Magic angle twisted bilayer graphene (MATBG)

1. ‘G’ in TBG
2. BM model for TBG
3. Strong correlation in MATBG

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HKU-UCAS young physicist forum

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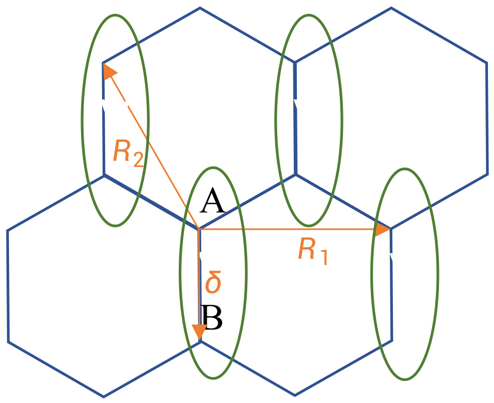
1. ‘G’ in TBG
   - Tight binding model
   - Symmetry and Dirac cone
   - Edge mode and topology
2. BM model for TBG
3. Strong correlation in MATBG

Tight binding model



$$H = t_1 \sum_{R_i} (c^{\dagger}_{R_i,A} c_{R_i,B} + c^{\dagger}_{R_i,A} c_{R_i+R_1+R_2,B} + c^{\dagger}_{R_i,A} c_{R_i+R_2,B} + \mathrm{h.}c.)$$

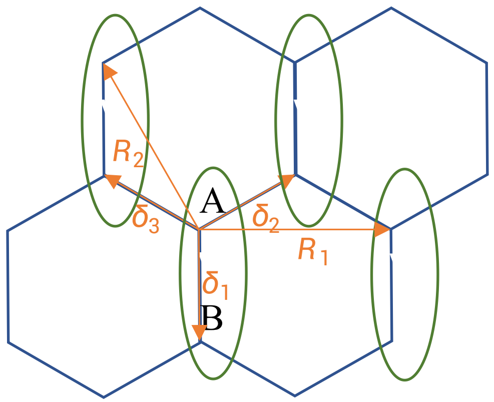
Fourier transformation

$$\begin{cases} c^{\dagger}_{R_i,A} = \frac{1}{\sqrt{N}} \sum_{k_1} e^{ik_1 \cdot R_i} c^{\dagger}_{k_1,A} \\ c^{\dagger}_{R_i,B} = \frac{1}{\sqrt{N}} \sum_{k_2} e^{ik_2 \cdot (R_i + \delta)} c^{\dagger}_{k_2,B} \end{cases} \& \begin{cases} c_{R_i,A} = \frac{1}{\sqrt{N}} \sum_{k_1} e^{-ik_1 \cdot R_i} c_{k_1,A} \\ c_{R_i,B} = \frac{1}{\sqrt{N}} \sum_{k_2} e^{-ik_2 \cdot (R_i + \delta)} c_{k_2,B} \end{cases}$$

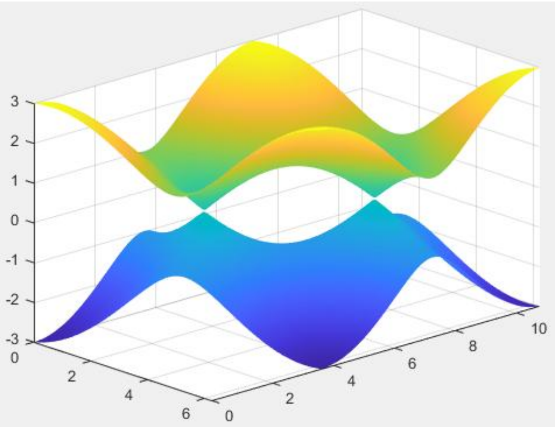
And orthogonal relation $\sum_{R_i} e^{i(k - k_0) \cdot R_i} = N\delta_{k,k_0}$

$$H = t_1 \sum_{k_1,k_2} \sum_{R_i} \frac{e^{i(k_1 - k_2) \cdot R_i}}{N} (e^{-ik_2 \cdot \delta} + e^{-ik_2 \cdot (R_1 + R_2 + \delta)} + e^{-ik_2 \cdot (R_2 + \delta)}) c^{\dagger}_{k_1,A} c_{k_2,B} + \mathrm{h.}c.$$
$$= t_1 \sum_{k} (e^{-ik \cdot \delta} + e^{-ik \cdot (R_1 + R_2 + \delta)} + e^{-ik \cdot (R_2 + \delta)}) c^{\dagger}_{k,A} c_{k,B} + \mathrm{h.}c.$$

Tight binding model



$R_1 = (\sqrt{3}a, 0)\,, R_2 = (-\frac{\sqrt{3}}{2}a, \frac{3}{2}a)$



$$H_k = t_1(e^{-ik\cdot\delta} + e^{-ik\cdot(R_1 + R_2 + \delta)} + e^{-ik\cdot(R_2 + \delta)})c_{k,A}^{\dagger}c_{k,B} + \mathrm{h.c.}$$

Written in matrix form

$$H_k = t_1 \begin{pmatrix} 0 & e^{-ik\cdot\delta_1} + e^{-ik\cdot\delta_2} + e^{-ik\cdot\delta_3} \\ e^{ik\cdot\delta_1} + e^{ik\cdot\delta_2} + e^{ik\cdot\delta_3} & 0 \end{pmatrix}$$

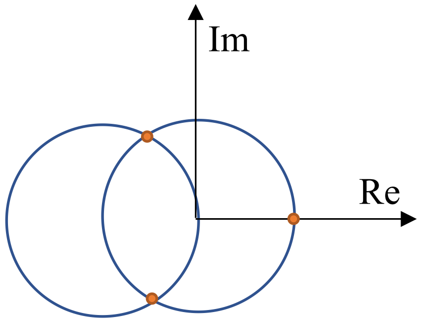
By solving the eigen value

$$E_k = \pm\, t_1|e^{ik\cdot\delta_1} + e^{ik\cdot\delta_2} + e^{ik\cdot\delta_3}|$$

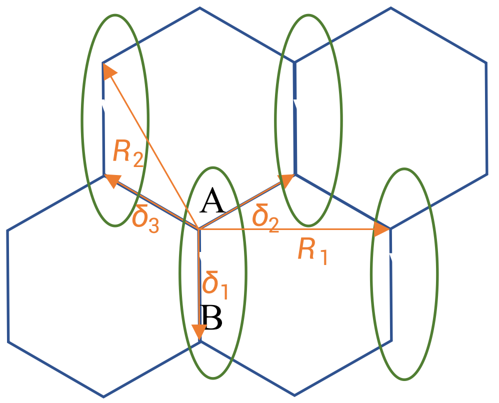
One can fine two degenerate points in the first Brillouin zone

$$e^{ik\cdot(\delta_1 - \delta_3)} + e^{ik\cdot(\delta_2 - \delta_3)} + 1 = 0 \Rightarrow e^{ik\cdot\delta_1} + e^{ik\cdot\delta_2} + 1 = 0$$

$$\Longrightarrow \begin{cases} k\cdot R_2 = \frac{2\pi}{3} \\ k\cdot R_1 = \frac{2\pi}{3} \end{cases} \text{or} \begin{cases} -k\cdot R_2 = \frac{2\pi}{3} \\ k\cdot R_1 = -\frac{2\pi}{3} \end{cases} \Longrightarrow \begin{cases} K_1 = \frac{2\pi}{3\sqrt{3}a}(1, \sqrt{3}) \\ K_2 = -\frac{2\pi}{3\sqrt{3}a}(1, \sqrt{3}) \end{cases}$$



Tight binding model



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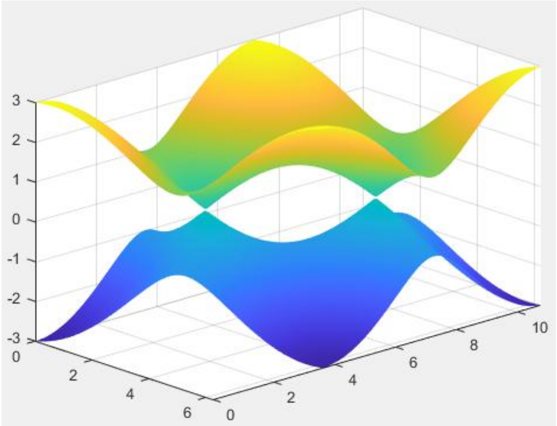


$$H_k = t_1 \begin{pmatrix} 0 & e^{-ik\cdot\delta_1} + e^{-ik\cdot\delta_2} + e^{-ik\cdot\delta_3} \\ e^{ik\cdot\delta_1} + e^{ik\cdot\delta_2} + e^{ik\cdot\delta_3} & 0 \end{pmatrix}$$

Expand H_k to linear order around K_1

$$H_{K_1+k} = t_1 \begin{pmatrix} 0 & e^{i\frac{2\pi}{3}} e^{-ik\cdot\delta_1} + e^{-i\frac{2\pi}{3}} e^{-ik\cdot\delta_2} + e^{-ik\cdot\delta_3} \\ e^{-i\frac{2\pi}{3}} e^{ik\cdot\delta_1} + e^{i\frac{2\pi}{3}} e^{ik\cdot\delta_2} + e^{ik\cdot\delta_3} & 0 \end{pmatrix}$$

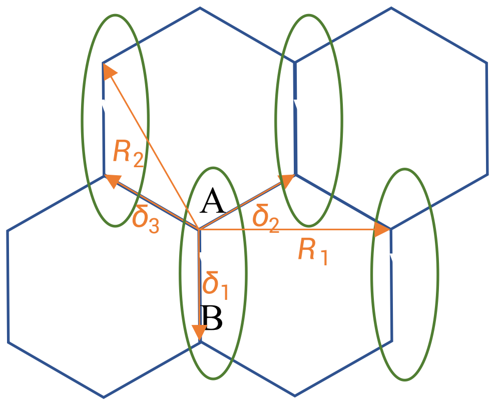
$$\approx t_1 \begin{pmatrix} 0 & -e^{i\frac{2\pi}{3}}\delta_1 - e^{-i\frac{2\pi}{3}}\delta_2 - \delta_3 \\ e^{-i\frac{2\pi}{3}}\delta_1 + e^{i\frac{2\pi}{3}}\delta_2 + \delta_3 & 0 \end{pmatrix} \cdot ik$$

$$= t_1 \begin{pmatrix} 0 & (-\frac{3}{4} + i\frac{3\sqrt{3}}{4})\, a(1,\ i) \\ (-\frac{3}{4} - i\frac{3\sqrt{3}}{4})\, a(1,\ -i) & 0 \end{pmatrix} \cdot k = \begin{pmatrix} 0 & (1,\ i) \\ (1,\ -i) & 0 \end{pmatrix} \cdot k'$$

Dispersion for $E_{k'}$ (Dirac cone)

$$E_{k'} = \pm\sqrt{k_x'^2 + k_y'^2}$$

Tight binding model



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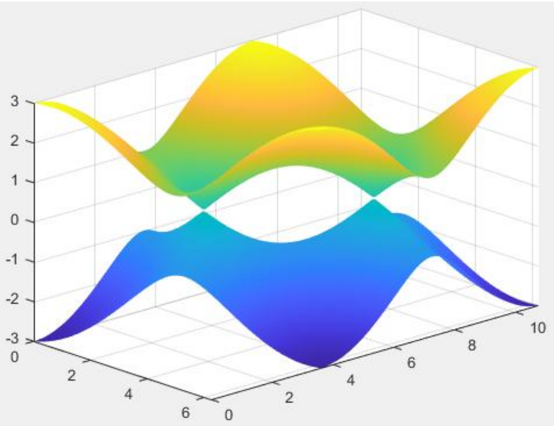


Conclusion for now

1. Nearest neighbor hopping tight binding model for graphene

$$H_k = t_1 \begin{pmatrix} 0 & e^{-ik\cdot\delta_1} + e^{-ik\cdot\delta_2} + e^{-ik\cdot\delta_3} \\ e^{ik\cdot\delta_1} + e^{ik\cdot\delta_2} + e^{ik\cdot\delta_3} & 0 \end{pmatrix}$$

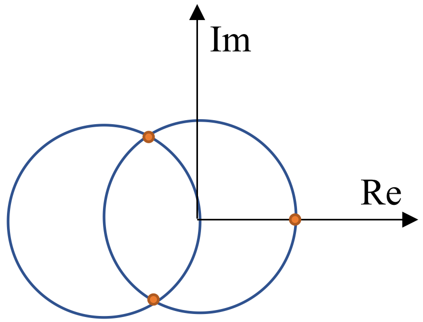
2. Two degenerate points at $\boldsymbol{K_1, K_2}$ in the first Brillouin zone

$$e^{iK\cdot\delta_1} + e^{iK\cdot\delta_2} + 1 = 0$$
$$(e^{iK\cdot\delta_1})^3 = (e^{iK\cdot\delta_2})^3 = (e^{iK\cdot\delta_3})^3 = 1$$

