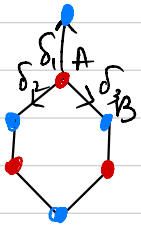
We have already seen that there are two inequivalent k points, and these are the dirac points, namely where the CB and the VB touches each other.

The Hamiltonian we have solved for graphene is

$$\hat{H} = -t \sum_{\langle ij \rangle} \left(c_{iA}^{+} c_{jB} + h.c \right)$$



$$c_{\vec{k},A} = \frac{1}{\sqrt{N}} \sum_j e^{-i \vec{k} \cdot \vec{x}_j} c_{jA}$$

$$c_{\vec{k},B} = \frac{1}{\sqrt{N}} \sum_j e^{-i \vec{k} \cdot x_j} c_{jB}$$

$$c_k = \begin{bmatrix} c_{\vec{k},A} \\ c_{\vec{k},B} \end{bmatrix}$$

$$\therefore \quad \hat{H} = \sum_{\vec{k}} c_k^{+} h(\vec{k}) c_{\vec{k}}$$

where $h(\vec{k}) = \begin{bmatrix} 0 & \sum_{i=1,2,3} e^{i \vec{k} \cdot \vec{\delta}_j} \\ \sum_{j=1,2,3} e^{-i \vec{k} \cdot \vec{\delta}_j} & 0 \end{bmatrix}$ no t_{AA} or t_{BB}.

Bloch Hamiltonian $h(\vec{k}) = \vec{d}(\vec{k}) \cdot \vec{\sigma} + d_0(\vec{k}) \cdot \sigma_0$

from Brillouin zone $\longrightarrow$ real space (Bloch sphere)

$$d_x(\vec{k}) = -t \sum_{j=1,2,3} \cos(\vec{k} \delta_j)$$

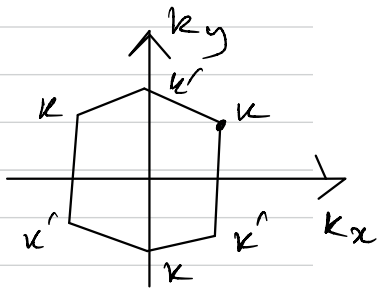
$$d_y(\vec{k}) = +t \sum \sin(\vec{k} \delta_j)$$

$d_z(\vec{k}) = 0 \Longrightarrow$ very important consequence

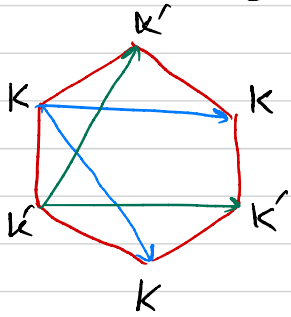
$$E_{\vec{k}} = \pm \sqrt{d_x^2(\vec{k}) + d_y^2(\vec{k})}$$

① $\pm$ → two bands as unit cell has two atoms.

② two valley K and K' simply because a triangular lattice has a hexagonal lattice in k-space.



