Insulating phases in twisted bilayer graphene

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Quantum Fluids of Light and Matter
July 2022

Acknowledgments

Theory


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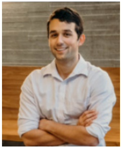
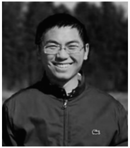
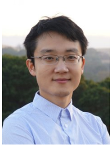

Aditya Cowsik


Zhi-Da Song


Biao Lian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Experiment


Myungchul Oh


Kevin P. Nuckolls


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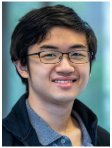

Ryan L. Lee

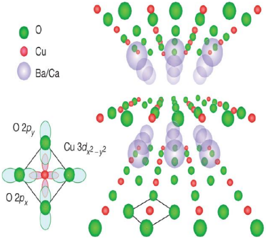

Ali Yazdani

References:

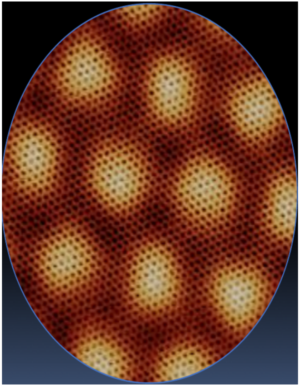
TBG I, II, III, IV, V, VI, PRB (2021), ArXiv:2110.15300, arxiv:220x.yyyyy.

Motivation: Engineering correlations

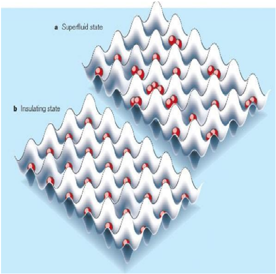
Material chemistry
few eVs



Moiré superlattices from 2D materials
$\simeq 10\mathrm{nm}$



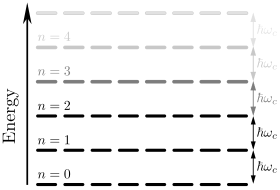
Cold atoms and optical lattices
$\simeq 1\mu\mathrm{m}$



See e.g. Kennes et al. Nature Physics (2021).

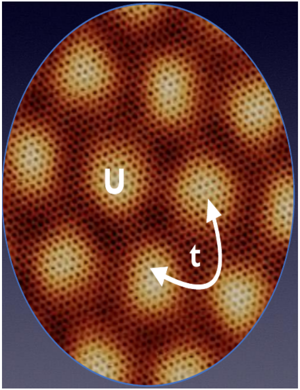
Motivation: Engineering correlations+topology

Flat bands with topology

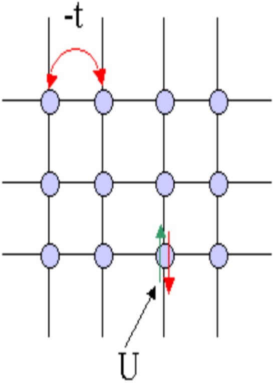


e.g., Landau levels.

Twisted bilayer graphene



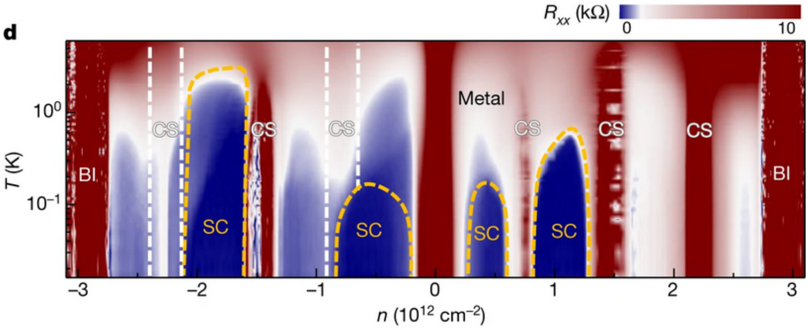
Correlated materials



e.g., Hubbard model

Goal: find simple analytical models to capture the emerging physics.

