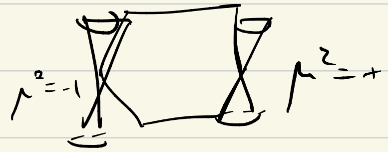
GRAPHENE LECTURES

2

Lecture 2

Last Time:

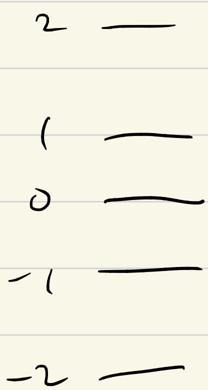
Graphene Review: TB $\to$ Dirac



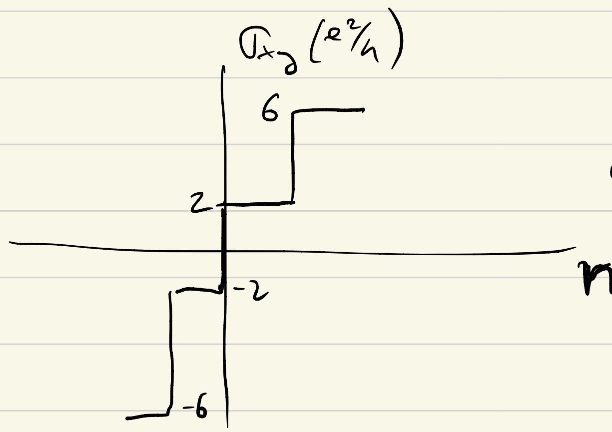
$$H_{eff} = v\left(k_x \mu^z \tau^x + k_y \tau^y\right)$$
$$= -iv\left(\mu^z \tau^x \partial_x + \tau^y \partial_y\right) \qquad = 4 \times \text{Dirac}$$

LLs: $\quad H_{Dirac} = -iv\,\vec{\tau}\cdot\left(\vec{\nabla} - ie\vec{A}\right)$

Solution: $\quad \varepsilon = \mathrm{sgn}(n)\sqrt{2|n|}\; v/\ell \qquad B\,2\pi\ell^2 = \varphi_0 = h/e$



$\Rightarrow$



etc.

# of states/LL $= p \times \left(\dfrac{BL^2}{\varphi_0}\right)$

$p = 4$ here

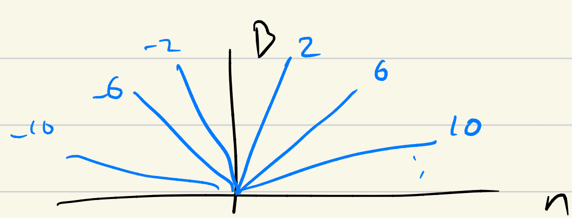
* Do I need to explain IQHE?? * If yes, edge states.

Fan Diagram: Plot minima of R_{xx} $\to$ occur when E_F is between LLs.

$$n = \frac{\sigma_{xy}}{(e^2/h)}\frac{B}{\varphi_0} = \left(\pm 2, \pm 6, \pm 10 \ldots\right) B/\varphi_0$$

$$\to B = \frac{n\varphi_0}{\pm 2, \pm 6, \pm 10, \ldots}$$

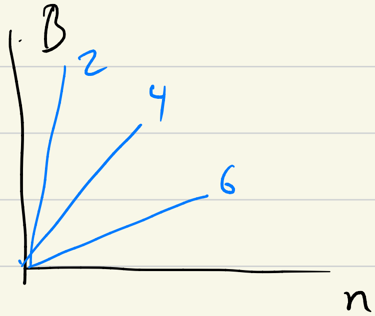
Colors $= 1/\text{slope}!$ $\longrightarrow$



Contrast

usual 2DEG

$H = \frac{k^2}{2m}$



(2 → spin deg.)

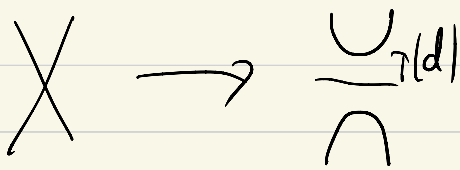
★ Incipient insulators → Zero magnetic field?