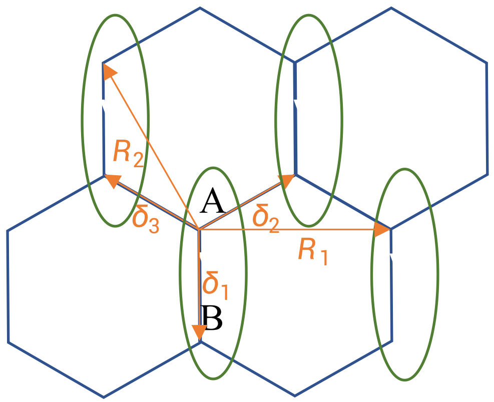
3. Linear dispersion and Dirac cone at $\boldsymbol{K_1, K_2}$

$$H_{K_1+k} \equiv H_{k'} = \begin{pmatrix} 0 & (1,\ i) \\ (1,\ -i) & 0 \end{pmatrix} \cdot k' = k'_x\sigma_x - k'_y\sigma_y$$

$$H_{K_2+k} \equiv H^*_{-k'} =- \begin{pmatrix} 0 & (1,\ -i) \\ (1,\ i) & 0 \end{pmatrix} \cdot k' =- k'_x\sigma_x - k'_y\sigma_y$$



Symmetry and Dirac cone



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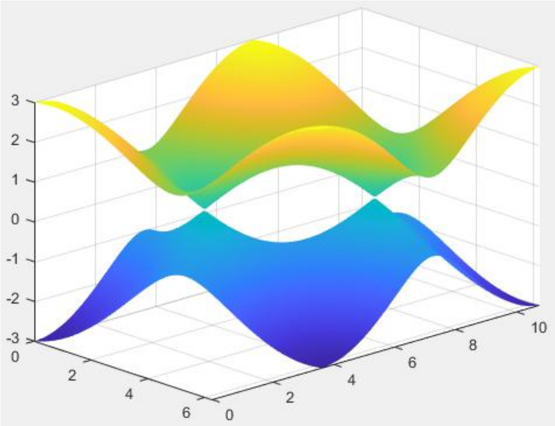


$$H_{K_1+k} \equiv H_{k'} = \begin{pmatrix} 0 & (1,\ i) \\ (1,\ -i) & 0 \end{pmatrix} \cdot k' = k'_x\sigma_x - k'_y\sigma_y$$

$$H_{K_2+k} \equiv H^*_{-k'} = -\begin{pmatrix} 0 & (1,\ -i) \\ (1,\ i) & 0 \end{pmatrix} \cdot k' = -k'_x\sigma_x - k'_y\sigma_y$$

Time reversal symmetry

$$\mathrm{h}(K+k)^* \equiv T\mathrm{h}(K+k)T^{-1} = \mathrm{h}(-K-k)$$

(One Dirac cone can be derived from the other one, TR alone will not protect Dirac cone from gapping)

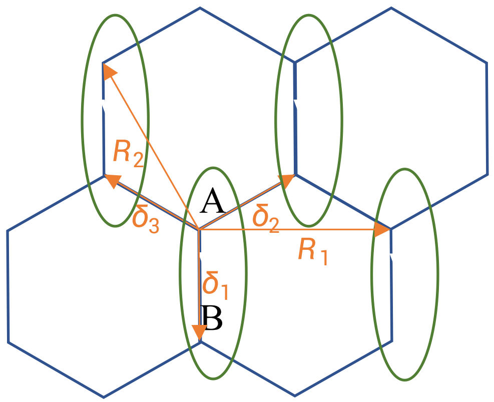
For example, we add BN term which preserves TR but open a gap

$$H = m\sum_{R_i}(c^\dagger_{R_i,A}c_{R_i,A} - c^\dagger_{R_i,B}c_{R_i,B})$$

$$\Rightarrow \begin{cases} H_{k'} = k'_x\sigma_x - k'_y\sigma_y + m\sigma_z \\ H^*_{-k'} = -k'_x\sigma_x - k'_y\sigma_y + m\sigma_z \end{cases} \Rightarrow \mathrm{h}(K+k)^* = \mathrm{h}(-K-k)$$

$$E_{k'=0} = \pm m$$

Symmetry and Dirac cone



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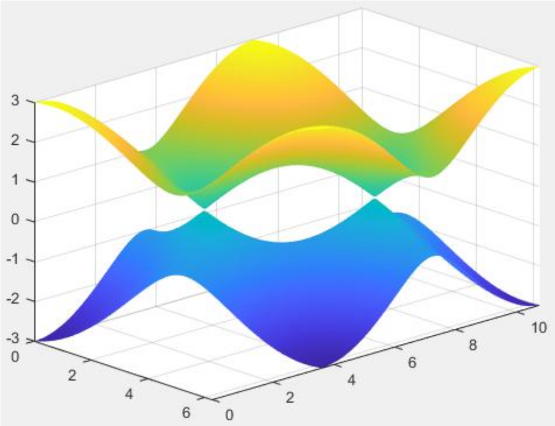


Inversion symmetry (C_{2z})

$$I c^{\dagger}_{R_i,A} I^{-1} = c^{\dagger}_{-R_i,B}, I c^{\dagger}_{R_i,B} I^{-1} = c^{\dagger}_{-R_i,A}$$

$$\sigma_x \mathrm{h}(-K-k)\sigma_x \equiv I\mathrm{h}(K+k)I^{-1} = \mathrm{h}(K+k)$$

Let us check BN term will break I

$$H = \sum_{R_i} (m_1 c^{\dagger}_{R_i,A} c_{R_i,A} - m_1 c^{\dagger}_{R_i,B} c_{R_i,B})$$

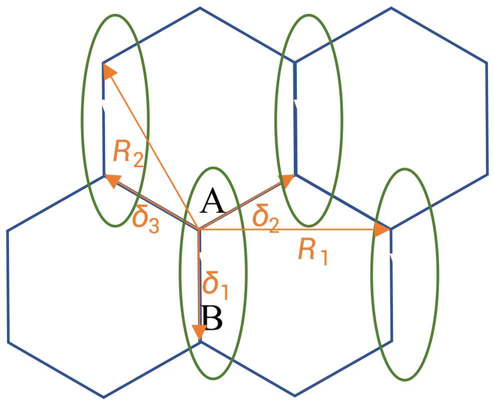
$$\Rightarrow \begin{cases} H_{k'} = k'_x\sigma_x - k'_y\sigma_y + m\sigma_z \\ H^*_{-k'} = -k'_x\sigma_x - k'_y\sigma_y + m\sigma_z \end{cases} \Rightarrow \sigma_x \mathrm{h}(-K-k)\sigma_x = \mathrm{h}(K+k) - 2m\sigma_z \neq \mathrm{h}(K+k)$$

But another kind of mass preserving I can also gap the Dirac cone

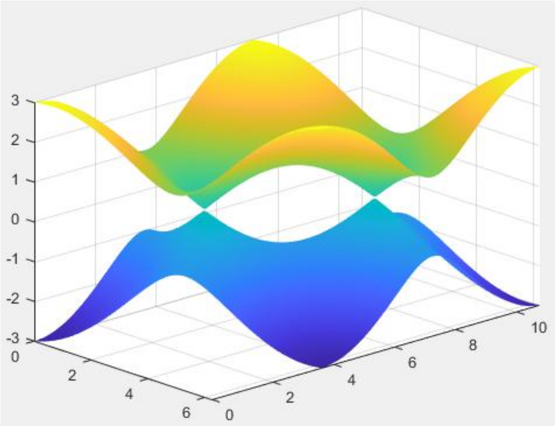
$$\begin{cases} H_{k'} = k'_x\sigma_x - k'_y\sigma_y + m\sigma_z \\ H^*_{-k'} = -k'_x\sigma_x - k'_y\sigma_y - m\sigma_z \end{cases} \Rightarrow \sigma_x \mathrm{h}(-K-k)\sigma_x = \mathrm{h}(K+k)$$

$$E_{k'=0} = \pm m, E^*_{-k'=0} = \mp m$$

Symmetry and Dirac cone



$R_1 = (\sqrt{3}a, 0)\,, R_2 = (-\frac{\sqrt{3}}{2}a, \frac{3}{2}a)$



TI symmetry

$$\sigma_x \mathrm{h}(K+k)^* \sigma_x \equiv (TI)\mathrm{h}(K+k)(TI)^{-1} = \mathrm{h}(K+k)$$

For any 2×2 matrix, one can write

$$M_{2D} = a\sigma_x + b\sigma_y + c\sigma_z + d\sigma_0$$

Without considering energy shift $d(k)\sigma_0$, constriction from TI requires

$$\begin{cases} a(k) = a(k)^* \\ b(k) = b(k)^* \\ c(k) = -c(k)^* \end{cases}$$

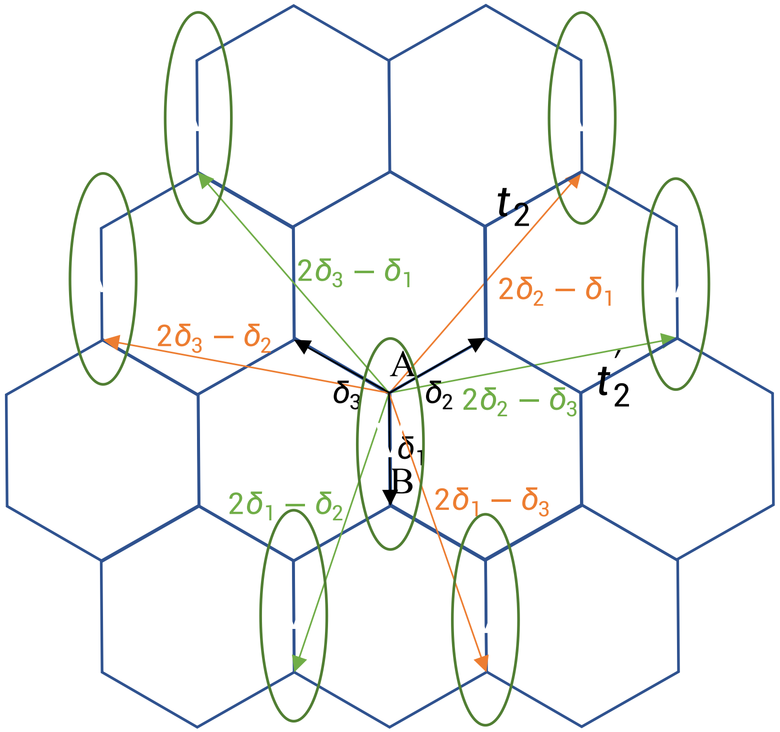
But Hermitian requires $c(k) = c(k)^*$ so that $c(k) = 0$ for Hamiltonian preserve TI

For perturbated Hamiltonian near K_1, it must have the form

$$H_{k'} = k_x' \sigma_x - k_y' \sigma_y + a\sigma_x + b\sigma_y$$

This just shift the Dirac point $k_x' \to k_x' + a, k_y' \to k_y' - b$, but the Dirac point itself will never open so long as the perturbation preserves TI (Local protected Dirac cone by TI symmetry)

Symmetry and Dirac cone



C_3 symmetry

t is unchanged under C_3 rotation (not only nearest neighbor is allowed)

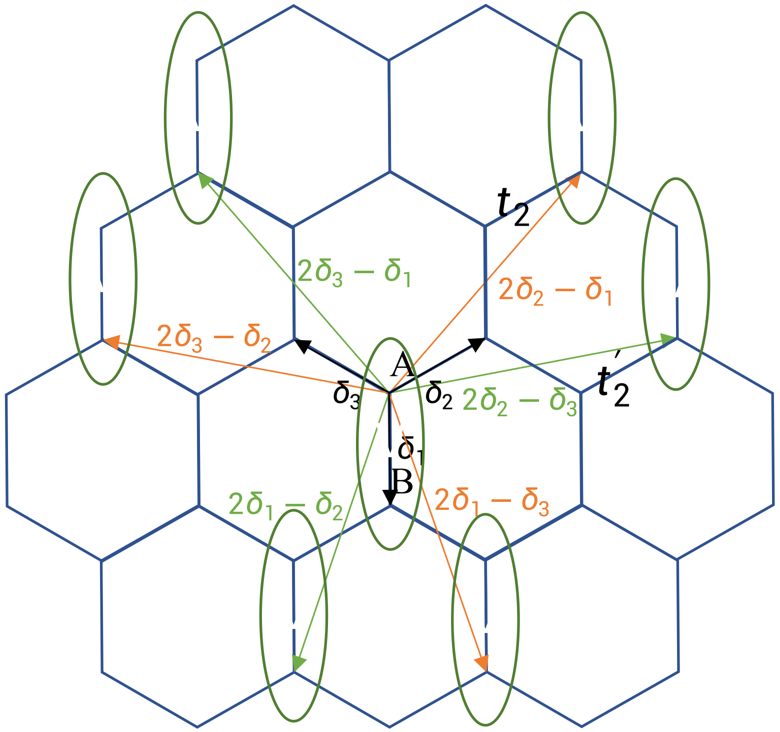
AA and BB hopping which are diagonal elements are forced to be 0 at Dirac point because of TI.