all the three K points are connected by vectors



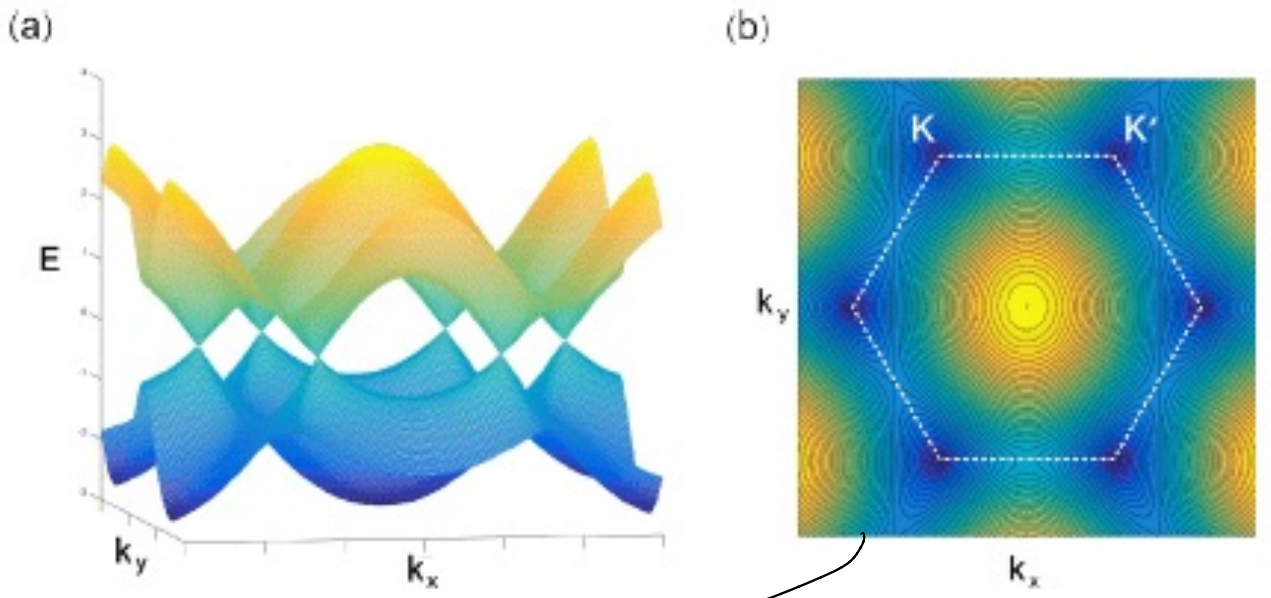
③ Charge neutral graphene means chemical potential is at $E_F = 0$

The conduction and valence band touches at the K and K' points, dispersion is linear and all the physics is happening there.

The wave func^n for Bloch hamiltonian

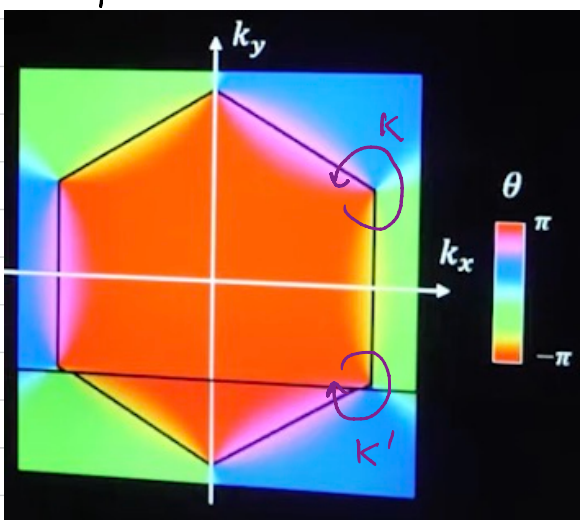
$$u_k = \frac{1}{\sqrt{2}} \begin{bmatrix} \pm 1 \\ e^{i\theta} \end{bmatrix} \quad \text{f. sendspin}$$

The wave func^n in graphene in terms of their magnitude are same on 'A' and 'B' sublattices but there is a relative phase θ between 'A' and 'B' sublattice..



as we go around the 'K' points the the phase evolves by 2π.

and this tells us the Dirac point is singular as the phase is not well defined.



The other important to note is that the evolution of ϕ around K and K' are completely opposite.

So we can define as at K we have vortex of the phase and at the K' we have anti vortex of the phase. This is where topology enters graphene and the singularity at the Dirac points and vortex and antivortex somehow protects this singularity.

We are only interested in near Dirac point physics only.

So, we are very close to the K point $\bar{K} + \tilde{k}$, where $|\tilde{k}| << |\bar{K}|$

$$d_x(\tilde{k}) = -t \sum_{j=1,2,3} \cos(\tilde{k}\delta_j) + t\tilde{k} \sum_{j=1,2,3} \delta_j \sin(\tilde{k}\delta_j)$$

$$d_y(k) = t \sum_{j=1,2,3} \sin(\tilde{k}\delta_j) + t\tilde{k} \sum_{j=1,2,3} \delta_j \cos(\tilde{k}\delta_j)$$

Taylor series expansion drops the terms at '$\tilde{k}$'

basis transformation

$$\vec{d} \to R_{-\pi/3}\vec{d},$$

unit vector rotated by $\pi/3$.