- Graphene at neutrality is semi-metal, neither ins. nor cond.
- In <u>theory</u>, it can be made insulating by various perturbations that lift deg. of DP
- <u>Dirac Mass</u>: Consider 1 DP (assume no K−K' mixing) ← spin-indep.

$$h_+ = v k_x \tau^x + v k_y \tau^y + h_+'$$

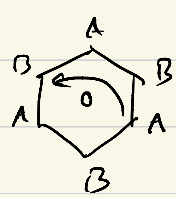
$$h_+' = a + b\tau^x + c\tau^y + d\tau^z$$

only this splits degeneracy.



Dirac "<u>mass</u>" $d \to m$

○ <u>Symmetry</u>: Inversion / C_2



$A \Leftrightarrow B$

$\tau^z \to -\tau^z$

$m \Rightarrow -m$.

also $K \to -K = K'$ switches valley

∘ Include valley.

$$h' = M\tau^z$$

$$M = m_0 + m_1 \mu^z$$

same sign for both valleys

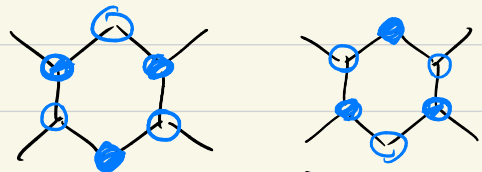
opposite sign for both valleys.

m_0 breaks C_2, preserves TR $(K \to -K)$

m_1 preserves C_2 $K \to -K$ $A \Leftrightarrow B$

but breaks TR

$m_0 > m_1 \longrightarrow$ "CDW"



sign of m

$m_1 > m_0 \longrightarrow$ "QAHE" $\to$ Haldane model.

· $\sigma_{xy} = \mathrm{sgn}(m_1)\,\dfrac{e^2}{h} \times p$ $\quad p = 2$ spin

Where does this come from??

Quick Summary of Topology + Graphene + Dirac

c.f. Jean-Noël

- Non-degenerate band $\quad \psi = e^{i\vec{k}\cdot\vec{r}}\, \phi_{nk}(\vec{r})$

$$\vec{A}_n(k) = \mathrm{Im}\, \langle \phi_{nk} | \vec{\nabla}_k | \phi_{nk} \rangle$$

Berry vect. pot.

Like vect. pot. $\quad \phi_{nk} \to e^{i\chi_n(k)} \phi_{nk}$

$$A \to A + \nabla \chi_n$$

$$B_n(k) = \frac{\partial A_n^x}{\partial k_y} - \frac{\partial A_n^y}{\partial k_x}$$

"flux"
= Berry Curvature.

- Symmetry: Inversion / C_2 $\quad B_n(-k) = B_n(k)$

TR $\quad B_n(k) = -B_n(k)$

$\Rightarrow \quad B_n = 0 \quad \forall k$ in B.Z.

applies to graphene.

- Dirac: Touch $\to$ $|\phi_{nk}\rangle$ not well-defined $\to$ neither is A or B.

// Check // $\quad \oint \vec{A}\cdot d\vec{k} = \pm\pi$ and DP

N.B. This gives top. reason for DP stability.
Like a "vortex"

Indeed $$h_\pm = v\begin{pmatrix} 0 & \pm k_x - ik_y \\ \pm k_x + ik_y & 0 \end{pmatrix}$$

Winds by $\pm 2\pi$ around $\vec{K}$ pnt.

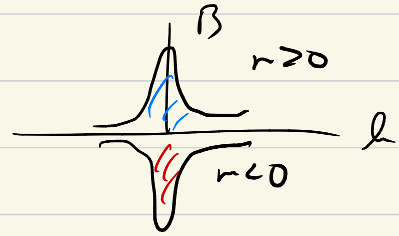
- Dirac mass:

N.D. at $m=0$, nascent Berry flux but sign undefined.

