GRAPHENE LECTURES

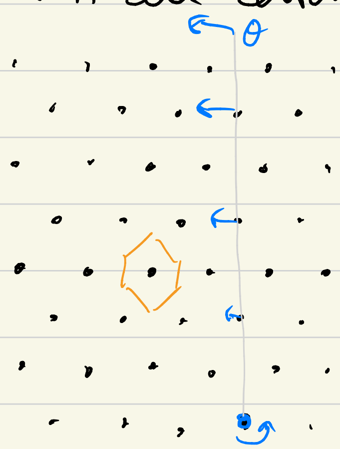
3

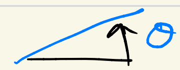
Twisting!

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.

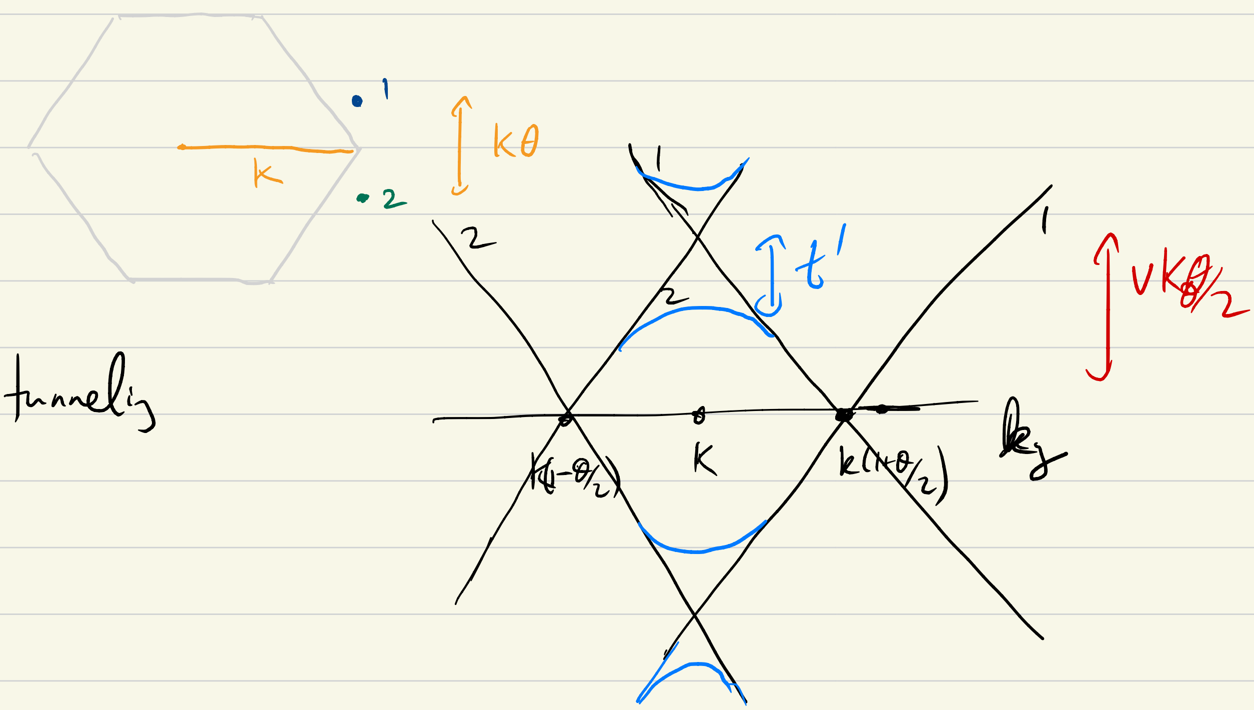
- Expect some kind of "adiabatic" approximation can apply, and local physics does not care if system is periodic or not.
- Indeed, turns out this is the case: exact lattice matching does not matter.

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

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

Simple argument

- Rotation by angle $\theta \rightarrow$ 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

* TBG w/ small angle looks locally like just a strained BG. Strain are small.

2d elasticity $\theta = \frac{\partial_x u_y - \partial_y u_x}{2}$

* So let's write down theory of BLG w/ strain/displacement.