$$H_2 = t_2 \sum_{R_i} (c^\dagger_{R_i,A} c_{R_i+2\delta_2-\delta_1-\delta_1,B} + c^\dagger_{R_i,A} c_{R_i+2\delta_3-\delta_2-\delta_1,B} + c^\dagger_{R_i,A} c_{R_i+2\delta_1-\delta_3-\delta_1,B} + \mathrm{h.c.})$$
$$+ t_2' \sum_{R_i} (c^\dagger_{R_i,A} c_{R_i+2\delta_2-\delta_3-\delta_1,B} + c^\dagger_{R_i,A} c_{R_i+2\delta_3-\delta_1-\delta_1,B} + c^\dagger_{R_i,A} c_{R_i+2\delta_1-\delta_2-\delta_1,B} + \mathrm{h.c.})$$

After Fourier transformation

$$H_{2,k} = t_2 (e^{-ik\cdot(2\delta_2-\delta_1)} + e^{-ik\cdot(2\delta_3-\delta_2)} + e^{-ik\cdot(2\delta_1-\delta_3)}) c^\dagger_{k,A} c_{k,B} + \mathrm{h.c.}$$
$$+ t_2' (e^{-ik\cdot(2\delta_2-\delta_3)} + e^{-ik\cdot(2\delta_3-\delta_1)} + e^{-ik\cdot(2\delta_1-\delta_2)}) c^\dagger_{k,A} c_{k,B} + \mathrm{h.c.}$$

Symmetry and Dirac cone



C_3 symmetry

$$H_{2,k} = t_2\left(e^{-iK\cdot(2\delta_2-\delta_1)} + e^{-iK\cdot(2\delta_3-\delta_2)} + e^{-iK\cdot(2\delta_1-\delta_3)}\right)c_{k,A}^{\dagger}c_{k,B} + \mathrm{h.}c.$$
$$+\, t_2'\left(e^{-iK\cdot(2\delta_2-\delta_3)} + e^{-iK\cdot(2\delta_3-\delta_1)} + e^{-iK\cdot(2\delta_1-\delta_2)}\right)c_{k,A}^{\dagger}c_{k,B} + \mathrm{h.}c.$$

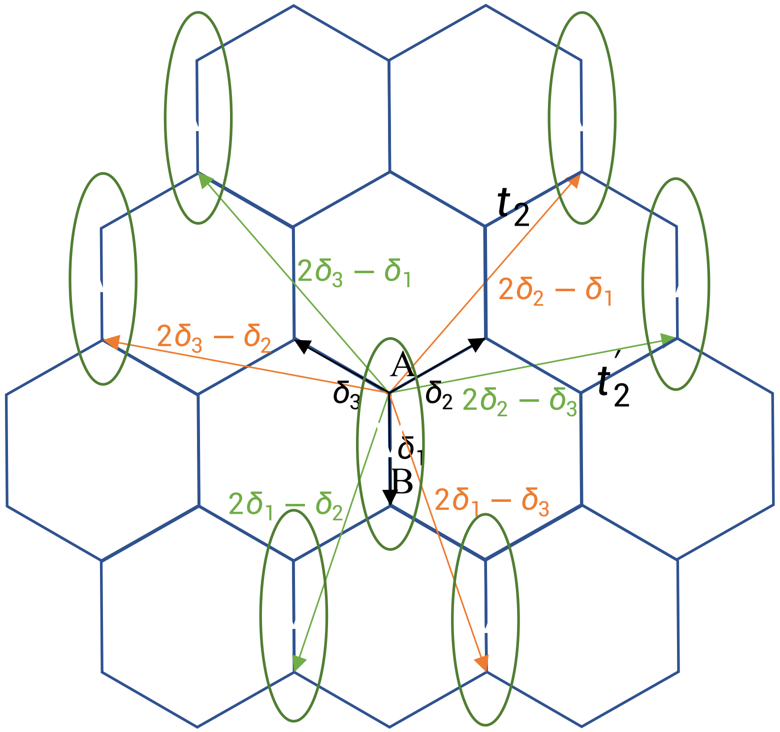
With conclusion 2 in our part one, we can check at K point, the coefficients with t_2 and t_2'

$$e^{-iK\cdot(2\delta_2-\delta_1)} + e^{-iK\cdot(2\delta_3-\delta_2)} + e^{-iK\cdot(2\delta_1-\delta_3)}$$
$$= e^{-iK\cdot(2\delta_2-\delta_1)}\left(1 + e^{-iK\cdot(2\delta_3-3\delta_2+\delta_1)} + e^{-iK\cdot(3\delta_1-2\delta_2-\delta_3)}\right)$$
$$= e^{-iK\cdot(2\delta_2-\delta_1)}\left(1 + e^{-iK\cdot\delta_1} + e^{-iK\cdot\delta_2}\right) = 0$$

$$e^{-iK\cdot(2\delta_2-\delta_3)} + e^{-iK\cdot(2\delta_3-\delta_1)} + e^{-iK\cdot(2\delta_1-\delta_2)}$$
$$= e^{-iK\cdot(2\delta_2-\delta_3)}\left(1 + e^{-iK\cdot(3\delta_3-2\delta_2-\delta_1)} + e^{-iK\cdot(2\delta_1-3\delta_2+\delta_3)}\right)$$
$$= e^{-iK\cdot(2\delta_2-\delta_3)}\left(1 + e^{-iK\cdot(-\delta_2)} + e^{-iK\cdot(-\delta_1)}\right) = 0$$

The other hopping preserving C_3 can also be proved give 0 matrix elements at K point
(C_3 symmetry promise Dirac cone at K point exactly)

Symmetry and Dirac cone



Conclusion for now

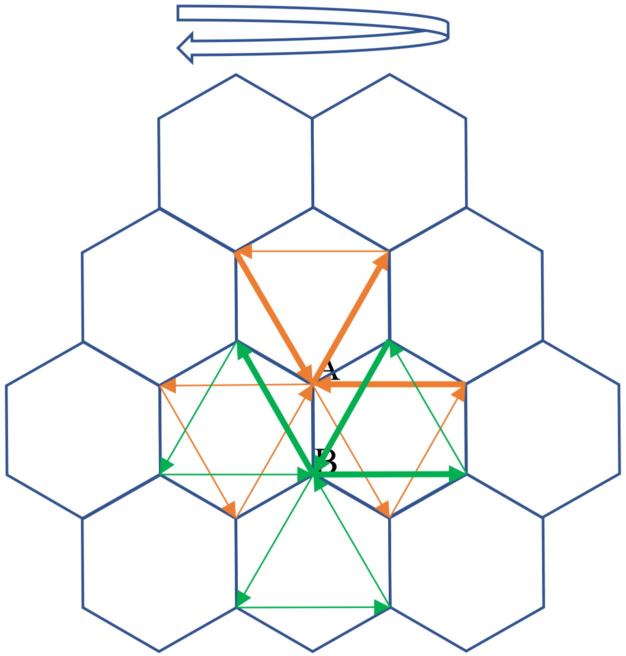
1. Dirac cone in graphene is robust (not only exist in nearest neighbor hopping model)

2. Perturbation preserves time reversal and inversion (like anisotropy of graphene induced by strain) will only shift the position of Dirac cone. TI makes sure Dirac cone perturbation stable

3. Hopping (even non-perturbation hopping) preserving C_3 promises Dirac cone located exactly at K point. C_3 makes sure Dirac cone globally stable

4. BN breaks inversion. If C_3 is preserved, it gaps Dirac cone exactly at K point

Edge mode and topology



$$H = t_1 \sum_{R_i} (c^\dagger_{R_i,A} c_{R_i,B} + c^\dagger_{R_i,A} c_{R_i+R_1+R_2,B} + c^\dagger_{R_i,A} c_{R_i+R_2,B} + \mathrm{h.}c.)$$

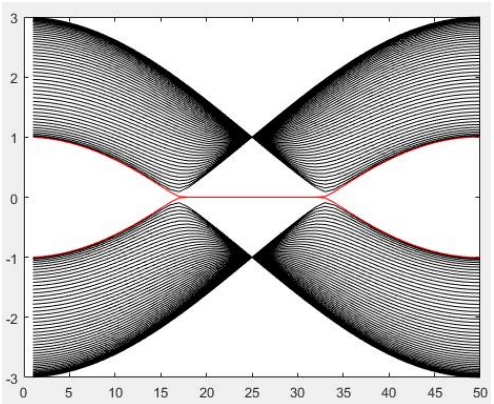
$$H_m = m \sum_{R_i} (c^\dagger_{R_i,A} c_{R_i,A} - c^\dagger_{R_i,B} c_{R_i,B})$$

$$H_\mathrm{h} = t_H \sum_{R_i} ic^\dagger_{R_i,A} c_{R_i+R_1+R_2,A} - ic^\dagger_{R_i,A} c_{R_i+R_1,A} - ic^\dagger_{R_i,A} c_{R_i+R_2,A} + \mathrm{h.}c.$$

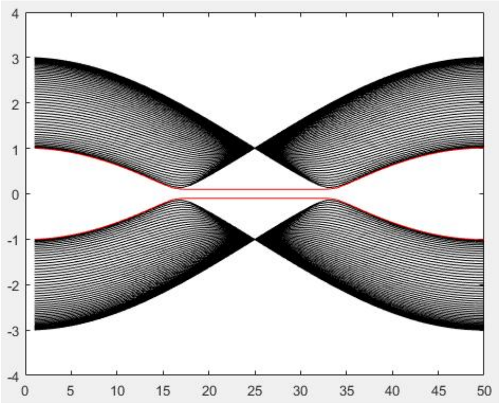
$$-ic^\dagger_{R_i,B} c_{R_i+R_1+R_2,B} + ic^\dagger_{R_i,B} c_{R_i+R_1,B} + ic^\dagger_{R_i,B} c_{R_i+R_2,B} + \mathrm{h.}c.$$

Periodic in one direction and zig-zag open boundary in the other direction

$t_1 = 1,\ m = 0,\ t_H = 0$



$t_1 = 1,\ m = 0.1,\ t_H = 0$



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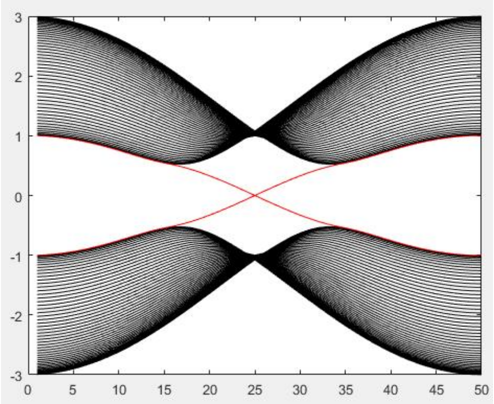