Turn on mass: $v k_x \mu^z \tau^x + v k_y \tau^y + m\tau^z$

Check: $$B = \frac{\mu^z m v^2}{2(v^2k^2+m^2)^{3/2}}$$

integral $= \pi\,\mathrm{sgn}(m)$



- Massive DP contributes $\int B = \pi\,\mathrm{sgn}(m\mu^z)$

  - Add these up.

Physics: Berry curvature $\to$ Hall effect.

$$\sigma_H = e^2 \sum_n \int \frac{d^2k}{(2\pi)^2} B_n(k)\, n_F(\varepsilon_{nk})$$

Valid for metals & insulators.

Filled Bands

$$\int d^2k \, B_n(k) = 2\pi \underbrace{C_n}_{\text{Integer = Chern \#}}$$

$$\sigma_H = \frac{e^2}{h} \sum_{n | \varepsilon_n < 0} C_n$$

IQHE

Chern Insulator

Dirac $\displaystyle \sum_n C_n = \sum_i \frac{1}{2} \operatorname{sgn}(m_i \mu_i^z)$ i = all non-deg. DPs

Example:

- CDW: $h' = m_0 \tau^z$ Same for both valleys. & spin.

$$\sum_n C_n = \underbrace{2}_{\text{spin}} \Big(\underbrace{+\frac{1}{2} \times \operatorname{sgn}(m_0)}_{\substack{\mu^z = +1 \\ K \text{ valley}}} \; \underbrace{- \frac{1}{2} \operatorname{sgn}(m_0)}_{\substack{\mu^z = -1 \\ K' \text{ valley}}} \Big) = 0$$

- Haldane $h' = m_0 \tau^z \mu^z$

$$\sum_n C_n = 2 \times \left(\frac{1}{2} \operatorname{sgn}(m_0) + \frac{1}{2} \operatorname{sgn}(m_0) \right)$$

$$= 2 \operatorname{sgn}(m_0) \quad \text{QAHE}$$

More nearby states? Break spin rot. sym.

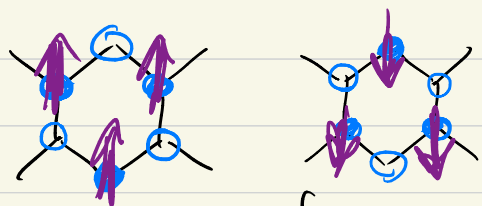
$$h' = m_2 \sigma^z \tau^z + m_3 \sigma^z \mu^z \tau^z$$

TR: $\tau^z \to \tau^z$, $\sigma^z \to -\sigma^z$, $\mu^z \to -\mu^z$

C_2: $\tau^z \to -\tau^z$, $\mu^z \to -\mu^z$

m_2: Break TR and Inv. $\to$ AF.

Like CDW of opposite sign for two spin



sign of m

m_3: Preserves TR, Inversion. Only breaks SU(2)

* Actually doesn't break any physical exact symmetries.

Would be generated by SOC

Kane-Mele model "QSHE" or $\mathbb{Z}_2$ TI.

Not very important for graphene $\to m_3 \sim \mu eV$

But WSe_2?

Summary

1-layer graphene → Dirac

• Many ~~nascent~~ incipient insulators due to DP Berry phase.

- Chern bands
- CDWs, AFs
- QSHE

Everything in TBG (actually all graphene) is a small perturbation on 1-layer graphene.

- Large effects only at low energy (small ε, small density, ...)