Why getting excited about moiré materials?

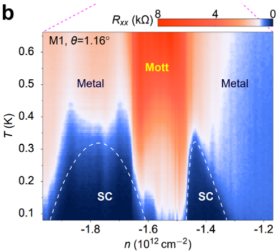


Lu et al. (Efetov Nature) (2019)

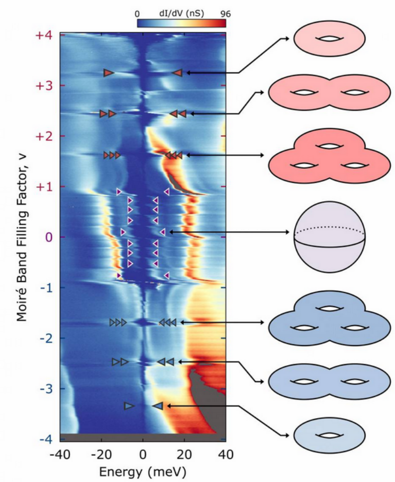
CS correlated state, SC superconducting state,...

Insulator states in TBG: Outline

- Single-particle physics
- Turning on the interaction
- Exact low energy states
- Reality check



Cao et al, Nature 556, 43 and 80 (2018).



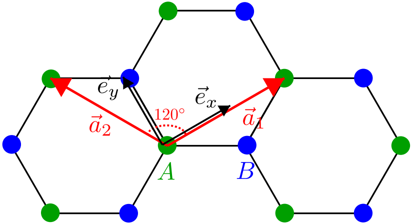
Nuckolls, K.P., Oh, M., Wong, D. et al. Nature (2020)

I- TBG: Single-particle physics

1- Graphene

Honeycomb lattice 2 atoms per unit cell

2 sublattices A and B.
(identical carbon atoms)



distance between two NN A and B atoms

$a \simeq 0.142$ nm

one π electron per carbon atom $\longrightarrow$ 2 e^- per unit cell, i.e., half filling taking into account spin.

$\vec{a_1} = \sqrt{3}\, a\, \vec{e_x}$, $\vec{a_2} = \frac{3}{2} a\, \vec{e_y} - \frac{\sqrt{3}}{2} a\, \vec{e_x}$

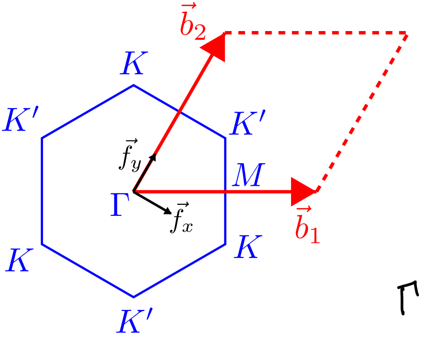
Brillouin zone

$$\vec{a}_i \cdot \vec{b}_j = 2\pi \, \delta_{i,j} \qquad \vec{e}_i \cdot \vec{f}_j = 2\pi \, \delta_{i,j}$$

$$\vec{b}_2 = \frac{4\pi}{3a} \vec{f}_y$$

$$\vec{b}_1 = \frac{2\pi}{3} \left(\vec{f}_x + \frac{1}{\sqrt{3}} \vec{f}_y \right)$$

$$= \frac{4\pi}{3a} \left(\frac{\sqrt{3}}{2} \vec{f}_x + \frac{1}{2} \vec{f}_y \right)$$



Γ, M, K and K' are the high symmetry points

Bloch Hamiltonian

$$\vec{k} = k_1 \vec{b}_1 + k_2 \vec{b}_2$$

hopping amplitude $t \simeq 3\,eV$

$$H(k) = t \begin{array}{c} \begin{pmatrix} 0 & 1 + e^{i\vec{k}\vec{a}_2} + e^{-i\vec{k}\vec{a}_1} \\ 1 + e^{-i\vec{k}\vec{a}_2} + e^{i\vec{k}\vec{a}_1} & 0 \end{pmatrix} \end{array} \begin{array}{c} A \\ B \end{array}$$