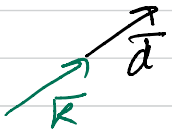
define Fermi velocity $v_F = \frac{\sqrt{3}\,t\,a}{2\hbar}$

Hamiltonian in the new basis.

$$H_K = \hbar v_F (k_x\sigma_x + k_y\sigma_y) \quad K \text{ point}$$

$$H_{K'} = \hbar v_F (k_x\sigma_x - k_y\sigma_y) \quad K' \text{ point}$$

implies at K point the $\vec{d}$ and $\vec{k}$ both goes in same direction say clock wise, while at K' it will be anti clockwise.



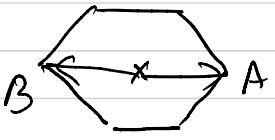
$$\therefore \boxed{H = \hbar v_F (k_x\sigma_x + \tau_z k_y\sigma_y)}, \quad \tau_z = \pm 1 \text{ for } K, K'$$

We have Dirac point, but why?

Let's discuss the symmetry:

Inversion / $C_2 Z_1$ Symmetry same for 2D.

Graphene has inversion symmetry



$$I\, C_{j,A}\, I^{-1} = C_{-j,B}$$

$$I\, C_{j,B}\, I^{-1} = C_{-j,A}$$

$$c_j = \begin{bmatrix} c_{j,A} \\ c_{j,B} \end{bmatrix} \qquad \mathcal{I}\, c_j \mathcal{I}^{-1} = \sigma_x c_{-j}$$

$$|c_{\bar{k}}|^{-1} = \frac{1}{\sqrt{N}} \sum_j e^{-i\bar{k}\cdot x_j}\, \mathcal{I}\, c_j \mathcal{I}^{-1} = \sigma_x c_{-\bar{k}}$$

$$\bar{k} \to -\bar{k}$$

$$H = \mathcal{I} H \mathcal{I}^{-1}$$

$$= \mathcal{I} \sum_{\bar{k}} c_{\bar{k}}^{\dagger} h(\bar{k}) c_{\bar{k}}\, \mathcal{I}^{-1} = \sum_{\bar{k}} c_{\bar{k}}^{\dagger} \sigma_x h(-\bar{k}) \sigma_x c_{\bar{k}}.$$

possible if for every $\bar{k}$

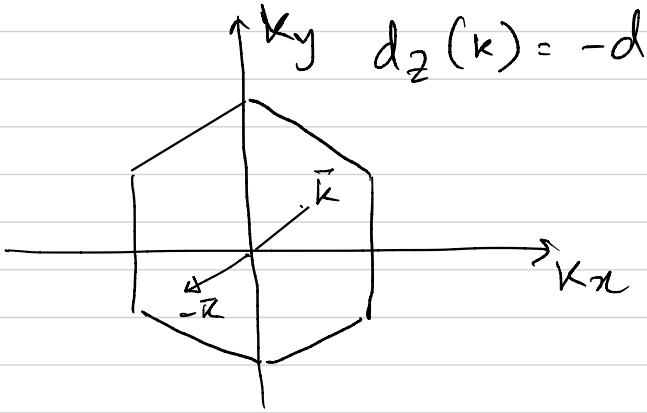
$$h(\bar{k}) = \sigma_x h(-\bar{k}) \sigma_x$$

Inversion symmetry puts some constraints on our $\vec{d}(k)$ vectors.

$$d_x(\bar{k}) = d_x(-\bar{k})$$

$$d_y(\bar{k}) = -d_y(-\bar{k}) \quad [\text{as } \sigma_y \text{ anti commutes with } \sigma_x]$$

$$d_z(k) = -d_z(-\bar{k})$$



for graphene

$$d_x(\bar{k}) = -t \sum_{j=1,2,3} \cos(\bar{k}\bar{a}_j)$$

symmetric in $\bar{k}$

$$d_y(\bar{k}) = t \sum_{j=1,2,3} \sin(\bar{k}\bar{a}_j)$$

antisymmetric in $\bar{k}$

∴ Graphene has inversion symmetry.