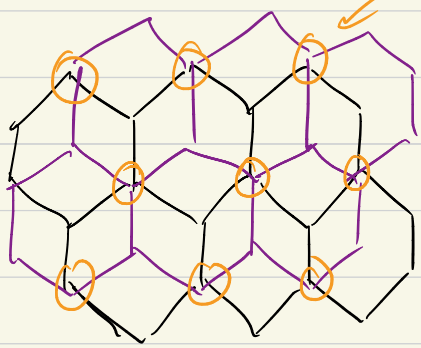
Next → Bilayers

Bilayer

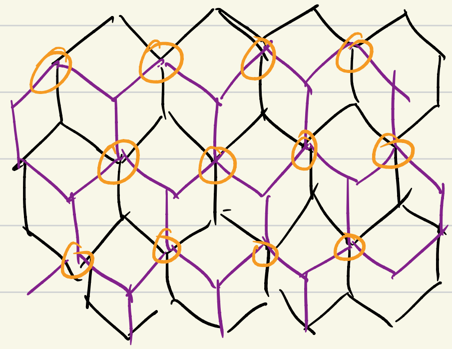
Structural Ground State

tunneling sites

A_1B_2

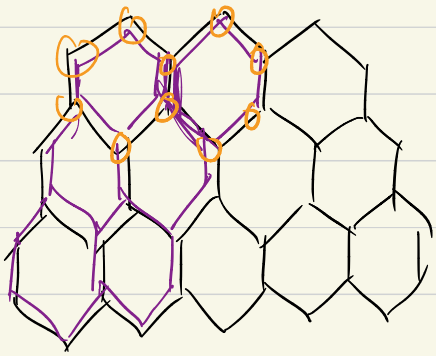


translate layer 2 by $-a\hat{y}$



B_1A_2

AA/BB



tunneling everywhere.

Maximum energy (worst stacking)

AB/BA Spectrum

$(\mu^z = +1 \quad K \text{ valley})$

$$H = v(k_x\tau^x + k_y\tau^y) - t'(\tau^-\gamma^+ + \tau^+\gamma^-)$$

$\vec{\gamma}$ = Pauli Matrix in layer space

$\gamma^z = 1$ upper layer

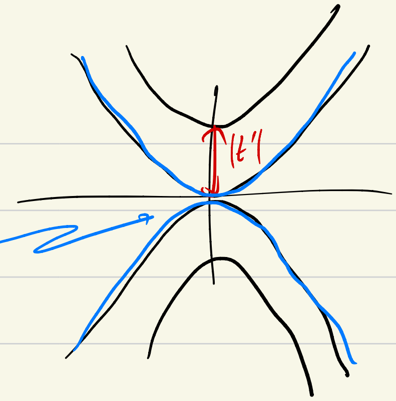
$ -1$ lower layer

τ^- : $A \to B$

τ^+ $B \to A$

$\tau^-\gamma^+$: $A_1 \to B_2$

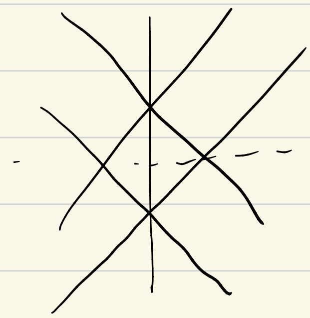
Result: $\varepsilon^2 = v^2k^2 + \frac{(t')^2}{2} \pm \sqrt{\left(\frac{(t')^2}{2}\right)^2 + (t')^2 v^2 k^2}$



$\varepsilon = \pm \frac{v^2 k^2}{|t'|}$

QBT semimetal

AA: $\varepsilon = \pm vk \pm |t'|$



Metal

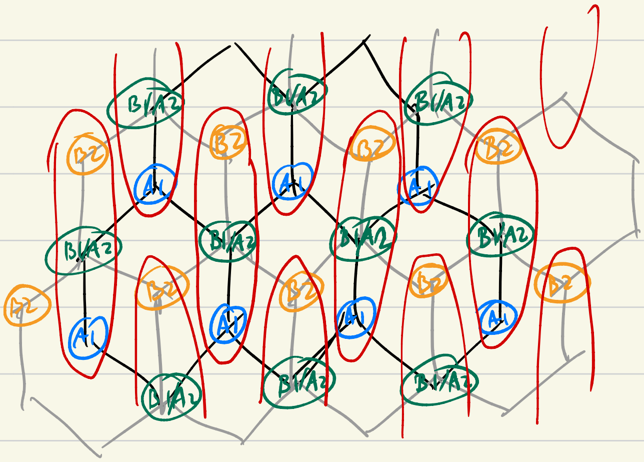
* Very big differences between 2 stackings.