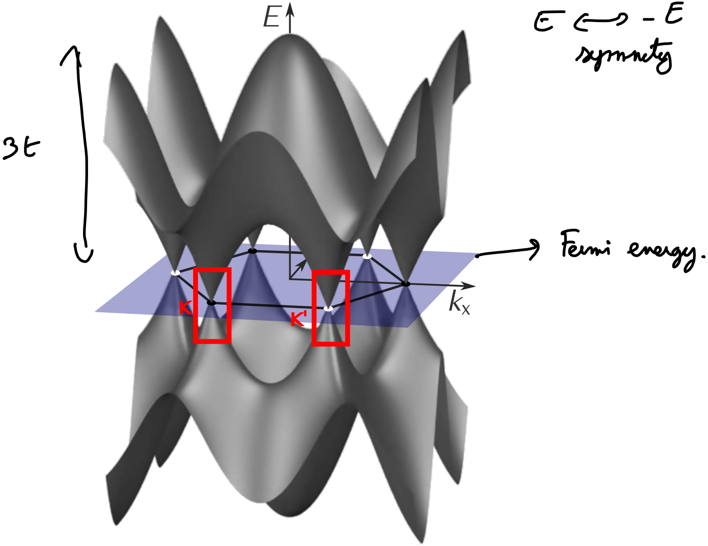
(bipartite lattice)

unit cell

$$H(k) = t \begin{pmatrix} 0 & f(\vec{k}) \\ f^*(\vec{k}) & 0 \end{pmatrix}$$

with $f(\vec{k}) = 1 + e^{-2\pi i k_1} + e^{2\pi i k_2}$

Graphene band structure



$E \longleftrightarrow -E$
symmetry

Dirac points

$k_1 = k_2 = \frac{1}{3}$ $\qquad \vec{K} = \left(\frac{\vec{b}_1}{3} + \frac{\vec{b}_2}{3}\right)$

$k_1 = k_2 = -\frac{1}{3}$ $\qquad \vec{K}' = -\left(\frac{\vec{b}_1}{3} + \frac{\vec{b}_2}{3}\right)$

$$f(k) = 1 + e^{-2\pi i k_1} + e^{2\pi i k_2}$$

$f(K) = f(K') = 0$ (root of unity)

$$\vec{K}' = -\frac{4\pi}{3a}\frac{\sqrt{3}}{3}\vec{f}_2$$

$$\vec{K} = \frac{4\pi}{3a}\frac{\sqrt{3}}{2}\vec{f}_2$$

- Effective Hamiltonian around K and K'

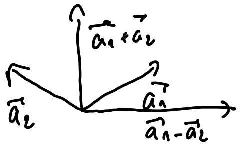
$$\vec{k} = \vec{K} + \delta\vec{k} \qquad \text{(focus on } \vec{K} \text{ first)}$$

$$f(\vec{k}) \simeq 1 + e^{-2\pi i K_1}(1 + i\,\delta\vec{k}\,\vec{a}_1) + e^{2\pi i K_2}(1 + i\,\delta\vec{k}\,\vec{a}_2)$$

$$\simeq i\left(-e^{-2\pi i K_1}\vec{a}_1 + e^{2\pi i K_2}\vec{a}_2\right)\cdot\delta\vec{k}$$

$$\simeq \left[\frac{\sqrt{3}}{2}\underbrace{(\vec{a}_1+\vec{a}_2)} + \frac{1}{2}\,i\,\underbrace{(\vec{a}_1-\vec{a}_2)}\right]\cdot\delta\vec{k}$$

orthogonal vectors.



$$|\vec{a}_1+\vec{a}_2|^2 = 3a^2 \qquad |a_1-a_2|^2 = 3a^2$$

You can define a new basis (x,y) from

$\vec{a}_1 - \vec{a}_2$ and $\vec{a}_1 + \vec{a}_2$

<u>Around K</u>

$$H_K(\delta\vec{k}) = \underbrace{\frac{\sqrt{3}}{2}\, t a}_{v_F \simeq \frac{c}{300}} \; \vec{\sigma}\cdot\delta\vec{k}$$