Let's look at time reversal symmetry (spinless for now)

$$T\, i\, T = -i \quad , \quad T = K \text{ complex conjugate}$$

$$T\, c_i\, T^{-1} = c_i \quad \text{(local operator } c\text{)}$$

but if we operate on a local operator which has explicit momentum k,

$$T\, c_{\bar{k}}\, T^{-1} = c_{-\bar{k}} \qquad \left[e^{ikx} \xrightarrow{T} e^{-ikx} \right]$$

If we require

$$T\, H\, T^{-1} = H$$

Then must be: $h(\bar{k}) = h^*(-k)$ for every $\bar{k}$

This will give us different set of constraints

$$d_x(\bar{k}) = d_x(-\bar{k})$$

$$d_y(\bar{k}) = -d_y(-\bar{k})$$

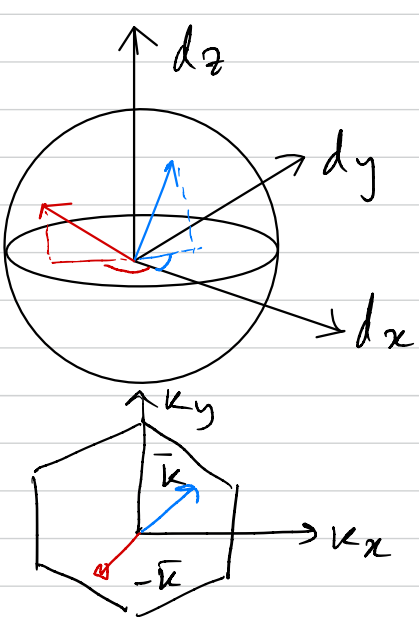
$$d_z(\bar{k}) = d_z(-\bar{k}) \quad \text{different from the Inversion constraint}$$

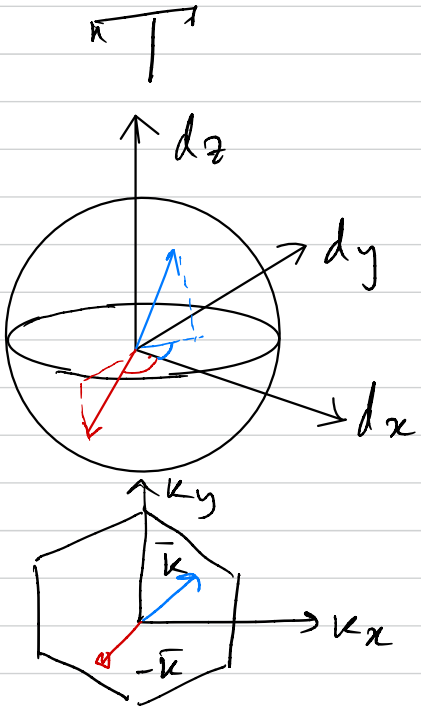
Let's see what are the consequences

Can this explain the presence of Dirac point.

It turns out in 2D generically there should not be any dirac point, unless protected by symmetry.

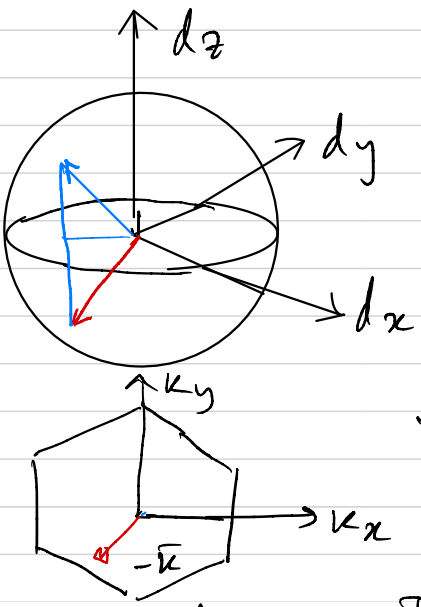
The Dirac point has to be fine tuned in 2D.





So, separately they do not protect

But under both $C_2T \Rightarrow C_2 \times T$



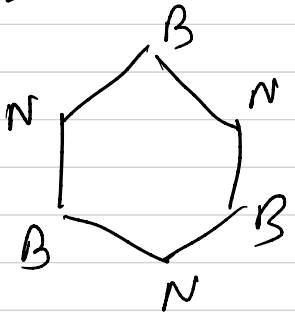
↓ guarantees $d_z = 0$

it fixes the $-\bar{k}$ vector.