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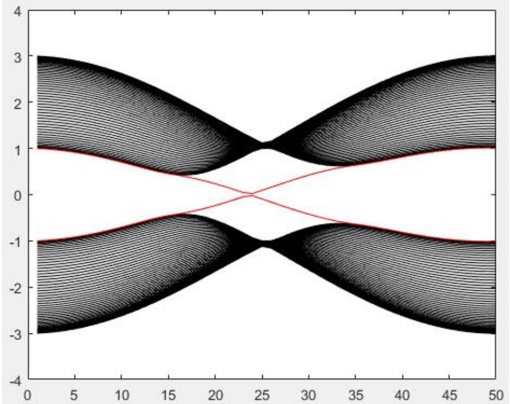
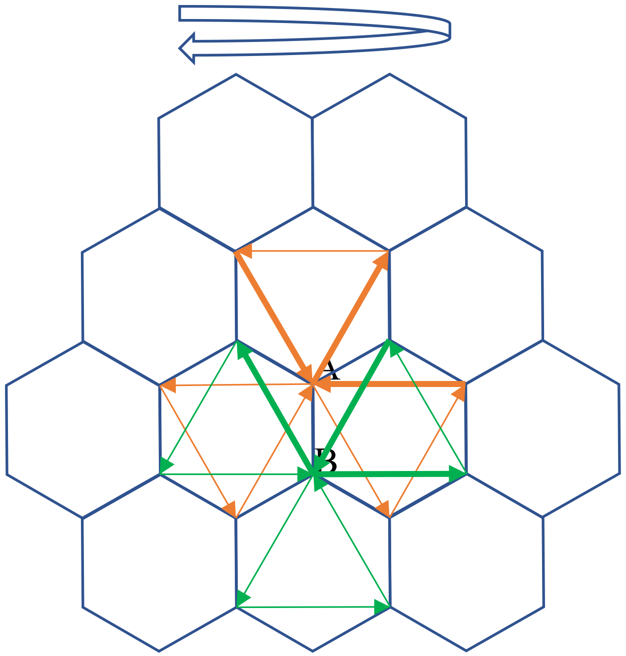
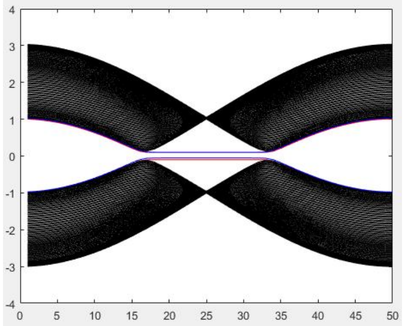
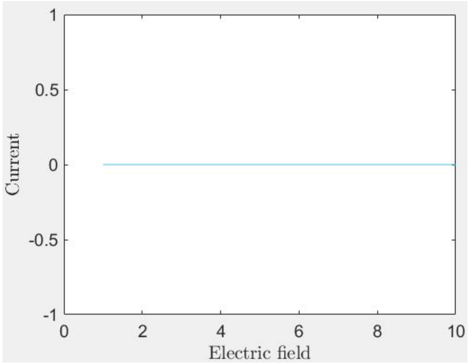


Edge mode and topology



$t_1 = 1,\ m = 0.1,\ t_H = 0$

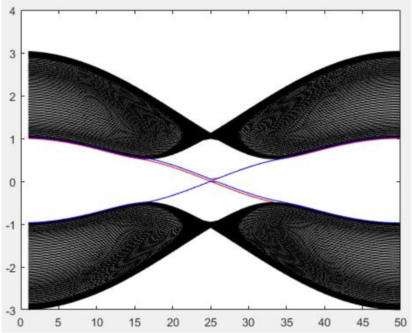


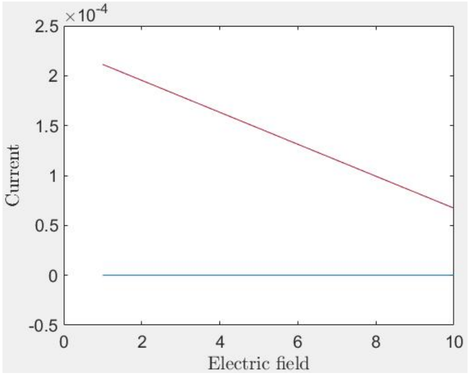



```
js1 =

     0
```

$t_1 = 1,\ m = 0,\ t_H = 0.1$

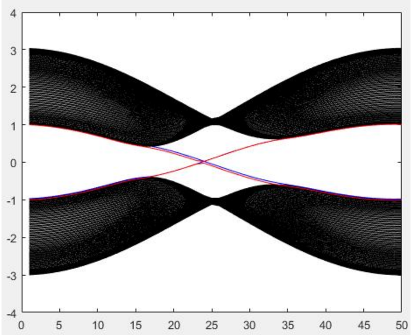


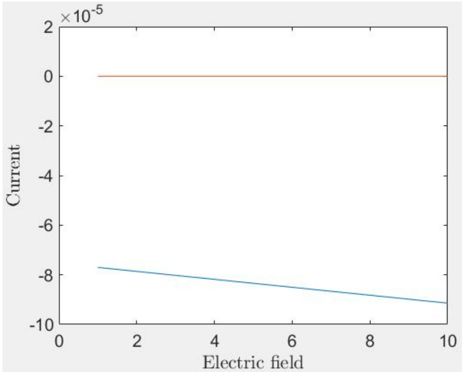



```
js1 =

  -1.0061 - 0.0000i
```

$t_1 = 1,\ m = 0.1,\ t_H = 0.1$



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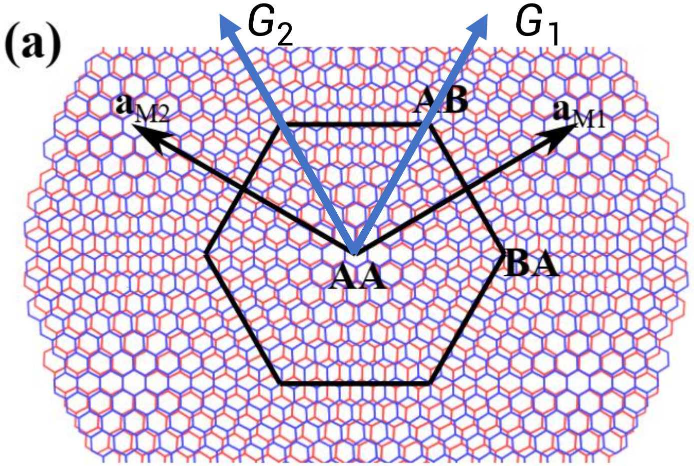
js1 =