Fermi velocity

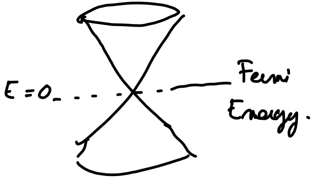
Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$$

Around K'

$$H_{K'}(\delta\vec{k}) = v_F \, \vec{\sigma}^{*}\cdot\delta\vec{k}$$

Two Dirac cones
(related by time reversal symmetry)



2- TBG: Bistritzer MacDonald (BM) model

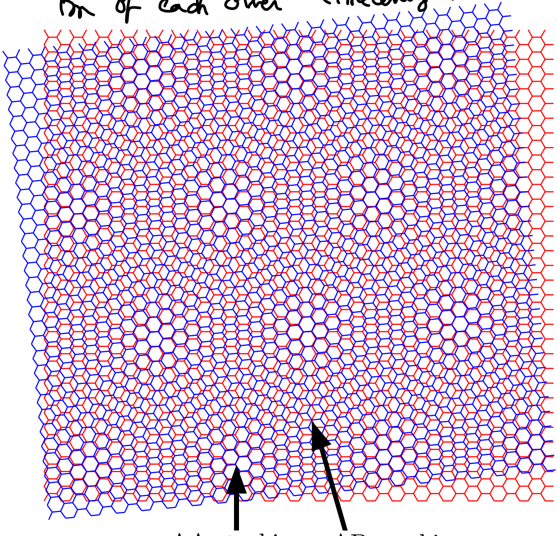
Moiré lattice

8cm

Take two layers of graphenes stacked exactly on top of each other (meaning A sites on top of A sites, B sites on top of B sites)

Now let's rotate ~~them~~ one of them by a small angle θ (rotate the top layer by $\frac{\theta}{2}$ and the bottom layer by $-\frac{\theta}{2}$)

We get a moiré pattern.

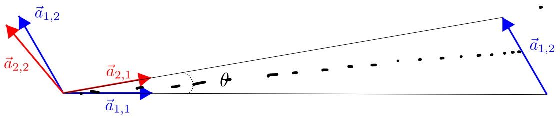


Notice that where you perform the rotation (i.e., the choice of the rotation center) does not matter (up to gauge transformation)

How large is the moiré unit cell?

A rough estimate

when do we meet another AA region



$$\text{length} \simeq \frac{\sqrt{3}\,a}{2\sin\frac{\theta}{2}} \simeq \frac{\sqrt{3}\,a}{\theta}.$$

volume of the moiré unit cell

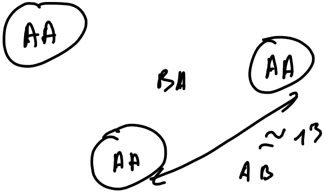
$\simeq \dfrac{1}{\theta^2}$ volume of the graphene unit cell.

for $\theta \simeq 1.05^\circ \simeq 1.83 \times 10^{-2}$ rad

How many carbon atoms within ~~the unit~~ cell.

$$\underbrace{2}_{\text{2 layers}} \times \underbrace{2}_{\substack{\text{2 atoms}\\ \text{per graphene}\\ \text{unit cell}}} \times \frac{1}{\theta^2} \simeq 1.2 \times 10^4 \text{ atoms per moiré unit cell}$$