Hence we have Dirac point

∴ if we $C_2\mathcal{T}$ symmetry the the Dirac pt. is destroyed.

How to do that, well we can use a substrate hBN (hexagonal Boron Nitride) also a hexagonal lattice, and



as 'A' and 'B' will not have same environment.

It will open a gap at the Dirac point.

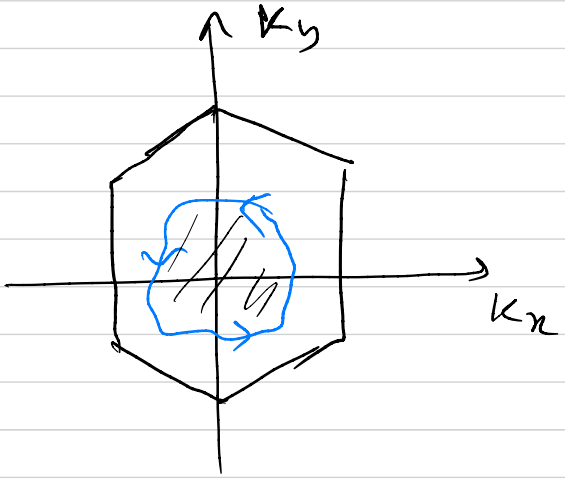
$$h_K = \begin{bmatrix} \Delta & 0 \\ 0 & -\Delta \end{bmatrix}$$

$$E_{\pm} = \pm \sqrt{(\hbar v_F k)^2 + \Delta^2}$$

effective mass $m = \Delta / v_F^2$

Is this enough for topological effect?

Haldane model



addition to dynamic phase, w.f can accuire a geometric phase

$$\gamma = \oint \bar{A}\, d\bar{k}$$

$$\bar{A}(\bar{k}) = i \langle u_k | \bar{\nabla}_k | u_k \rangle$$

Berry's curvature $\Omega(\bar{k}) = \bar{\nabla} \times \bar{A}$

One special trajectory that is for entire BZ

$$C = \frac{1}{2\pi} \int_{BZ} \Omega \, dk^2 = n \quad \text{Chern number}$$

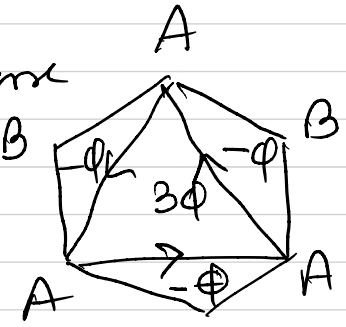
$n \neq 0$ Topological

The bands in graphene are trivial as K and K' has opposite Ω, so when integrated over entire BZ $C = 0$.

Let's add 2nd nearest neighbour

$j \xrightarrow{t_2 e^{i\phi}} i$

we acquire a phase



magnetic flux over all zero ϕ

for 'B' opposite orientation

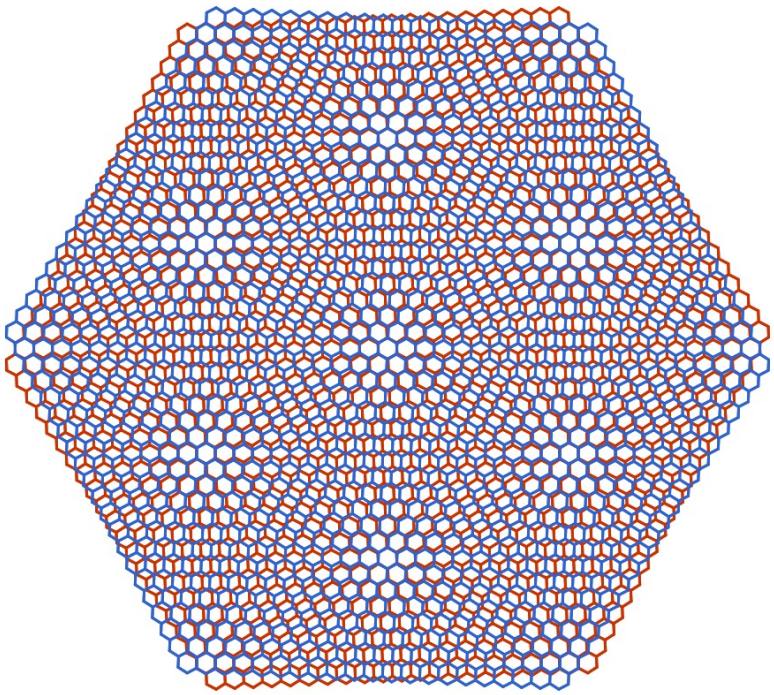
Point to note that this interaction add diagonal term in the H.