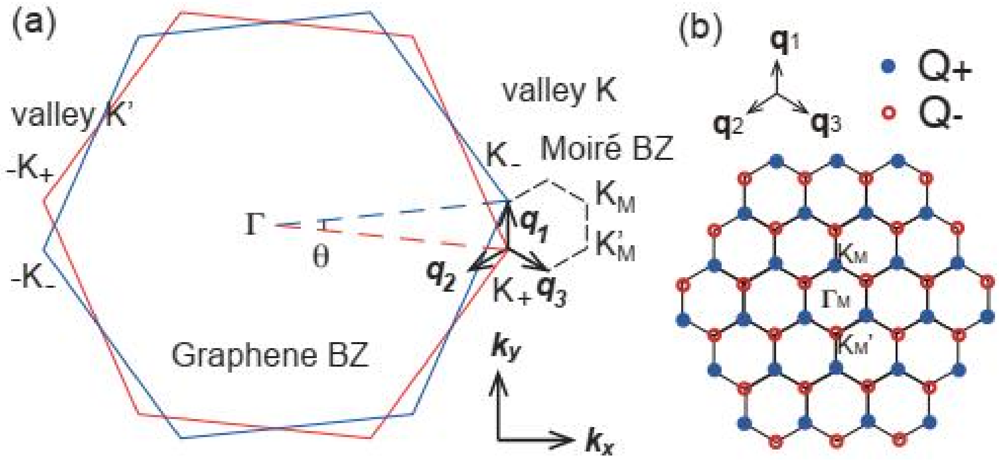
  -1.0049 - 0.0000i
```

Magic angle twisted bilayer graphene (MATBG)

1. ‘G’ in TBG
2. BM model for TBG
   - Moiré potential
   - Momentum space form and dispersion
   - Symmetry breaking and transport
3. Strong correlation in MATBG

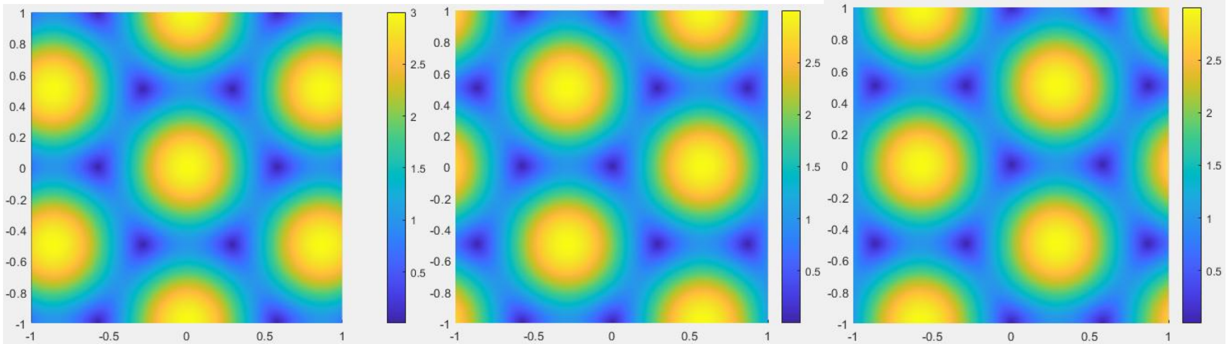
Moiré potential and symmetry





$$H(r) = -iv_F \begin{pmatrix} \partial_r \cdot \sigma & 0 \\ 0 & \partial_r \cdot \sigma \end{pmatrix} + \begin{pmatrix} 0 & T(r) \\ T^\dagger(r) & 0 \end{pmatrix}$$

$$T(r) = \sum_{j=1}^{3} e^{-iq_j \cdot r} \cdot \begin{pmatrix} u_0 & u_1 e^{-i\frac{2\pi(j-1)}{3}} \\ u_1 e^{i\frac{2\pi(j-1)}{3}} & u_0 \end{pmatrix}$$



AA hopping | BA hopping | AB hopping

$$q_1 = \frac{G_2 + G_1}{3}, \; q_2 = \frac{G_2 - 2G_1}{3}, q_3 = \frac{G_1 - 2G_2}{3}$$

$$r_{BA} = \frac{a_{M1} - a_{M2}}{3}, \; r_{AB} = \frac{2a_{M1} + a_{M2}}{3}$$

Momentum space form and dispersion

$$H(r) = -iv_F \begin{pmatrix} \partial_r \cdot \sigma & 0 \\ 0 & \partial_r \cdot \sigma \end{pmatrix} + \begin{pmatrix} 0 & T(r) \\ T^\dagger(r) & 0 \end{pmatrix}$$

$$T(r) = \sum_{j=1}^{3} e^{-iq_j \cdot r} \cdot \begin{pmatrix} u_0 & u_1 e^{-i\frac{2\pi(j-1)}{3}} \\ u_1 e^{i\frac{2\pi(j-1)}{3}} & u_0 \end{pmatrix}$$

$$c_r^\dagger = \frac{1}{\sqrt{N}} \sum_{k_1} e^{ik_1 \cdot r} c_{k_1}^\dagger$$

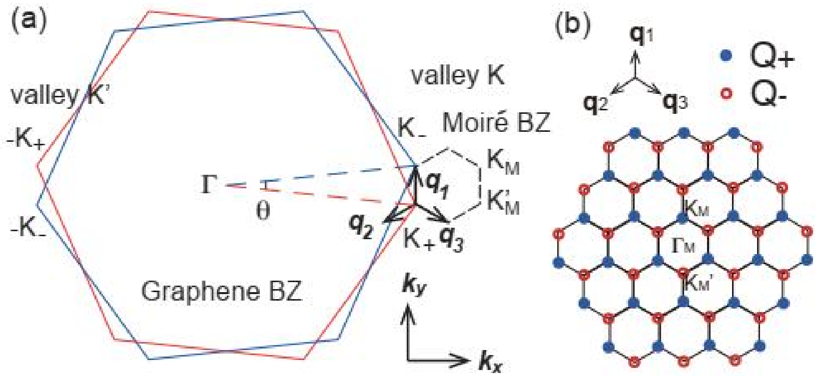
$$c_r = \frac{1}{\sqrt{N}} \sum_{k_2} e^{-ik_2 \cdot r} c_{k_2}$$

From $H(r)$ to $H^\tau(k)$

$$-iv_F \begin{pmatrix} \partial_r \cdot \sigma & 0 \\ 0 & \partial_r \cdot \sigma \end{pmatrix} \to v_F \begin{pmatrix} (k-K_-) \cdot \sigma & 0 \\ 0 & (k-K_+) \cdot \sigma \end{pmatrix} \delta_{k_1,k_1'}$$

$$\sum_{j=1}^{3} e^{-iq_j \cdot r} \to \frac{1}{N\Omega} \sum_{j=1}^{3} \sum_{k_1} \sum_{k_2} \int d^2 r \, e^{i(k_1 - k_2 - q_j) \cdot r}$$
$$= \frac{1}{N} \sum_{j=1}^{3} \sum_{k_1} \sum_{k_2} \delta_{k_1,\, k_2+q_j} = \sum_{k_1} \sum_{j=1}^{3} \delta_{k_1,k_1'-q_1+q_j}$$
$$= \sum_{k_1} (\delta_{k_1,k_1'} + \delta_{k_1,k_1'-G_1} + \delta_{k_1,k_1'-G_2})$$

$$T(r) \to \begin{pmatrix} u_0 & u_1 \\ u_1 & u_0 \end{pmatrix} \delta_{k_1,k_1'} + \begin{pmatrix} u_0 & u_1 e^{-i\frac{2\pi}{3}} \\ u_1 e^{i\frac{2\pi}{3}} & u_0 \end{pmatrix} \delta_{k_1,k_1'-G_1} + \begin{pmatrix} u_0 & u_1 e^{i\frac{2\pi}{3}} \\ u_1 e^{-i\frac{2\pi}{3}} & u_0 \end{pmatrix} \delta_{k_1,k_1'-G_2}$$



$$q_1 = \frac{G_2 + G_1}{3},\ q_2 = \frac{G_2 - 2G_1}{3}, q_3 = \frac{G_1 - 2G_2}{3}$$

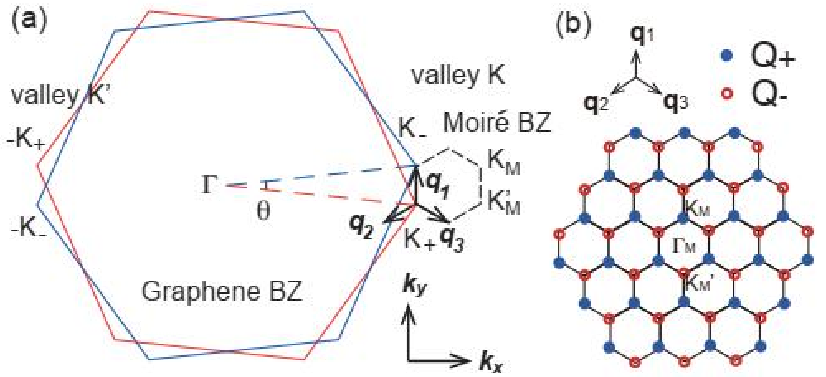
Momentum space form and dispersion

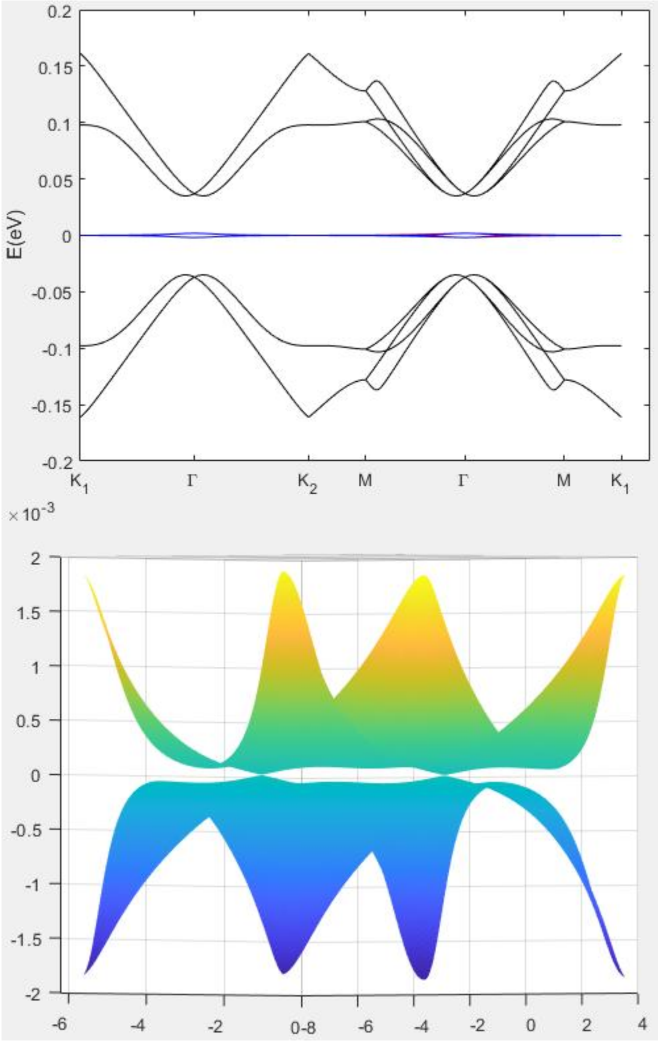
$$H^{\tau}(k) = v_F \begin{pmatrix} (k-K_-)\cdot\sigma & 0 \\ 0 & (k-K_+)\cdot\sigma \end{pmatrix} \delta_{k_1,k_1'} + \begin{pmatrix} 0 & U^{\tau} \\ U^{\tau\dagger} & 0 \end{pmatrix}$$

$$U^{\tau} = \begin{pmatrix} u_0 & u_1 \\ u_1 & u_0 \end{pmatrix} \delta_{k_1,k_1'} + \begin{pmatrix} u_0 & u_1 e^{-i\frac{2\pi}{3}} \\ u_1 e^{i\frac{2\pi}{3}} & u_0 \end{pmatrix} \delta_{k_1,k_1'-G_1} + \begin{pmatrix} u_0 & u_1 e^{i\frac{2\pi}{3}} \\ u_1 e^{-i\frac{2\pi}{3}} & u_0 \end{pmatrix} \delta_{k_1,k_1'-G_2}$$

$$H^{-\tau}(k) = v_F \begin{pmatrix} (-k-K_-)\cdot\sigma^* & 0 \\ 0 & (-k-K_+)\cdot\sigma^* \end{pmatrix} \delta_{k_1,k_1'} + \begin{pmatrix} 0 & U^{-\tau} \\ U^{-\tau\dagger} & 0 \end{pmatrix}$$

$$U^{-\tau} = \begin{pmatrix} u_0 & u_1 \\ u_1 & u_0 \end{pmatrix} \delta_{k_1,k_1'} + \begin{pmatrix} u_0 & u_1 e^{i\frac{2\pi}{3}} \\ u_1 e^{-i\frac{2\pi}{3}} & u_0 \end{pmatrix} \delta_{k_1,k_1'+G_1} + \begin{pmatrix} u_0 & u_1 e^{-i\frac{2\pi}{3}} \\ u_1 e^{i\frac{2\pi}{3}} & u_0 \end{pmatrix} \delta_{k_1,k_1'+G_2}$$





$$(\theta, v_F/a_0, u_0, u_1) = (1.08°, 2.38eV, 0.08eV, 0.11eV)$$

Symmetry breaking and transport

- $C_{2z}T$

$$(\sigma_x K)H(r)(\sigma_x K) = H(-r)$$