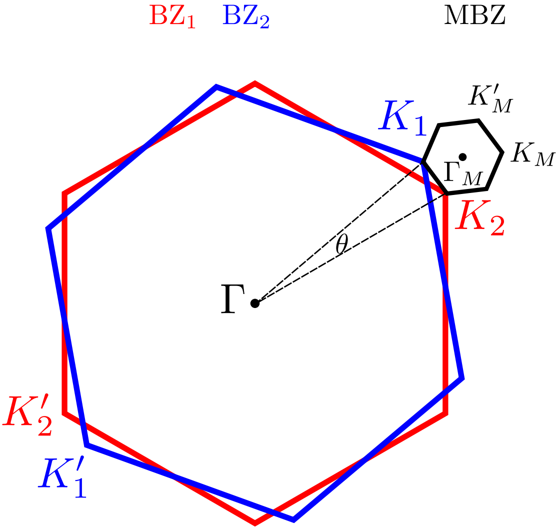
We don't want to deal with a lattice / tight binding model with so many sites $\rightarrow$ continuous model



$\simeq 13$ nm at $\theta \simeq 1.05^\circ$

triangular lattice of AA stacking.

Moiré Brillouin zone



What ingredient do we need?

1) For each layer, simplify by considering only Dirac cone dispersion, assuming no cross talking between K and K'.

2) A continuous description for the coupling between the two layers.

Dirac cone in real space

$$\vec{\sigma} \cdot \vec{k} \longrightarrow -i \vec{\partial} \cdot \vec{\sigma}$$

rotate the top layer by $\frac{\theta}{2}$ $\longrightarrow$

$$i \partial_x \left(\cos\frac{\theta}{2} \sigma_x - \sin\frac{\theta}{2} \sigma_y \right)$$
$$-i \partial_y \left(\cos\frac{\theta}{2} \sigma_y + \sin\frac{\theta}{2} \sigma_x \right)$$

$$\underset{\text{small angles}}{\sim} -i \vec{\partial} \cdot \vec{\sigma} + i \frac{\theta}{2} \vec{\partial} \wedge \vec{\sigma}$$

* rotate the bottom layer by $-\frac{\theta}{2}$: $-i\vec{\partial}\cdot\vec{\sigma} - i\frac{\theta}{2}\vec{\partial}\wedge\vec{\sigma}$.

$$H_0(\vec{r}) = i v_F \begin{pmatrix} \vec{\partial}\cdot\vec{\sigma} + \frac{\theta}{2}\vec{\partial}\wedge\vec{\sigma} & 0 \\ 0 & \vec{\partial}\cdot\vec{\sigma} - \frac{\theta}{2}\vec{\partial}\wedge\vec{\sigma} \end{pmatrix}$$

top layer

bottom layer.

$$= i v_F \left(\tau_0 \, \vec{\partial}\cdot\vec{\sigma} + \frac{\theta}{2} \tau_z \, \vec{\partial}\wedge\vec{\sigma} \right)$$

Pauli matrices for the layer index

Pauli matrices for the sublattice index.

Interlayer hopping

$$H_{\text{interlayer}} = \begin{pmatrix} 0 & T(\mathbf{r}) \\ T^\dagger(\mathbf{r}) & 0 \end{pmatrix}$$

generic expression.
(no intralayer coupling)

BM model

$$T(\mathbf{r}) = \sum_{j=1}^{3} T_j e^{i\mathbf{q}_j \cdot \mathbf{r}}$$

$$T_j = w_0\sigma_0 + w_1 \left[\sigma_x \cos\left(\frac{2\pi(j-1)}{3}\right) + \sigma_y \sin\left(\frac{2\pi(j-1)}{3}\right)\right]$$

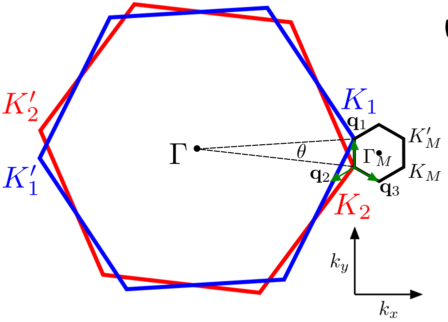
couples A with A, B with B

couple A with B, B with A

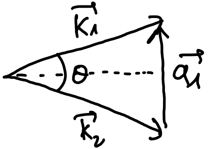
$$T(0) = w_0 \sigma_0$$

origin at AA stacking.