that is it adds mass (in a way)

if calculated formerly, one can show that $d_z(k)$ will have different mass term for the K and K' valleys.

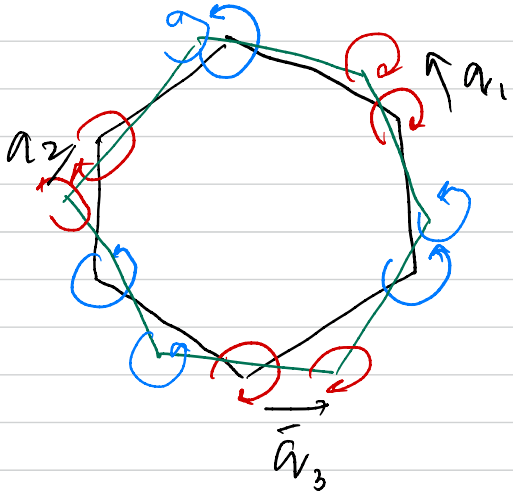
Twisted bilayer graphene.

'Moir - misalignment



$\lambda \sim 14\,nm$

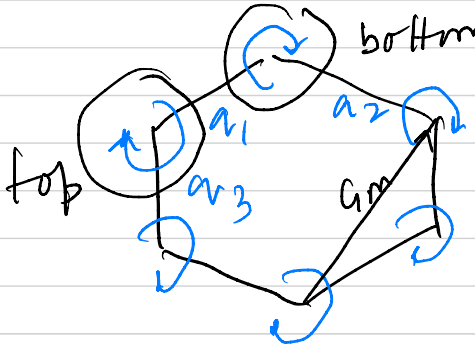
$a_0 = 1.4\,\text{Å}$



$$|q_i| = k_\theta = \frac{2\pi\theta}{a}$$

The new periodicity allows scattering related to the reciprocal lattice vectors.

There are mini BZ



$q_{1t} - q_{1b} = q_m$

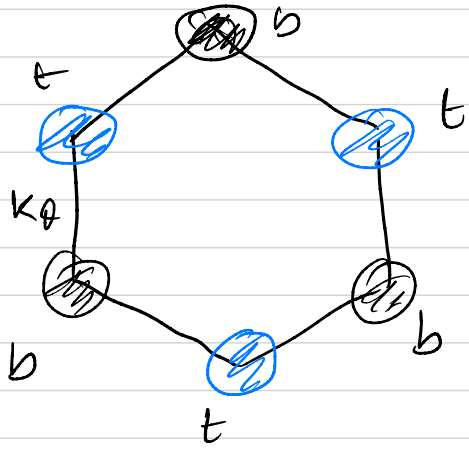
if θ is small this is small.

Also we can decouple this region of momentum space from the original 'K' valley of graphene

The original K, K' can be regarded as internal degree of freedom.

$$G_{1m} = \frac{2\pi}{\lambda} \Rightarrow \lambda = \frac{\sqrt{3}a}{\theta}$$

Low energy TBG is similar to low energy of graphene.



b → bottom graphene

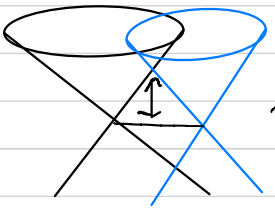
t → top graphene.

Important point is all the Dirac points are inequivalent have same chirality

i.e explicitly TRS is broken!

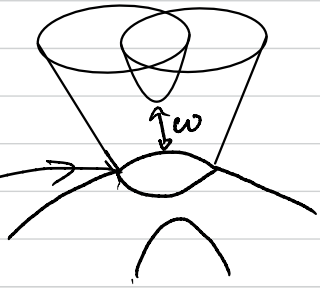
However, as this is locally broken, the C_2T is still there, so that will protect the vorticity of Dirac points.