- C_{3z}

$$e^{i\frac{2\pi}{3}\sigma_z}H(r)e^{-i\frac{2\pi}{3}\sigma_z} = H(C_{3z}r)$$

- C_{2x}

$$(\tau_x\sigma_x)H(r)(\tau_x\sigma_x) = H(C_{2x}r)$$

- P

$$(i\tau_y)H(r)(-i\tau_y) =- H(-r)$$

$$H(r) =- iv_F\begin{pmatrix} \partial_r\cdot\sigma & 0 \\ 0 & \partial_r\cdot\sigma \end{pmatrix} + \begin{pmatrix} 0 & T(r) \\ T^{\dagger}(r) & 0 \end{pmatrix}$$

$$T(r) = \sum_{j=1}^{3} e^{-iq_j\cdot r}\cdot\begin{pmatrix} u_0 & u_1 e^{-i\frac{2\pi(j-1)}{3}} \\ u_1 e^{i\frac{2\pi(j-1)}{3}} & u_0 \end{pmatrix}$$

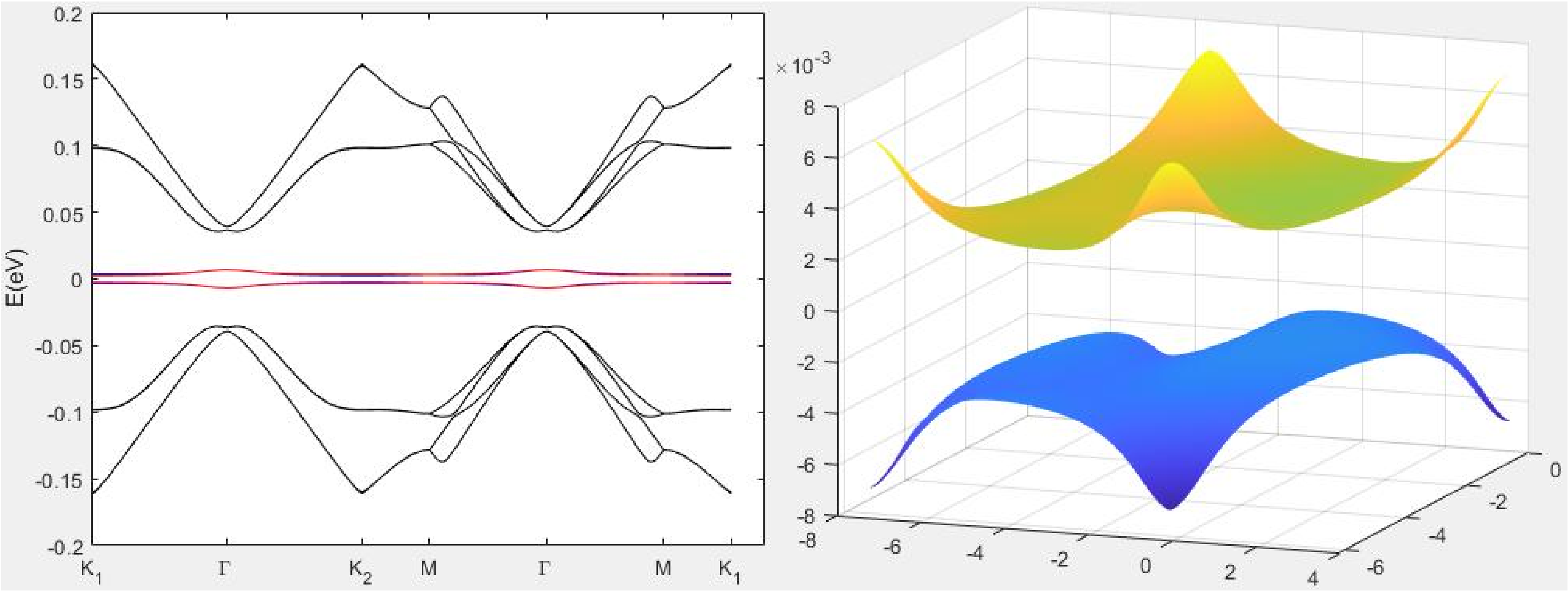
Symmetry breaking and transport

- Break $C_{2z}T$ with hBN term

$$H_{\Delta}^{T} = \delta_{\boldsymbol{k},\boldsymbol{k}'} \begin{pmatrix} \Delta_1 \sigma_z & 0 \\ 0 & \Delta_2 \sigma_z \end{pmatrix}$$

Valley hall effect is allowed

(*T* is not broken)



$\Delta_1 = 0, \Delta_2 = 0.017\text{eV}$

Symmetry breaking and transport

- Break C_{3z} with strain

$$\boldsymbol{x}' = \begin{pmatrix} \frac{1}{1+\epsilon} & 0 \\ 0 & \frac{1}{1-\delta\epsilon} \end{pmatrix} \boldsymbol{x} \approx \begin{pmatrix} 1-\epsilon & 0 \\ 0 & 1+\delta\epsilon \end{pmatrix} \boldsymbol{x}$$

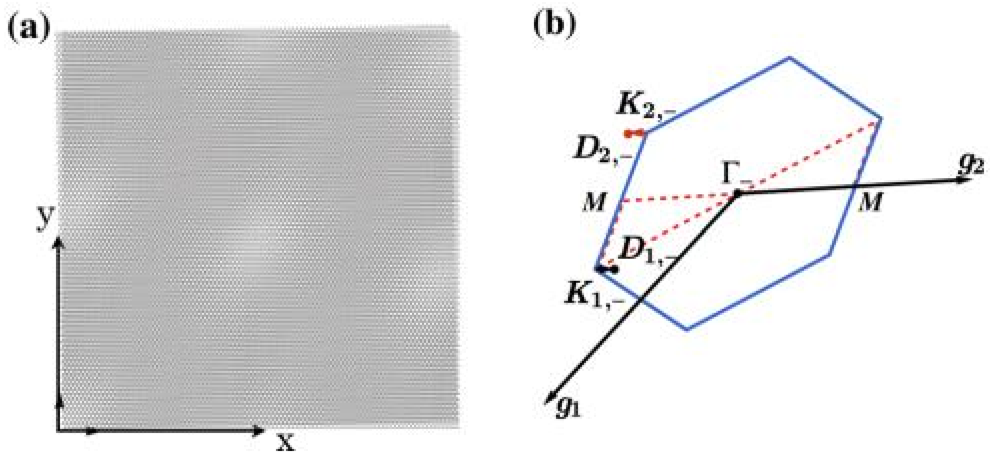
$$S(\epsilon,\theta) = \begin{pmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{pmatrix} \begin{pmatrix} 1-\epsilon & 0 \\ 0 & 1+\delta\epsilon \end{pmatrix} \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix}$$

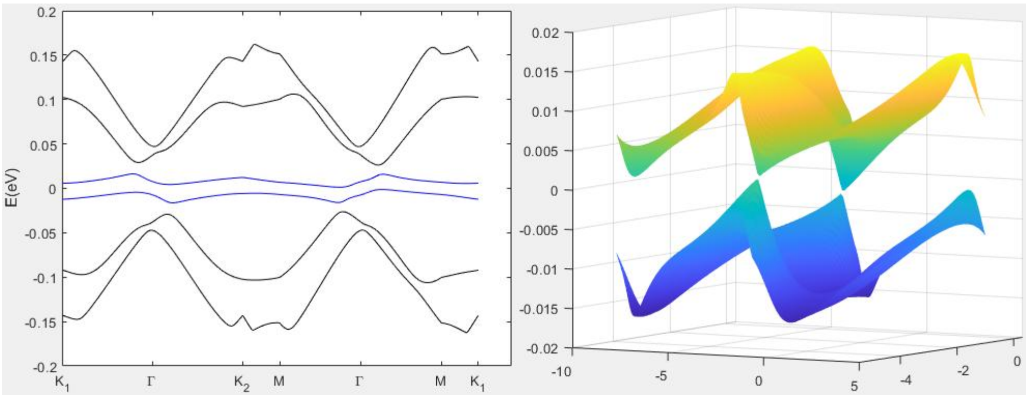
$$\boldsymbol{p}' = S^{-1}(\epsilon,\theta)\boldsymbol{p}$$
$$\boldsymbol{G}_i' = S^{-1}(\epsilon,\theta) \begin{pmatrix} 1 & -a \\ a & 1 \end{pmatrix} \boldsymbol{G}_i - \boldsymbol{G}_i$$

Second harmonic hall effect is allowed once Dirac cone gaps

$$H^{\tau}(k) = v_F \begin{pmatrix} (k-K_-')\cdot\sigma & 0 \\ 0 & (k-K_+')\cdot\sigma \end{pmatrix} \delta_{k_1,k_1'} + \begin{pmatrix} 0 & U'^{\tau} \\ U'^{\tau\dagger} & 0 \end{pmatrix}$$

$$U'^{\tau} = \begin{pmatrix} u_0 & u_1 \\ u_1 & u_0 \end{pmatrix} \delta_{k_1,k_1'} + \begin{pmatrix} u_0 & u_1 e^{-i\frac{2\pi}{3}} \\ u_1 e^{i\frac{2\pi}{3}} & u_0 \end{pmatrix} \delta_{k_1,k_1'-G_1'} + \begin{pmatrix} u_0 & u_1 e^{i\frac{2\pi}{3}} \\ u_1 e^{-i\frac{2\pi}{3}} & u_0 \end{pmatrix} \delta_{k_1,k_1'-G_2'}$$





$\epsilon = 0.4\%, \delta = 0.16, \theta = 45^{\circ}$

Symmetry breaking and transport

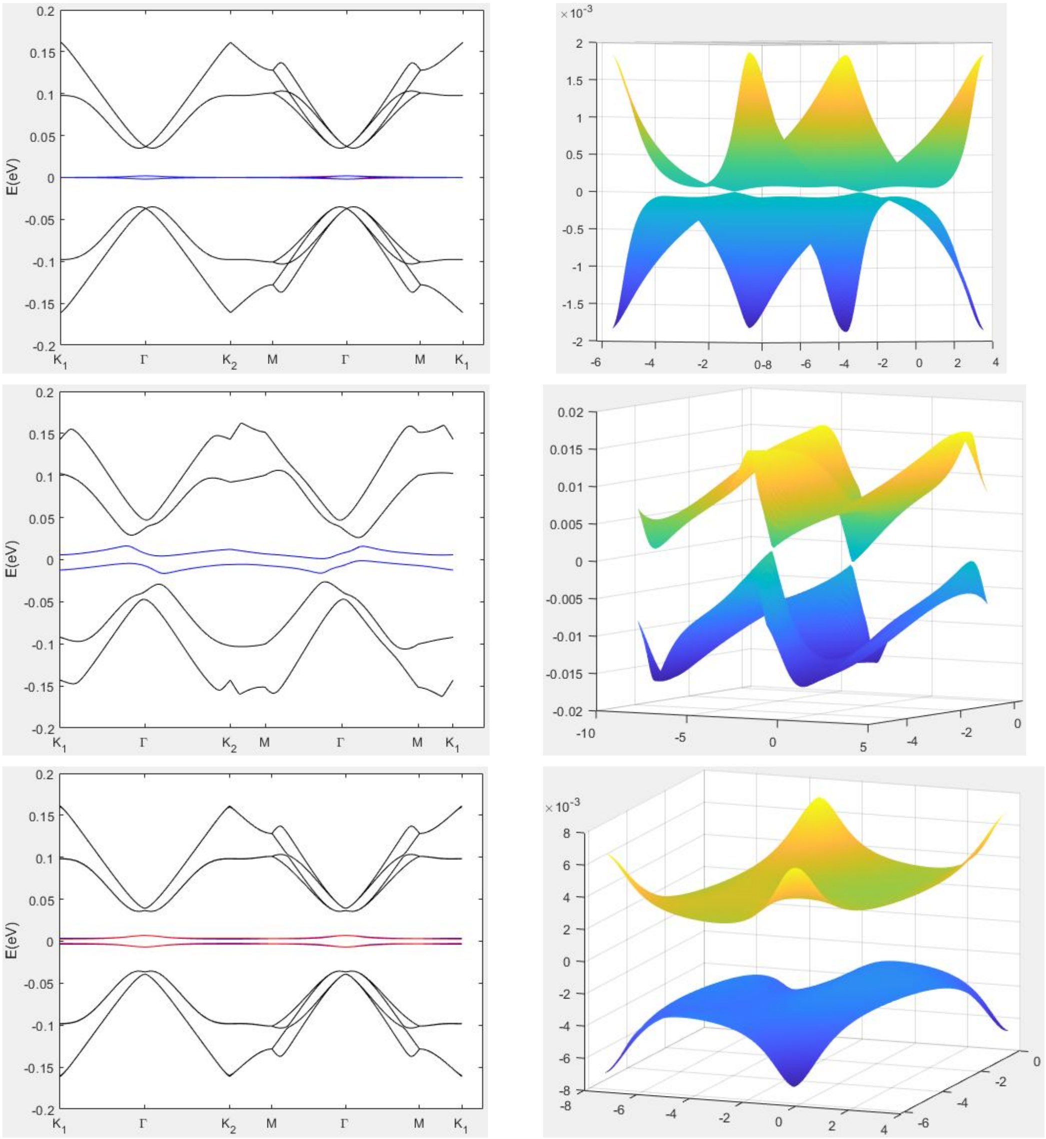
Conclusion for now

1. Original BM model preserve TI and C_{3z} so that Dirac cone will not move or gap.

2. Strain can move Dirac cone away from K point but will not gap it.

3. hBN can gap Dirac cone by breaking Inversion (or C_{2z}) and give non-trivial topology to flat bands.

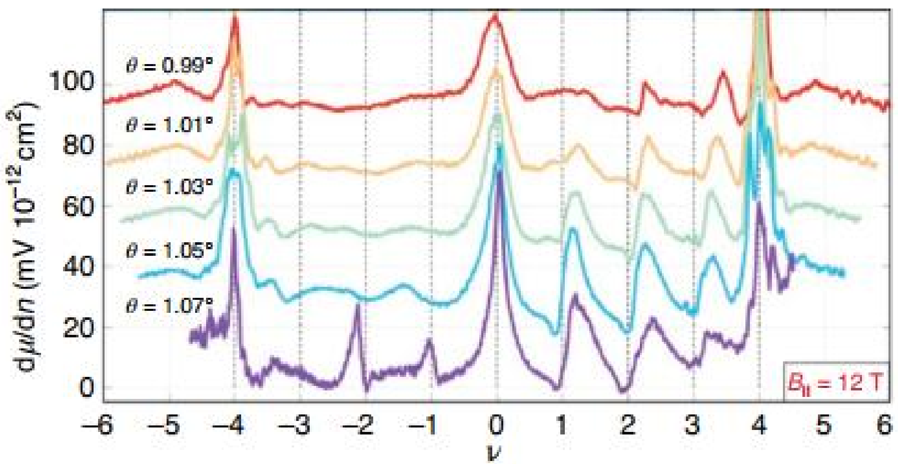
4. T is not broken either by strain or hBN so that no total linear order anomalous hall (second harmonic is allowed).

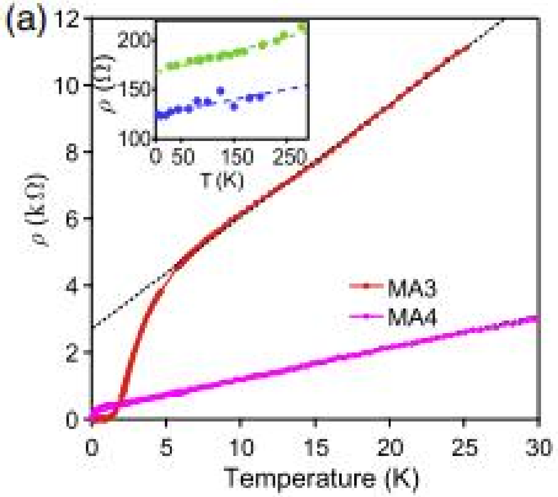


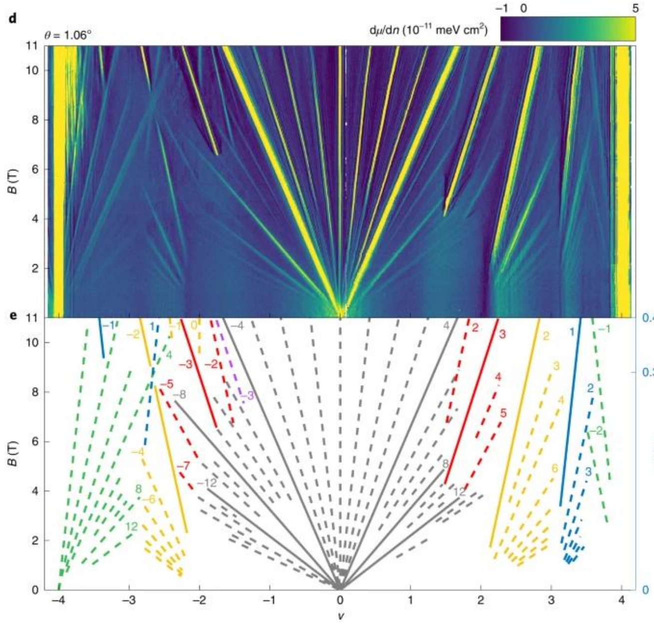
Magic angle twisted bilayer graphene (MATBG)

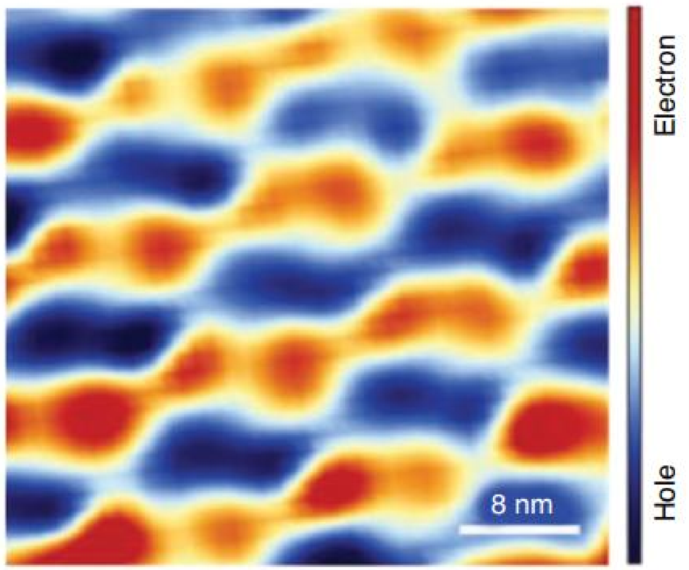
1. ‘G’ in TBG
2. BM model for TBG
3. Strong correlation in MATBG
   - Brief experimental observations
   - Coulomb interaction projected on flat bands
   - Chiral limit and symmetry
   - Exact solutions at integer fillings (take $\nu = 1$ as example)

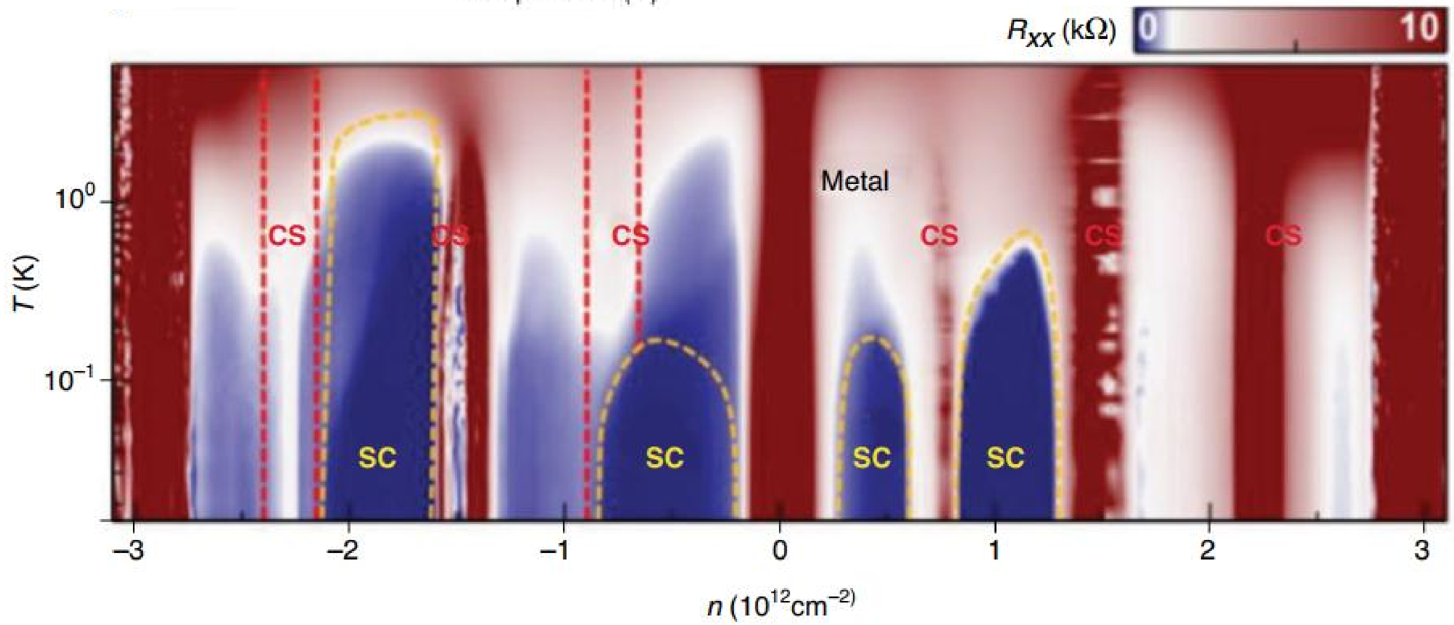
Brief experimental observations











Coulomb interaction projected on flat bands

$$H_I = \frac{1}{2\Omega} \sum_{Q} \sum_{q \in mBZ} V(q+Q)\delta\rho_{q+Q}\delta\rho_{-q-Q}$$

$$\delta\rho_{q+Q} = \sum_{s,\tau} \sum_{k \in mBZ} \sum_{K,X} \left(c^{\dagger}_{k,s,\tau;K,X} c_{k+q,s,\tau;K+Q,X} - \frac{\upsilon+4}{8}\delta_{q,0}\delta_{Q,0}\right) = \delta\rho^{\dagger}_{-q-Q}$$

H_0 diagonalized transformation

$$c^{\dagger}_{k,s,\tau;n} = \sum_{K,X} u_{n,\tau;K,X}(k)\, c^{\dagger}_{k,s,\tau;K,X}$$