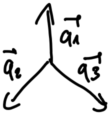
The $\vec{q_i}$'s enforce the periodicity and are related to the distance between 2 K points of the two layers with the same helicity / chirality.



call $|K| = |K_1| = |K_2| = \frac{4\pi}{3\sqrt{3}a} = \frac{4\pi}{3|\vec{a_1}|}$

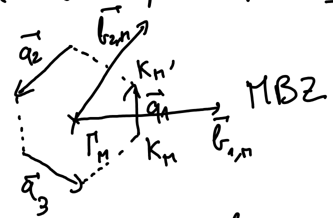


$|\vec{q_1}| = 2|K|\sin\frac{\theta}{2}$



$\vec{q_2}$ and $\vec{q_3}$ obtained by a $\frac{2\pi}{3}$ and $\frac{4\pi}{3}$ rotation.

$|\vec{q}_1|$ is also the distance between the two K points of the moiré Brillouin zone (K_M and K_M')



order of magnitude for w_0 and w_1

$w_1 \simeq 110$ meV

$v_F \simeq 5.9$ eVÅ

(including all the $\hbar$ factors, ...
i.e, $\hbar = c = 2\pi = 1$:))

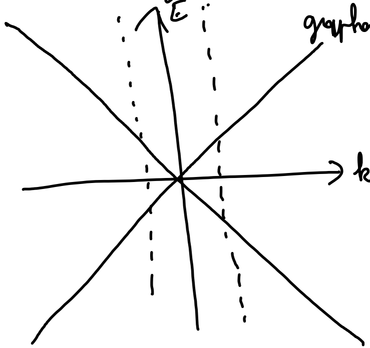
$\frac{w_0}{w_1}$ is of the order of $0.6 - 0.8$ (due to relaxation and corrugation effect)

Band structure

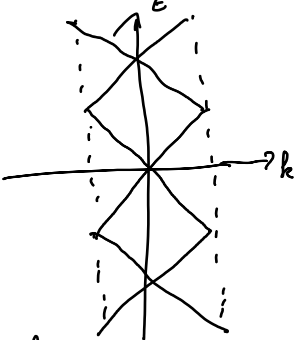
First, discard the $\vec{\partial}\cdot\vec{\sigma}$ term and $T(\vec{r})$.

Paving the graphene BZ with moiré BZ

$\rightarrow$ folding the graphene dispersion (here reduced to a single Dirac cone) into the moiré BZ



$\Longrightarrow$



(remember that $\theta \simeq 10^{-2}$)

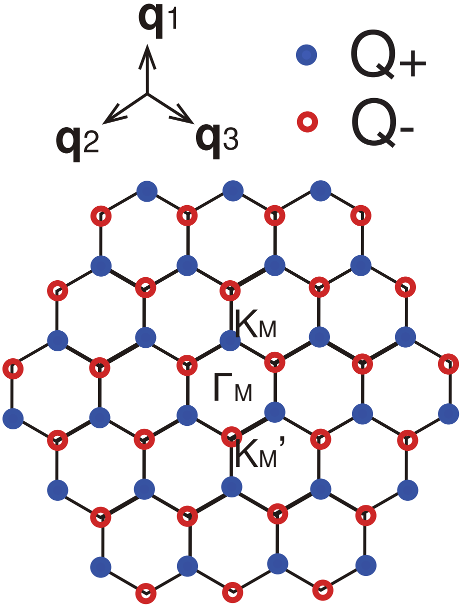
BM in momentum space

$$\hat{H}_0 = \sum_{\mathbf{k}\in \mathrm{MBZ}} \sum_{\eta\alpha\beta s} \sum_{\mathbf{Q}\mathbf{Q}'\in \mathcal{Q}_\pm} \left[h_{\mathbf{Q},\mathbf{Q}'}\left(\mathbf{k}\right)\right]_{\alpha\beta} c^{\dagger}_{\mathbf{k},\mathbf{Q},\alpha} c_{\mathbf{k},\mathbf{Q}',\beta}$$