* Exercises:
  - Derive AB spectrum.
  - What is low energy model for the QBT?
  - What happen for ABC trilayer?

Extra Notes on bilayer

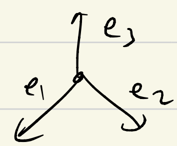
Bilayer – Different ways to align 2 graphene layers.

A-B Stacking



Really need to check convention.

Ok?



σ = sublattice

Interlayer: $B1 \leftrightarrow A2$ k-independent.

$$\boxed{H = v\left(k_x \tau^z \sigma^x + k_y \sigma^y\right) - w\left(\sigma^- \mu^+ + \sigma^+ \mu^-\right)}$$

$$\begin{array}{c|cccc} & A1 & B1 & A2 & B2 \\ \hline A1 & & & & \\ B1 & & & & \\ A2 & & & & \\ B2 & & & & \end{array} \quad \begin{pmatrix} 0 & v(k_x - ik_y) & 0 & 0 \\ v(k_x + ik_y) & 0 & w & 0 \\ 0 & w & 0 & v(k_x - ik_y) \\ 0 & 0 & v(k_x + ik_y) & 0 \end{pmatrix}$$

$$\begin{array}{c|cccc} & A1 & A2 & B1 & B2 \\ \hline A1 & & & & \\ A2 & & & & \\ B1 & & & & \\ B2 & & & & \end{array} \quad \begin{pmatrix} 0 & 0 & v(k_x - ik_y) & 0 \\ 0 & 0 & -w & v(k_x - ik_y) \\ v(k_x + ik_y) & -w & 0 & 0 \\ 0 & v(k_x + ik_y) & 0 & 0 \end{pmatrix}$$

skip

$vk \ll w$. P.T.

$k = 0$: $\left(\sigma^+ \mu^- + \sigma^- \mu^+\right)^2$

$= \sigma^+ \mu^- \sigma^- \mu^+ + h.c.$

$= \left(\frac{1+\sigma^z}{2}\right)\left(\frac{1-\mu^z}{2}\right) + \left(\frac{1-\sigma^z}{2}\right)\left(\frac{1+\mu^z}{2}\right)$

$= \frac{1}{2} - \frac{\mu^z \sigma^z}{2} = (0, 1)$

$\sigma^+ \mu^- + \sigma^- \mu^+ = \underbrace{0, 0}_{(A1,\, B2)}, +1, -1$

Extra notes bilayer

$$H = \begin{pmatrix} 0 & \Gamma \\ \Gamma^{\dagger} & 0 \end{pmatrix} \Rightarrow H^2 = \begin{pmatrix} \Gamma\Gamma^{\dagger} & \\ & \Gamma^{\dagger}\Gamma \end{pmatrix}$$

$$\Gamma = v(k_x - ik_y) + w\sigma^-$$
$$\Gamma^{\dagger} = v(k_x + ik_y) + w\sigma^+$$

$$\Gamma^{\dagger}\Gamma = \begin{pmatrix} v^2k^2 + w^2 & wv(k_x - ik_y) \\ wv(k_x + ik_y) & v^2k^2 \end{pmatrix}$$

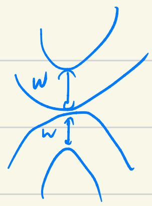
$$\Gamma v = \varepsilon u \quad \to$$
$$\Gamma^{\dagger} u = \varepsilon v$$

$$= v^2k^2 + \frac{w^2}{2} + \frac{w^2}{2}\sigma^z + wvk_x\sigma^x + wvk_y\sigma^y$$

show $\to$

$$\Rightarrow \boxed{\varepsilon^2 = v^2k^2 + \frac{w^2}{2} \pm \sqrt{\left(\frac{w^2}{2}\right)^2 + w^2v^2k^2}}$$

$$f = \sqrt{a+x}$$
$$f' = \frac{1}{2\sqrt{a+x}}$$
$$f'' = -\frac{1}{4(a+x)^{3/2}}$$