$$\delta\rho_{q+Q} = \sum_{k,s,\tau} \sum_{K,X} \left(\sum_{m,n} u^{*}_{K,X;n,\tau}(k) u_{K+Q,X;m,\tau}(k+q)\, c^{\dagger}_{k,s,\tau;n} c_{k+q,s,\tau;m} - \frac{\upsilon+4}{8}\delta_{q,0}\delta_{Q,0}\right)$$

$$= \sum_{k,s,\tau} \sum_{K,X} \left(\sum_{m,n} u^{*}_{K,X;n,\tau}(k) u_{K+Q,X;m,\tau}(k+q)\, \left(c^{\dagger}_{k,s,\tau;n} c_{k+q,s,\tau;m} - \frac{\upsilon+4}{8}\delta_{q,0}\delta_{m,n}\right)\right)$$

$$= \sum_{k,s,\tau} \sum_{m,n} \lambda_{n,m,\tau}(k, k+q+Q)\, \left(c^{\dagger}_{k,s,\tau;n} c_{k+q,s,\tau;m} - \frac{\upsilon+4}{8}\delta_{q,0}\delta_{m,n}\right)$$

Define form factor

$$\lambda_{n,m,\tau}(k, k+q+Q) \equiv \sum_{K,X} u^{*}_{K,X;n,\tau}(k) u_{K+Q,X;m,\tau}(k+q)$$

All the symmetry information is hidden in λ now

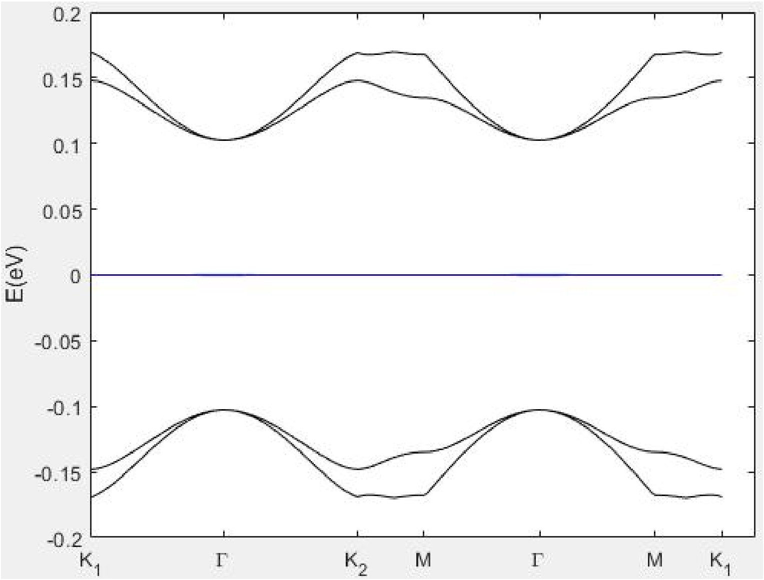
Coulomb interaction projected on flat bands

$$H = \frac{1}{2\Omega} \sum_{Q} \sum_{q \in mBZ} V(q+Q)\,\delta\rho_{q+Q}\,\delta\rho_{-q-Q}$$

$$\delta\rho_{q+Q} = \sum_{k,s,\tau} \sum_{m,n} \lambda_{n,m,\tau}(k, k+q+Q)\left(c^{\dagger}_{k,s,\tau;n} c_{k+q,s,\tau;m} - \frac{\upsilon+4}{8}\delta_{q,0}\delta_{m,n}\right)$$

Ignore remote bands and flat bands dispersion below

Chiral limit and symmetry



BM model review

$$H^{\tau}(k) = v_F \begin{pmatrix} (k-K_-)\cdot\sigma & 0 \\ 0 & (k-K_+)\cdot\sigma \end{pmatrix} \delta_{k_1,k_1'} + \begin{pmatrix} 0 & U^{\tau} \\ U^{\tau\dagger} & 0 \end{pmatrix}$$

$$U^{\tau} = \begin{pmatrix} u_0 & u_1 \\ u_1 & u_0 \end{pmatrix} \delta_{k_1,k_1'} + \begin{pmatrix} u_0 & u_1 e^{-i\frac{2\pi}{3}} \\ u_1 e^{i\frac{2\pi}{3}} & u_0 \end{pmatrix} \delta_{k_1,k_1'-G_1} + \begin{pmatrix} u_0 & u_1 e^{i\frac{2\pi}{3}} \\ u_1 e^{-i\frac{2\pi}{3}} & u_0 \end{pmatrix} \delta_{k_1,k_1'-G_2}$$ ($u_0 = 0$ for chiral limit)

At chiral limit

$$\sigma_z H^{\tau}(k)\sigma_z = -H^{\tau}(k)$$

$$H^{\tau}(k)|\psi_E\rangle = E|\psi_E\rangle = 0$$ ($E = 0$ for chiral limit flat bands)

$$H^{\tau}(k)\sigma_z|\psi_E\rangle = -E\sigma_z|\psi_E\rangle = 0$$

Diagonalize flat bands according to eigenvalue of σ_z (Equivalent to apply an hBN perturbation which gives two bands Chern number ± 1)

$$\begin{pmatrix} \langle\psi_1|\sigma_z|\psi_1\rangle & \langle\psi_1|\sigma_z|\psi_2\rangle \\ \langle\psi_2|\sigma_z|\psi_1\rangle & \langle\psi_2|\sigma_z|\psi_2\rangle \end{pmatrix} \Longrightarrow \begin{cases} |\psi_+\rangle = |\psi_1\rangle + \sigma_z|\psi_1\rangle \\ |\psi_-\rangle = |\psi_1\rangle - \sigma_z|\psi_1\rangle \end{cases} \Longrightarrow \begin{pmatrix} \langle\psi_+|\sigma_z|\psi_+\rangle & \langle\psi_+|\sigma_z|\psi_-\rangle \\ \langle\psi_-|\sigma_z|\psi_+\rangle & \langle\psi_-|\sigma_z|\psi_-\rangle \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

(Chern basis)

Chiral limit and symmetry

Projected Coulomb interaction at flat chiral limit

$$H = \frac{1}{2\Omega}\sum_{G}\sum_{q\in mBZ} V(q+G)\delta\rho_{q+G}\delta\rho_{-q-G}$$

$$\delta\rho_{q+G} = \sum_{k,m,n,s,\tau} \lambda_{m,n,\tau}(k,k+q+G)\left(c^{\dagger}_{k,m,s,\tau}c_{k+q,n,s,\tau} - \frac{\nu+4}{8}\delta_{q,0}\delta_{m,n}\right)$$

$$= \sum_{k,m,n} \lambda_{m,n,\tau}(k,k+q+G)\left(c^{\dagger}_{k,m,s,\tau}c_{k+q,n,s,\tau} + c^{\dagger}_{k,m,-s,\tau}c_{k+q,n,-s,\tau} + \tilde{c}^{\dagger}_{k,m,s,-\tau}\tilde{c}_{k+q,n,s,-\tau} + \tilde{c}^{\dagger}_{k,m,-s,-\tau}\tilde{c}_{k+q,n,-s,-\tau} - \frac{\nu+4}{2}\delta_{q,0}\delta_{m,n}\right)$$

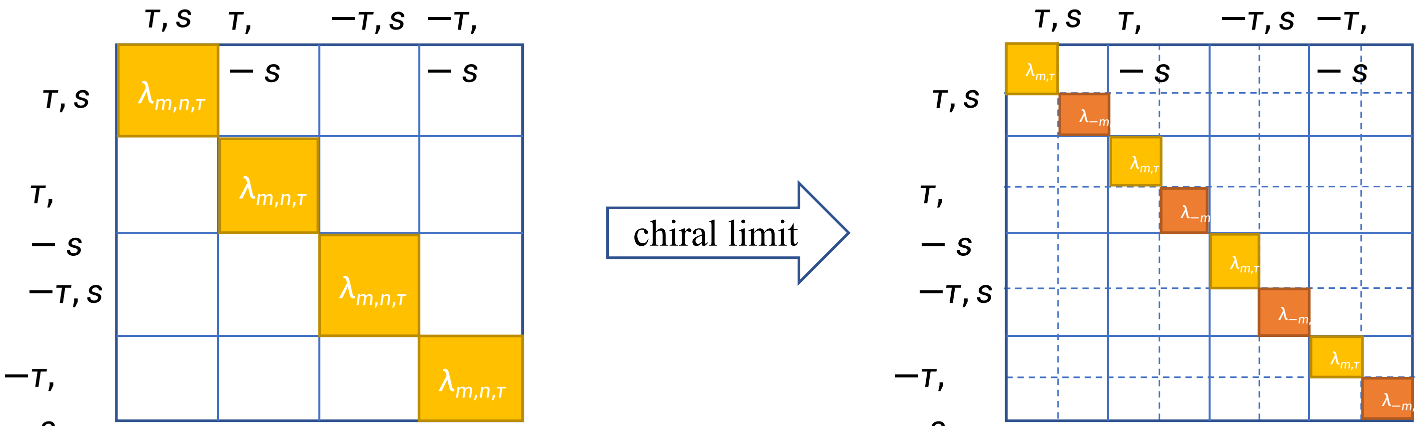
$$= \sum_{k,m} \lambda_{m,\tau}(k,k+q+G)\left(c^{\dagger}_{k,m,s,\tau}c_{k+q,m,s,\tau} + c^{\dagger}_{k,m,-s,\tau}c_{k+q,m,-s,\tau} + \tilde{c}^{\dagger}_{k,m,s,-\tau}\tilde{c}_{k+q,m,s,-\tau} + \tilde{c}^{\dagger}_{k,m,-s,-\tau}\tilde{c}_{k+q,m,-s,-\tau} - \frac{\nu+4}{2}\delta_{q,0}\right)$$