define in the MBZ

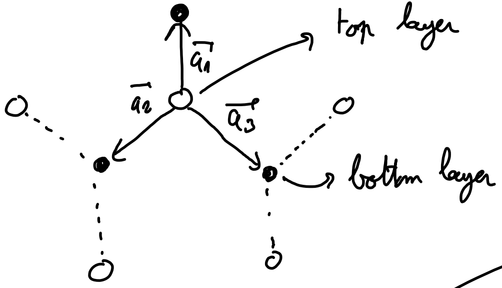
$$h_{\mathbf{Q},\mathbf{Q}'}\left(\mathbf{k}\right) = \underbrace{v_F(\mathbf{k}-\mathbf{Q})\cdot\sigma\delta_{\mathbf{Q},\mathbf{Q}'}}_{\text{Dirac dispersion}} \underbrace{- \lambda v_F \frac{\theta}{2}\xi_Q \delta_{\mathbf{Q},\mathbf{Q}'}\left(\mathbf{k}-Q\right)\wedge\sigma}_{\text{contribution due to the rotation}} + \overbrace{\sum_{j=1}^{3} T_j \delta_{\mathbf{Q},\mathbf{Q}'\pm\mathbf{q}_j}}^{\text{interlayer coupling.}}$$

$$\xi_Q = \begin{cases} +1 & \text{for } Q\in\mathcal{Q}_+ \\ -1 & \text{for } Q\in\mathcal{Q}_- \end{cases}$$



q1
q2
q3
Q+
Q-
KM
ΓM
KM'

What is $q_\pm$? Momentum lattice



q_+ top layer

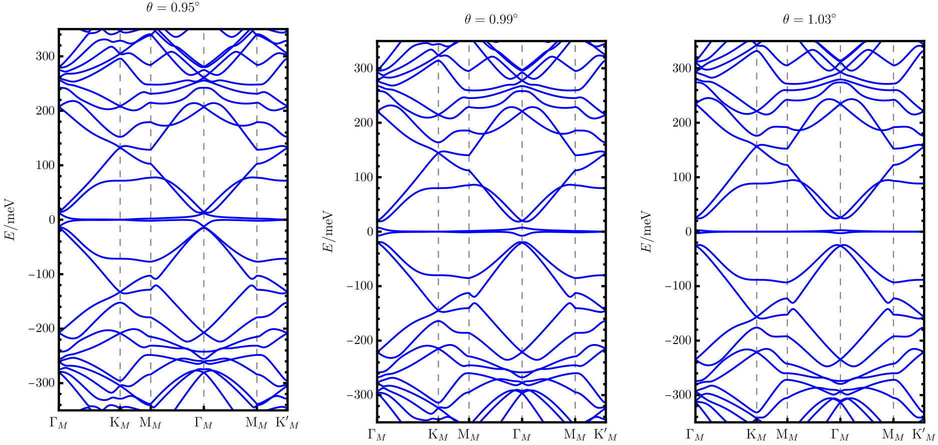
q_- bottom layer.

We encode both which copy of the MBZ and which layer you are looking at.

becomes a "band index" for the folded bands.

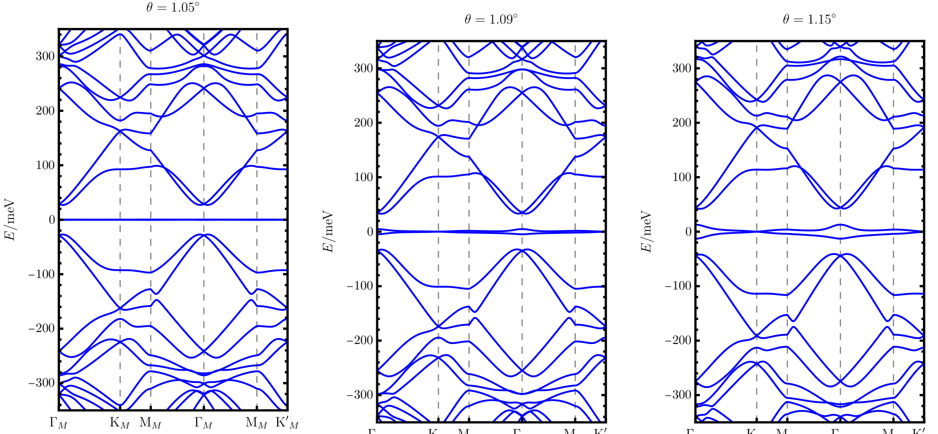
You can center this lattice at different positions (does not matter if you perform an infinite sum, up to a gauge transformation) Most usually Γ or $K_\pm$