* 3 Effects

① Pure geometry: strain changes lengths. If we have different strain in the two layers, we have to take into account relative shifts of $\vec{x} \leftrightarrow \vec{x}$. e.g. DPs move etc.

SAVE!!

② Intra-layer energetics: strain leads to "gauge fields" well-known in graphene. Basically equal & opposite for the two valleys. [Secondary]

③ Inter-layer coupling: very dependent upon relative displacement of the 2 layers. Eg. AA vs AB.

– These are the only effects that depend on $\vec{u}$ and not $\partial_i u_j$. Position not strain.

① Pure geometrical effects. We need this because of different strains in different layers.

Textbook: $\vec{x} = \vec{R} + \vec{u}(\vec{R})$

actual position of atom — ideal position of u.c. — displacement / phonon field

"Lagrangian coordinates" → awkward. $u(\vec{R})$

Eulerian $\vec{x} = \vec{R} + \vec{u}(\vec{x})$

implicitly defines $\vec{u}(\vec{x})$
almost the same but
not for long distances.

Better because $\vec{u}(\vec{x})$
actually describes geometry
at real coord. $\vec{x}$.

Apply to graphene: $C(\vec{x}) \sim \psi_+(R)\, e^{i\vec{K}\cdot\vec{R}} = \psi_+(R)\, e^{i\vec{K}\cdot(\vec{x}-\vec{u}(\vec{x}))}$

$$= \underbrace{\left(\psi_+(R)\, e^{-i\vec{K}\cdot\vec{u}(x)}\right)}\, e^{i\vec{K}\cdot\vec{x}}$$

$$\boxed{\psi_+(\vec{x}) = \psi_+(R)\, e^{-i\vec{K}\cdot\vec{u}(x)}}$$

$$\boxed{\psi_+(R) = \psi_+(\vec{x})\, e^{i\vec{K}\cdot\vec{u}(x)}}$$

How does this affect H_{Dirac}?

$$H_{Dirac} = \int d^2R\, \psi_+^\dagger\, (-iv\,\vec{\sigma}\cdot\vec{\nabla}_R)\, \psi_+$$

Change variables to $\vec{x}$

$$d^2R = d^2x \left|\frac{\partial R}{\partial x}\right| , \quad \frac{\partial}{\partial R_\mu} = \frac{\partial x_\nu}{\partial R_\mu}\frac{\partial}{\partial x_\nu}$$

Some algebra: to $O(u)$

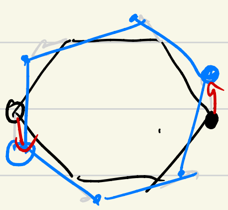
ℓ = layer.

$$= \int d^2x\, \psi^\dagger_{\ell *}(x) \Big[-iv \Big(\sigma^\mu + \underbrace{\sigma^\nu \frac{\partial u^{(\ell)}_\mu}{\partial x_\nu}}_{\text{local coord. rots/scalings.}} - \underbrace{\nabla\cdot u^{(\ell)}}_{\text{density change}} \sigma^\mu \Big) \frac{\partial}{\partial x_\mu} - \underbrace{v(\vec{k}\cdot\partial_\mu \vec{u}^{(\ell)})\sigma^\mu}_{\text{biggest effect: Shift of } \vec{K} \text{ point.}} \Big] \psi_{\ell x}$$

Emphasize: This is all just geometry. For 1 layer it is not actually significant. But for two layers, need $\vec{u}_1$ & $\vec{u}_2$, and then relative shifts are important.

$\boxed{\text{Main effect}}$

BZ Lh



K-point shift with rotation or strain.

$$\delta k^\mu = -\vec{K}\cdot\partial_\mu \vec{u}$$

② Intra-layer energetics: Strain stretches bonds
$\Rightarrow$ "Artificial gauge fields"

Kind of standard results (Ando 2006 + RMP)

$$\vec{\nabla} \to \vec{\nabla} - i\vec{A} \quad , \quad \vec{A} \sim \frac{\gamma}{a} \mu^z \begin{pmatrix} \epsilon_{xx} - \epsilon_{yy} \\ 2\epsilon_{xy} \end{pmatrix} \qquad \gamma = O(1)$$

Strain tensor
$\epsilon_{\mu\nu} = \frac{1}{2}(\partial_\mu u_\nu + \partial_\nu u_\mu)$

There are similar effects as the

Can compare $\vec{A} \sim \frac{\gamma}{a} \partial_\mu u_\nu$ to $\vec{K} \cdot \partial_\mu \vec{u}$

Same order of magnitude.