Low energy band $\to$ $-$ sign

$$\varepsilon^2 \simeq v^2k^2 + \frac{w^2}{2} - \left(\frac{w^2}{2} + \frac{w^2v^2k^2}{2\left(\frac{w^2}{2}\right)} - \frac{(w^2v^2k^2)^2}{8\left(\frac{w^2}{2}\right)^3} \right)$$

$$\simeq v^2k^2 + \frac{w^2}{2} - \left(\frac{w^2}{2} + v^2k^2 - \frac{(v^2k^2)^2}{w^2} \right)$$

$$\varepsilon^2 \simeq \left(\frac{v^2k^2}{w}\right)^2 \Rightarrow \boxed{\varepsilon = \pm \frac{v^2k^2}{|w|}}$$

SKIP TO HERE

(21) $H_{\text{eff}}^{(GS)} = E_0 + \mathcal{P}H'(E_0 - H_0)^{-1}H'\mathcal{P}.$ $= -PH'\frac{1}{H_0}H'P$

$$H = \underbrace{v(k_x\tau^z\sigma^x + k_y\sigma^y)}_{H'} - \underbrace{w(\sigma^-\mu^+ + \sigma^+\mu^-)}_{H_0}$$

$-$ sign is corrected

Extra Notes Bilayer

$E_0 = 0$

P = projector on 0-energy states of H_0 $(A1, B2)$

$$\tau^2 = +1$$

$$H' = v(h_x - ih_y)\sigma^+ + v(h_x + ih_y)\sigma^-$$

$$H'|A1\rangle = v(h_x + ih_y)|B1\rangle$$

eigenstates of H_0: $\frac{1}{\sqrt{2}}\left(|A2\rangle + |B1\rangle\right)$ $\quad E_0 = -w$

$\frac{1}{\sqrt{2}}\left(|A2\rangle - |B1\rangle\right)$ $\quad E_0 = +w$

I guess $H_0^{-1} = \frac{H_0}{w^2} = -\frac{1}{w}\left(|A2\rangle\langle B1| + |B1\rangle\langle A2|\right)$ in this subspace

$$H_0^{-1} H' |A1\rangle = -\frac{v(h_x + ih_y)}{w} |A2\rangle$$

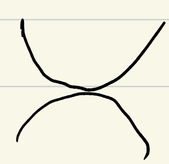
$$-H' H_0^{-1} H' |A1\rangle = +\frac{v^2 (h_x + ih_y)^2}{w} |B2\rangle$$

So in $\begin{pmatrix} |A1\rangle \\ |B2\rangle \end{pmatrix}$ subspace

$$H_{eff} = +\begin{pmatrix} 0 & \frac{v^2}{w}(h_x - ih_y)^2 \\ \frac{v^2}{w}(h_x + ih_y)^2 & 0 \end{pmatrix}$$

This is good. NB. $w \sim 100\,meV$

$v \sim 10^6\,m/s$?

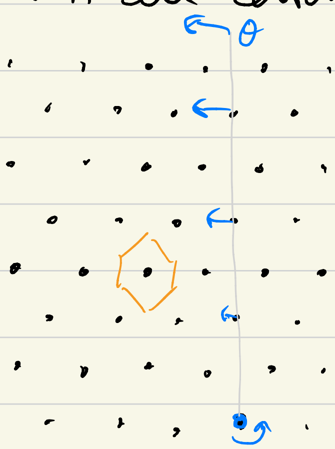


Twisting!

SLIDES 1-5

- Rotate 2 layers relative to one another
- Moiré pattern. Anyone know where the name comes from?

Consider unit cell centers



Generic angles:
- Sites will never coincide
- NOT periodic
- Quasi-periodic

Quasi-periodic systems are complex (and nasty!)
- No Bloch Theorem - Can be localization, ...