Let's look at the coupling of the top and the bottom layer.



$\hbar v_F k_\theta \rightarrow$

Let's look at important energy scales momentum space separation of same chirality



additionally, coupling between the two layers, will open a gap decided by how much tunneling is allowed between the two layers.

- One energy scale decides tunneling between diff moiré unit cells in same layer.
- Second energy scale decides tunneling between top and the bottom layer.

i.e There can be a resonance condition that may appear. if and when the energy scales are comparable.

as w increases and becomes comparable to moire energy scale, then this bands are going to flatten out and the electrons can actually completely freeze!

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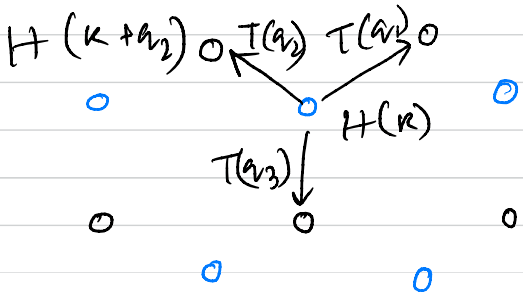
Magic angle → where the effective velocity of Dirac fermion goes to zero.

There are series of angle (Reading assignment)



In momentum space again.

Here scattering is now possible between 'black' to 'blue' in momentum space.

so, we have to use momentum dependent hopping matrix $T(q)$

$$H(k+Q) = \hbar v_F (k+Q) \cdot \sigma$$

$$T(Q \cdot Q') = \sum_{j=1,2,3} T_j (\delta_{Q-Q', q_j} + \delta_{Q'-Q, q_j})$$

scattering between 2 Q's separated by q_j

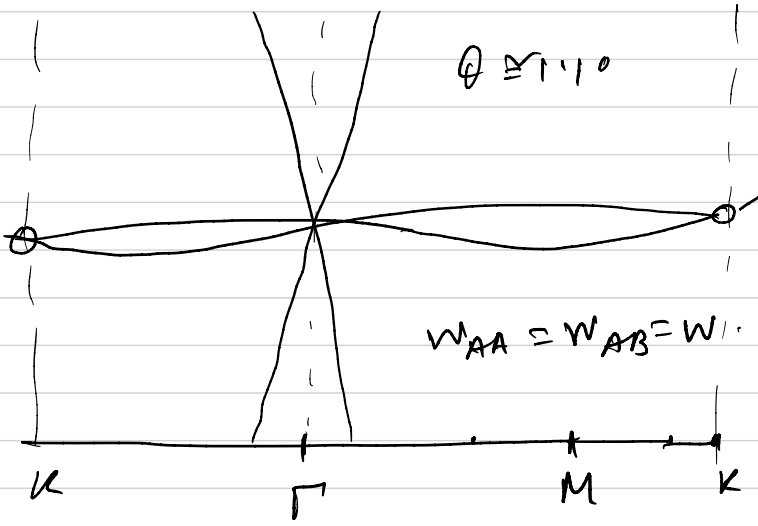
Sublattice space (C_2 preserved) $T_j = w_{AA}\sigma_0 + w_{AB}\left(\cos\frac{2\pi j}{3}\sigma_x + \sin\frac{2\pi j}{3}\sigma_y\right)$

for graphene naturally AB stacking is favoured known as Bernal stacking.

So, naturally 'AA' regions will shrink a bit and 'AB' regions will grow a bit and the top and bottom layers will get a bit closer between the AA and AB regions. In real system $w_{AB} > w_{AA}$

But the reading assignment paper has $w_{AB} = w_{AA}$

We can again diagonalize this hamiltonian and the band structure can be found.



$$\alpha = \frac{wa}{\hbar v_F \theta}$$

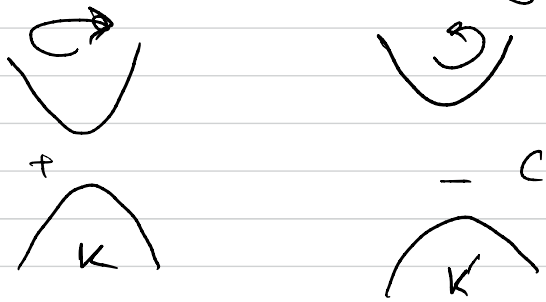
If w_{AA} and w_{AB} are taken realistically

$$w_{AA} = 0.95\, w_{AB}$$

Then realistic.