But $\epsilon = 0$ for pure rot.

So let's neglect it

③ Inter-layer interactions.

- Let's assume main effect is tunneling. This is sensible since this describes well the untwisted bilayer in expt.

So we seek a term like

$$H = \int d^2x \; \psi^\dagger_{2+} \underline{\underline{T}}(u_1,u_2)\, \psi_{1+} \quad + h.c.$$

tunneling from lower to upper layer near K point.

LOGIC Do it in R-coords, then transform

Symmetry considerations

① Slide both layers together $\vec{u}_1 \to \vec{u}_1 + \vec{d}$, $\vec{u}_2 \to \vec{u}_2 + \vec{d}$

No change!

So

$$T_R(\vec{u}_1, \vec{u}_2) = T_R(\vec{u}_1 - \vec{u}_2)$$

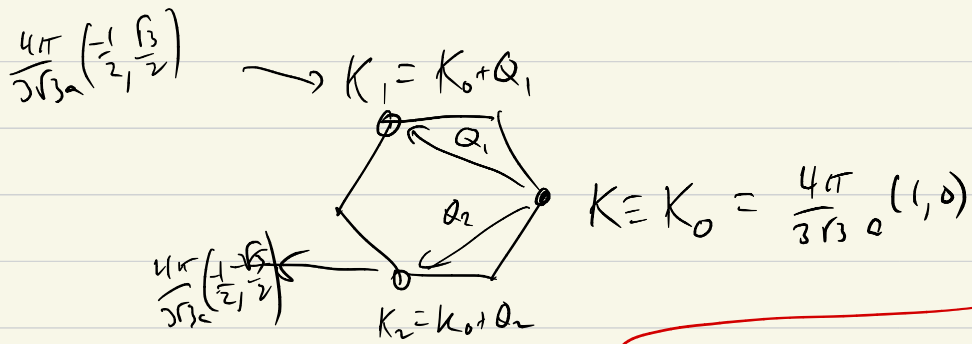
$R = x + u(x)$

② Shift one layer by one lattice spacing.

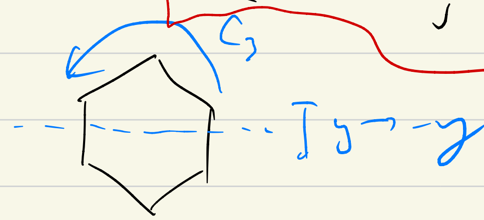
$$\vec{u}_1 \to \vec{u}_1 + \vec{a}$$
$$\psi_1 \to \psi_1 e^{+i\vec{k}\cdot\vec{a}}$$

Then we need $T_R(\vec{u}+\vec{a}) = e^{-i\vec{k}\cdot\vec{a}}\, T_R(\vec{u})$

Means $T_R(\vec{u}) = e^{-i\vec{K}\cdot\vec{u}} \sum_{\vec{Q}\in RL} T_Q\, e^{i\vec{Q}\cdot\vec{u}} \simeq \sum_j T_j\, e^{-i\vec{k}_j\cdot\vec{u}}$



From 1+2, we have $\boxed{T_R(\vec{u}) = \sum_j T_j\, e^{-i\vec{k}_j\cdot\vec{u}}}$



③ Point symmetries

Ⓐ C_3 Rotation: $T_{j+1} = e^{2\pi i\sigma^z/3}\, T_j\, e^{-2\pi i\sigma^z/3}$

Ⓑ R_y: $T_0 = \tau^x T_0 \tau^x$

Ⓒ $C_2^x TR$: $T_0 = \tau^x T_0^* \tau^x$

$$\boxed{T_j = u\mathbb{I} + w(\tau^+\zeta^j + \tau^-\bar{\zeta}^j)}$$

Ⓑ+Ⓒ $\Rightarrow$ $T_0 = u\mathbb{I} + w\tau^x = u + w(\tau^+ + \tau^-)$

Ⓐ $T_1 = u\mathbb{I} + w(\zeta\tau^+ + \bar{\zeta}\tau^-)$

$T_2 = u\mathbb{I} + w(\bar{\zeta}\tau^+ + \zeta\tau^-)$

$\zeta = e^{2\pi i/3}$ $\quad \bar{\zeta} = 1/\zeta = \zeta^2$

★ Now Transform: $\psi(R) = \psi(k)\, e^{ik_0\cdot u} \longrightarrow T_X(u) = \sum_j T_j\, e^{-i(\vec{k}_j - \vec{k}_0)\cdot u}$