TBG band structure: effect of θ



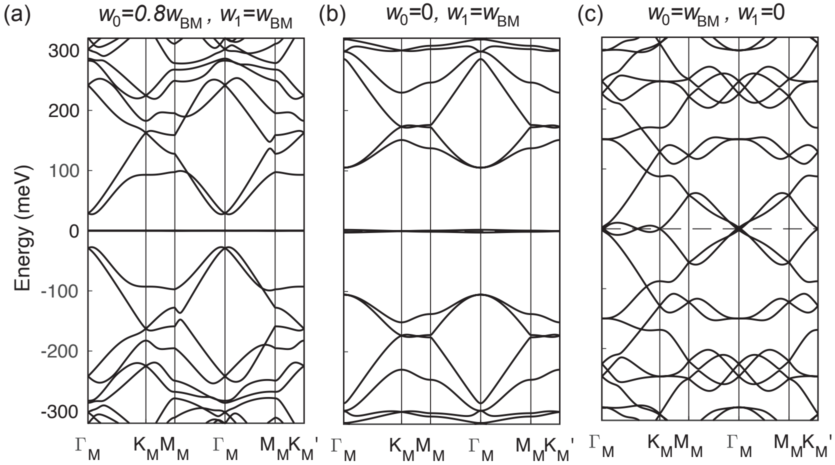
$w_{\mathrm{BM}} = 110\mathrm{meV}, w_0/w_1 = 0.8$

TBG band structure: effect of θ



$w_{\mathrm{BM}} = 110\mathrm{meV}, w_0/w_1 = 0.8$

TBG band structure: effect of w_0, w_1

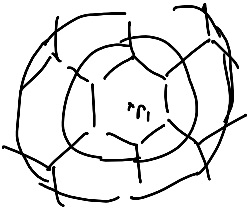


$w_{\mathrm{BM}} = 110\mathrm{meV}, \theta = 1.05^\circ$

For fixed values of w_0 and w_1, certain values of θ lead to two flat bands near zero energy (first magic angle) or more (second magic angles → four flat bands) separated by a clear gap from the other bands

How do we practically compute the band structure?

You can use shells centered around Γ_n.



$$\begin{pmatrix} Sh_{1-1} & Sh_{2-1} & 0 & \cdots & \cdots \\ Sh_{1-2} & Sh_{2-2} & Sh_{3-2} & 0 & \cdots \\ 0 & S_{2-3} & Sh_{3-3} & & \\ \vdots & 0 & & & \end{pmatrix}$$

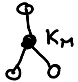
The size of these matrices depends on the shells

How to find the magic angle?

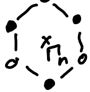
BM → look at the velocity at the K_M point.
and make it vanish for the band.

How to capture it roughly?

* Tripod approximation (lattice centered around K_M)
→ magic angle



* Hexagonal approximation (lattice centered around Γ_M)
→ magic angle + flatness of the band



How many terms in the sum over $q_\pm$?

For the flat bands, the upper left block in the hexagonal approximation. Adding more shells will add corrections converging <u>exponentially</u> with the number of shells

While the magic angle and the flatness
are "relatively" easy to capture, getting a large gap
between the two active bands and the other
passive bands is more difficult. The bandwidth
is of the order of 1 meV while the gap
is typically of the order of 30 meV.

3- TBG: Symmetry and topology