But: For small angles, and weak coupling between layers,

the system locally looks regular & periodic

- So one could see regions that look locally AA-like, AB-like, etc.

- Expect some kind of "adiabatic" approximation can apply, and local physics does not care if system is periodic or not.
- Indeed, turns out this is the case: exact lattice matching does not matter.

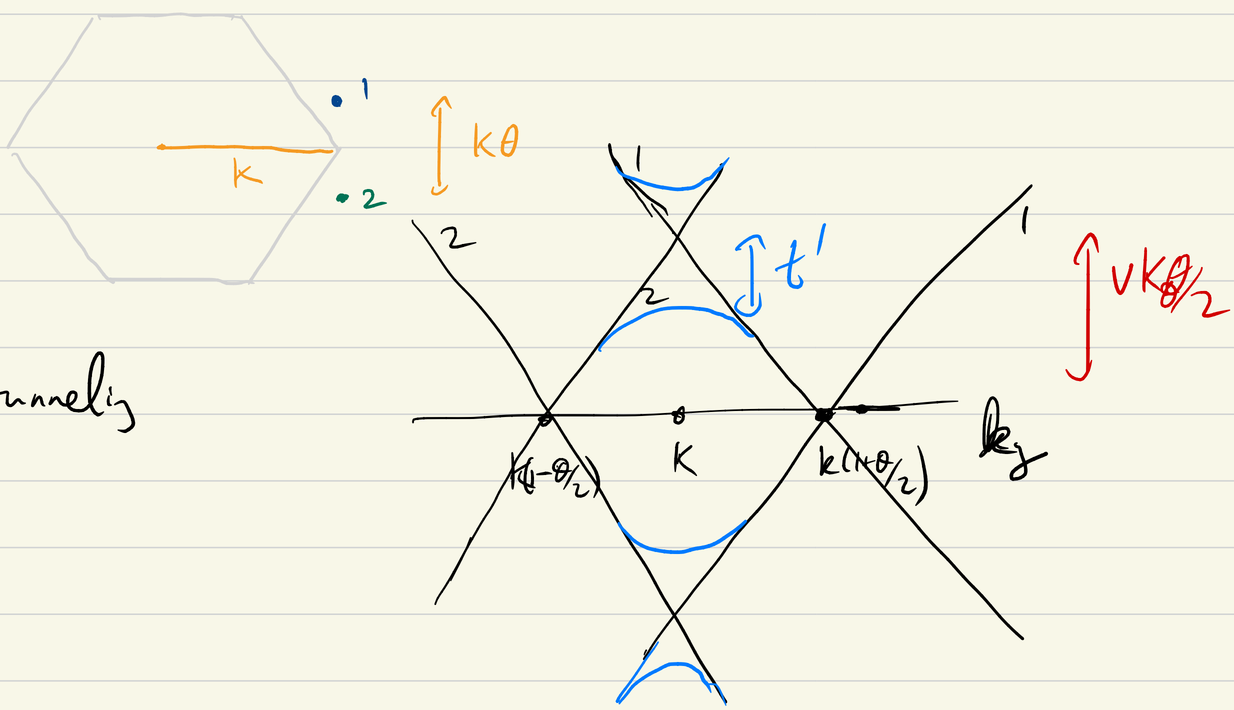
Almost:

$$\theta L_y = a_{u.c.} = \sqrt{3} a_{cc}$$

Moiré unit cell length $L = \sqrt{3} a / \theta$

Simple argument

- Rotation by angle θ $\rightarrow$ Shifts DPs by $K\theta\hat{y}$



Zero tunneling

Tunneling lowers gaps $\rightarrow$ when $t' \sim vK_\theta$ $\rightarrow$ especially flat.

How to make this sharp?

Bistritzer - MacDonald, PNAS 108, 12233 (2011).

- Showed how quasi-periodicity $\approx$ periodicity
- Calculations!
- Elegantly identify dimensionless parameter