Check

$\vec{u} = 0$: AA

$$T = \sum_j T_j = 3u\,\mathbb{I} \quad \checkmark \qquad u = \frac{t'_{AA}}{3}.$$

$\vec{u} = (0, a)$

$$\vec{k}_0 \cdot \vec{u} = 0 \qquad e^{-ik_0 \cdot u} = 1$$
$$\vec{k}_1 \cdot \vec{u} = \frac{2\pi}{3} \qquad e^{-ik_1 \cdot u} = \bar{\zeta}$$
$$\vec{k}_2 \cdot u = -\frac{2\pi}{3} \qquad e^{-ik_2 \cdot u} = \zeta$$

$$T = T_0 + \zeta T_1 + \bar{\zeta} T_2 = 3w\tau^+ = \begin{pmatrix} 0 & 3w \\ 0 & 0 \end{pmatrix}$$

$$v = \frac{t'_{AB}}{3}$$

So our unknown parameters are known! (approx).

$u \simeq w = 100\,\mathrm{meV}$

Symmetry does not relate u + w, so they can differ somewhat.

Now let us apply this all to TBG (dropped all terms)

$$\mathcal{H} \simeq \psi_1^\dagger (-iv\vec{\tau}\cdot\vec{\nabla})\psi_1 + \psi_2^\dagger(-iv\vec{\tau}\cdot\vec{\nabla})\psi_2 - v\psi_1^\dagger \vec{k}\cdot\partial_\mu \vec{u}_1 \sigma^\mu \psi_1$$
$$- v\psi_2^\dagger \vec{k}\cdot\partial_\mu \vec{u}_2 \sigma^\mu \psi_2$$
$$- \sum_j \left(e^{-i(\vec{k}_j - \vec{k}_0)\cdot\vec{u}} \, \psi_1^\dagger T_j \psi_2 + h.c. \right)$$

TWIST

$$\vec{u}_1 = \frac{\theta}{2}\hat{z}\times\vec{r} \qquad \vec{u}_2 = -\frac{\theta}{2}\hat{z}\times\vec{r}$$

$$\vec{K}\cdot\partial_\mu\vec{u}_1\sigma^\mu = K\partial_\mu u_1^x \sigma^\mu = -\frac{K\theta}{2}\sigma^y$$

$$K\cdot\partial_\mu\vec{u}_2\sigma^\mu = +\frac{K\theta}{2}\sigma^y$$

$$(\vec{K}_j-\vec{K}_0)\cdot\vec{u} = (\vec{K}_j-\vec{K}_0)\,\theta\,\hat{z}\times\vec{r} = \vec{q}_j\cdot\vec{r}$$

$$\boxed{\vec{q}_j = \theta(\vec{K}_j-\vec{K}_0)\times\hat{z}}$$

$$\Rightarrow \boxed{\begin{aligned}\mathcal{H} \simeq\ &\psi_1^\dagger(i v\vec{\tau}\cdot\vec{\nabla})\psi_1 + \psi_2^\dagger(-iv\vec{\tau}\cdot\vec{\nabla})\psi_2 + \frac{vK\theta}{2}\left(\psi_1^\dagger\sigma^y\psi_1 - \psi_2^\dagger\sigma^y\psi_2\right)\\ &-\sum_j\left(e^{-i\vec{q}_j\cdot\vec{r}}\psi_1^\dagger T_j\psi_2 + h.c.\right)\end{aligned}}$$

$$\boxed{\mathcal{H}_{1p} = -iv\vec{\tau}\cdot\vec{\nabla} + \frac{vK\theta}{2}\tau^y\gamma^z - \sum_j\left(e^{-i\vec{q}_j\cdot\vec{r}}T_j\gamma^+ + h.c.\right)}$$

$$\boxed{T_j = u + w(\zeta^j\tau^+ + \bar{\zeta}^j\tau^-)}$$

BM model $\quad u \sim t'_{AA}/3 \quad w \sim t'_{AB}/3$

You can check that $\vec{q}_1, \vec{q}_2$ are RLVs of Moiré pattern!!!

