m_2G_2)$$

$$\cdot \underbrace{e^{-i(m_1G_1+m_2G_2)\cdot\tau_n + i(m_1G_1'+m_2G_2')\cdot\tau_{n'}}}$$

$$= e^{-i((m_1G_1+m_2G_2)\cdot\tau_n - (m_1G_1'+m_2G_2')\cdot\tau_{n'})}$$

this is exponentially small if

$(m_1 G_1 + m_2 G_2)\cdot \tau_n >> (m_1 G_1' + m_2 G_2')\cdot \tau_{n'}$

for Graphene: 2 atoms in unit cell

So $\tau_x = \tau_A , \tau_B$

$\tau_A = 0 , \tau_B = -(a_1 + 2a_2)/3$

$\tau_{A'} = d e_z + \tau_0$

$\tau_{B'} = d e_z + \tau_0 - (a_1' + 2a_2')/3$

lets try with the 1st case,

$\tau_x = 0 , \tau_x = d e_z + \underbrace{\tau_0}_{\tau = \begin{pmatrix} \tau_1 \\ \tau_2 \end{pmatrix}}$

then we have, for

$$G_1 = \begin{pmatrix} 2\pi/a \\ 2\pi/\sqrt{3}a \end{pmatrix} , G_2 = \begin{pmatrix} 2\pi/a \\ -2\pi/\sqrt{3}a \end{pmatrix}$$

& $m R(\theta) G = R(\theta)(mG)$

$$\Rightarrow \frac{2\pi}{a}\left(\begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}\begin{pmatrix} m_1 + m_2 \\ 1/\sqrt{3}(m_1 - m_2) \end{pmatrix}\right)\cdot \begin{pmatrix} \tau_1 \\ \tau_2 \end{pmatrix} << 0$$