Let's compare with single layer graphene.

in graphene by breaking C_2T symmetry the K K' can be gapped.



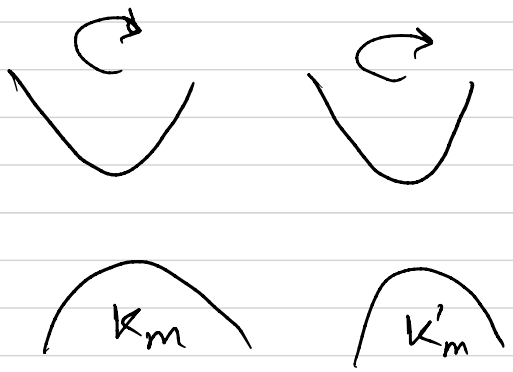
$C = \pm 1/2$

Breaking time reversal symmetry

$m_K = -m_{K'}$

opposite masses → $C = \pm 1$ Haldane

But in twisted bilayer graphene.



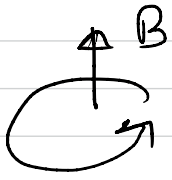
the chirality is same for both valleys

So breaking C_2 symmetry

$C = \pm 1$

anomalous Hall effect

Comparison with QHE



AB effect

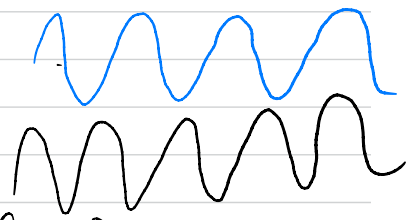
$$\Delta\theta = \frac{e}{\hbar c} \times B \times \text{Area}.$$

$\Delta\theta = 2\pi$ defines new unit cell

magnetic length $l_B = \sqrt{\frac{\hbar c}{eB}} \sim 10\,nm$ @ 7 T

QHE is new insulating states when density 'n' commensurates with magnetic unit cell.

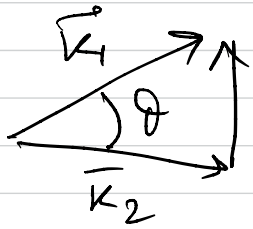
Moire $V_\pm(x) = \sin[(k \pm \delta)x]$



$$V_+(x) + V_-(x) = 2\cos(\delta x)\sin(kx)$$

superlattice with approximate period

$$a_{moire} = \frac{2\pi}{\delta} \gg \frac{2\pi}{k}$$



$\delta = |\bar{K}_1 - \bar{K}_2| \sim 2 k_i \sin\theta/2 \approx |\bar{k}_i| \theta$

$|\bar{k}_i| \sim \frac{2\pi}{a_{lattice}}$ if $a_{lattice} \sim 0.3nm$

$\theta \sim 1.5°$

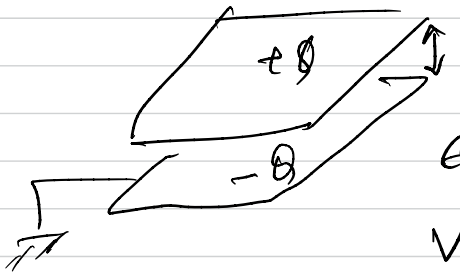
$a_{moire} = \frac{2\pi}{\delta} \sim \frac{a_{lattice}}{\theta} \sim 10nm.$

Just as magnetic field modifies the kinetic energy of free electrons, moire modifies $\mathcal{E}(k)$

$\Rightarrow$ flat bands with small kinetic energy = strong correlations.

many possible combinations & parameters

new physics!



$\epsilon_r \sim 10$

$V \sim 1V$

$n_e = \frac{Q}{A} = \frac{CV}{A} = \frac{\epsilon V}{d}$

$n \sim \frac{1 \text{ electron}}{(10nm)^2}$

$= 10^{-3}$ /unit cell

length scale of 10nm?