✱ This is a Bloch Hamiltonian: Periodic under

$\vec{r} \to \vec{r} + \vec{A}$

$\vec{q}_i \cdot \vec{A} = 2\pi \mathbb{Z}$ — define Moiré lattice

So we can seek $\psi(\vec{x}) = e^{i\vec{q}\cdot\vec{x}} \phi_{\vec{q}}(\vec{x})$ ← Periodic.

✱ Dimensional Analysis

- Choose length in $1/k_\theta$ $\quad k_\theta \vec{x} \to \vec{x}$ $\quad \vec{q}_j = k_\theta \bar{q}_j$
- Energy $v k_\theta$

$$\boxed{\frac{\mathcal{H}_{1p}}{v k_\theta} = \underbrace{-i\vec{\tau}\cdot\vec{\nabla} + \frac{1}{2}\tau^y \gamma^z}_{= -i\vec{\tau}\cdot(\nabla + i\frac{\gamma^z}{2}\hat{y})} - \frac{w}{v k_\theta}\left(\sum_j e^{-i\bar{q}_j\cdot\vec{x}} \bar{T}_j \gamma^+ + h.c.\right)}$$

$\bar{T}_j = \frac{u}{w} + \bar{\zeta}^j \tau^+ + \bar{\zeta}^{\bar{j}} \tau^-$

4x4 matrix Dirac-like eqn. for each spin & each valley.

1-particle Dirac-Bloch equation

With unit cell of size 1

Only 1 dimensionless parameter $\frac{w}{v k_\theta}$ $\left(\text{also } \frac{u}{w} \text{ but } \simeq 1\right)$

✱ What is accomplished? Two microscopic small parameters:

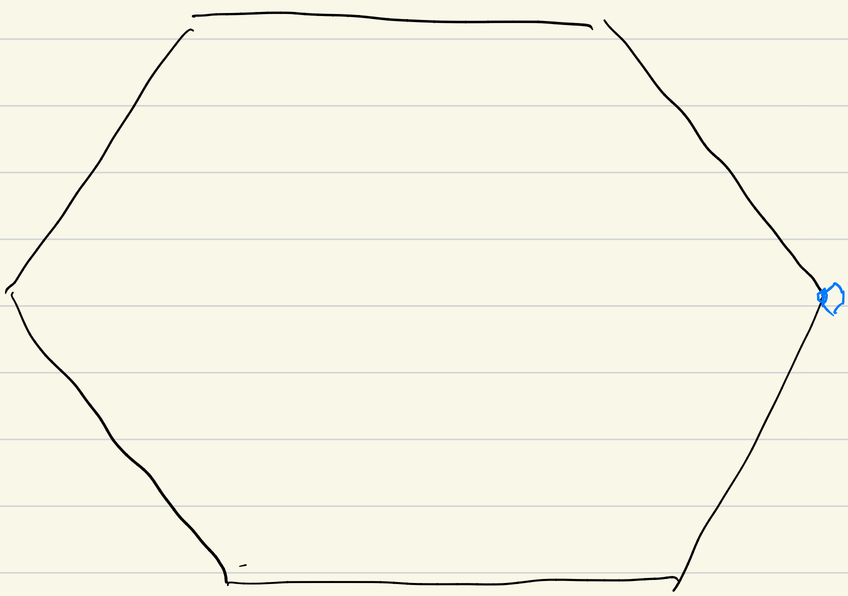
$w \ll W \sim t$

$v k_\theta \ll W \sim t$

$\boxed{\text{BUT}}$ $\frac{w}{v k_\theta}$ can be arbitrary.

SLIDES

$\theta = 1^\circ = \frac{\pi}{180} = \frac{1}{60}$



Realistic Scale!

Continuum model allows us to focus directly on this tiny scale!!