$C_{2z}P$ symmetry, $\lambda_{m,n,\tau}(k,k+q+G) = m\cdot n\cdot\lambda_{-m,-n,-\tau}(k,k+q+G)$

$\tilde{c}^{\dagger}_{k,-m,s,-\tau} = m c^{\dagger}_{k,m,s,-\tau}$

chiral limit

$\langle\psi_+|\psi_-\rangle = 0$



U(4)

U(4) × U(4)

Exact solutions at integer fillings

Find a ground state

$$H_I = \frac{1}{2\Omega}\sum_{G}\sum_{q\in mBZ} V(q+G)\delta\rho_{q+G}\delta\rho_{-q-G}$$

$$\delta\rho_{q+G} = \sum_{k,m}\lambda_{m,\tau}(k,k+q+G)\left(c^{\dagger}_{k,m,s,\tau}c_{k+q,m,s,\tau} + c^{\dagger}_{k,m,-s,\tau}c_{k+q,m,-s,\tau} + \tilde{c}^{\dagger}_{k,m,s,-\tau}\tilde{c}_{k+q,m,s,-\tau} + \tilde{c}^{\dagger}_{k,m,-s,-\tau}\tilde{c}_{k+q,m,-s,-\tau} - \frac{\nu+4}{2}\delta_{q,0}\right)$$

Full fill n Chern bands is one of ground states

$\delta\rho_{q+G}|\psi_0\rangle = \sum_k \lambda_{m,\tau}(k,k+G)(n-(\nu+4))\,|\psi_0\rangle = 0$, when $n-(\nu+4)=0$

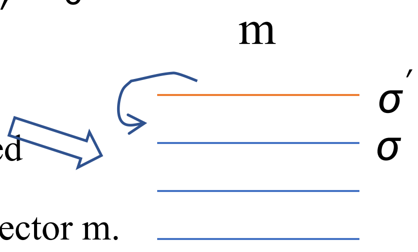
Raising operators within U(4) applying on ground states are also ground states

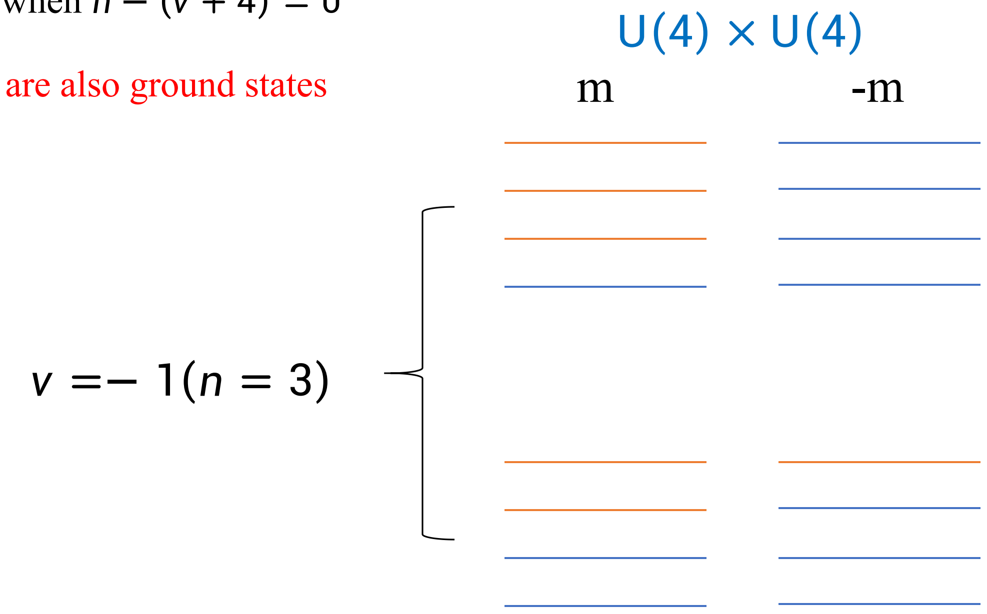
$H_I\Delta^{\dagger}_{m,\sigma,\sigma'}|\psi_0\rangle = \Delta^{\dagger}_{\sigma,\sigma'}H_I|\psi_0\rangle = 0$

$\Delta^{\dagger}_{m,\sigma,\sigma'} \equiv \sum_k c^{\dagger}_{k,m,\sigma}c_{k,m,\sigma'}$

$\sigma,\ \sigma'$ for empty and occupied

spin-valley U(4) in Chern sector m.



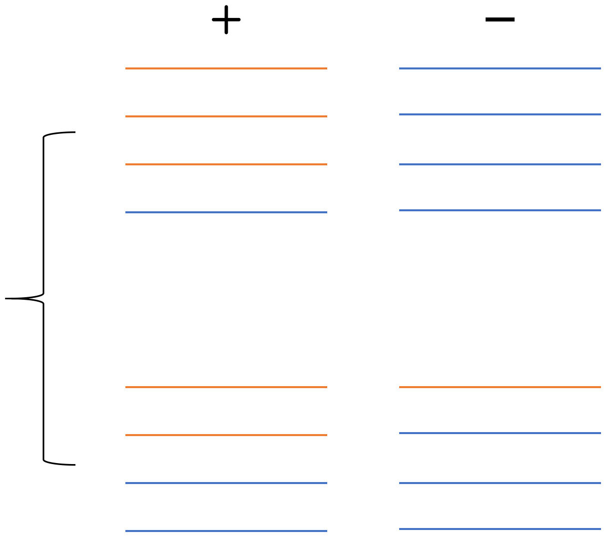


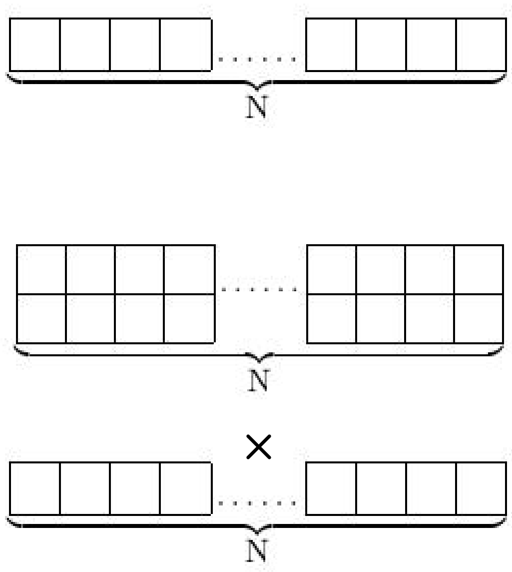
Exact solutions at integer fillings

Ground state degeneracy by SU(4) Young diagram

$U(4) \times U(4)$	Young diagram	Degeneracy	Chern number
		$\dfrac{(N+3)(N+2)(N+1)}{3!}$	$C = 3$
		$\dfrac{(N+3)^2(N+2)^3(N+1)^2}{3!\,3!\,2!}$	$C = 1$

$v =- 1(n = 3)$





Exact solutions at integer fillings

All ground states can be expressed by a given ground state and U(4) generators

$|\psi_g\rangle = \prod_{\sigma,\sigma',m} (\Delta^\dagger_{m,\sigma,\sigma'})^{a_{m,\sigma,\sigma'}} |\psi_0\rangle \qquad (\Delta^\dagger_{m,\sigma,\sigma'} \equiv \sum_k c^\dagger_{k,m,\sigma} c_{k,m,\sigma'})$

Single particle excitation

$H_I c^\dagger_{k,m,\sigma}|\psi_g\rangle = [H_I, c^\dagger_{k,m,\sigma}]|\psi_g\rangle$

$= \frac{1}{2\Omega}\sum_G \sum_{q\in mBZ} V(q+G)\delta\rho_{q+G}[\delta\rho_{-q-G}, c^\dagger_{k,m,\sigma}]\,|\psi_g\rangle$

$= \frac{1}{2\Omega}\sum_G \sum_{q\in mBZ} V(q+G)\,[\delta\rho_{q+G},[\delta\rho_{-q-G}, c^\dagger_{k,m,\sigma}]]\,|\psi_g\rangle$

$= \frac{1}{2\Omega}\sum_G \sum_{q\in mBZ} V(q+G)\lambda_{m,\sigma}(k+q+G,k)\lambda_{m,\sigma}(k,k+q+G)\; c^\dagger_{k,m,\sigma}|\psi_g\rangle$

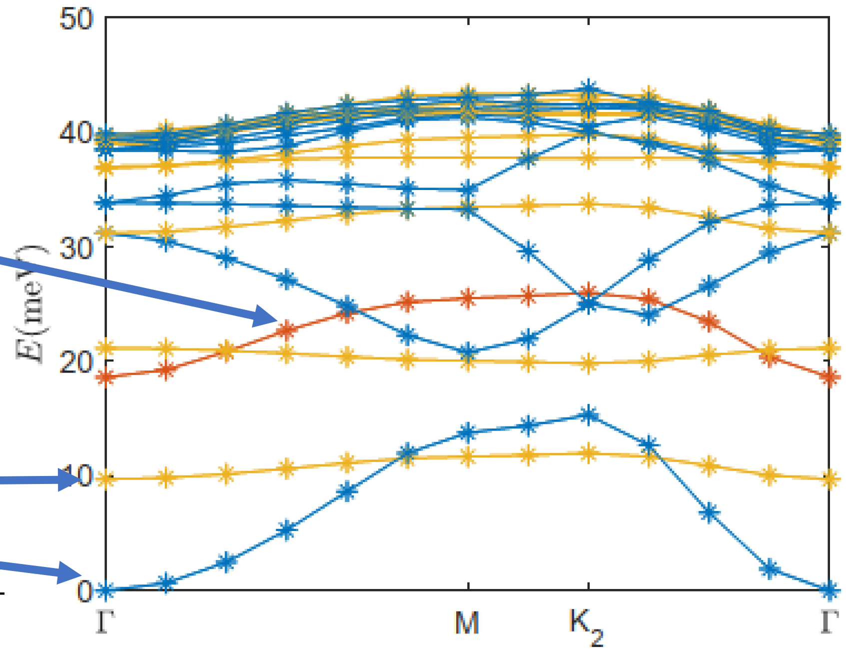
Two particle charge neutral excitation

$H_I c^\dagger_{k,m,\sigma_1} c_{k+p,n,\sigma_2}|\psi_g\rangle = [H_I, c^\dagger_{k,m,\sigma_1} c_{k+p,n,\sigma_2}]|\psi_g\rangle$

$= \frac{1}{2\Omega}\sum_G \sum_{q\in mBZ} V(q+G)\,[\delta\rho_{q+G},[\delta\rho_{-q-G}, c^\dagger_{k,m,\sigma_1} c_{k+p,n,\sigma_2}]]\,|\psi_g\rangle$

$= \frac{1}{2\Omega}\sum_G \sum_{q\in mBZ} V(q+G)[\lambda_{m,\sigma_1}(k,k+q+G)\lambda_{m,\sigma_1}(k+q+G,k)c^\dagger_{k,m,\sigma_1} c_{k+p,n,\sigma_2}$

$-2\lambda_{m,\sigma_1}(k+p,k+p+q+G)\lambda_{n,\sigma_2}(k+q+G,k)c^\dagger_{k+q,m,\sigma_1} c_{k+q+p,n,\sigma_2} + \lambda_{n,\sigma_2}(k+p+q+$



Main References

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4. Correlated Hofstadter spectrum and flavour phase diagram in magic-angle twisted bilayer graphene, Jiachen Yu, etc.
5. Strange Metal in Magic-Angle Graphene with near Planckian Dissipation, Yuan Cao, etc.
6. Designing flat bands by strain, Zhen Bi, etc.
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Thanks

Next time:

Quantum Monte Carlo (QMC) in momentum space

2.1 Write down QMC in momentum space

2.2 Sign problem and sign bounds theory

2.3 QMC for 2D flat bands systems