③ Graphene

$$h_{eff}(\vec{q}) = v(\tau^z \sigma^x q_x + \sigma^y q_y)$$

3.1 TRS

$$\mathcal{H} = \sum_{\vec{k}} c_k^\dagger h(\vec{k}) c_k$$

$$\boxed{[\mathcal{H}, \Theta] = 0 \iff h(\vec{k}) = \Theta^{-1} h(-\vec{k}) \Theta}$$

$$\Theta = U \underbrace{\mathbb{K}}$$

complex conjugation.

* TRS in graphene ?

First guess : $\Theta = \mathbb{K}$

(spinless graphene)

TRS $\Leftrightarrow$ $h_{eff}(\vec{q}) = h_{eff}(-\vec{q})^*$

$\Leftrightarrow$ $v(\tau^z \sigma^x q_x - \sigma^y q_y)$

$= v(-\tau^z \sigma^x q_x - \sigma^y q_y)$

Doesn't work. $\Rightarrow$ graphene breaks TRS !?

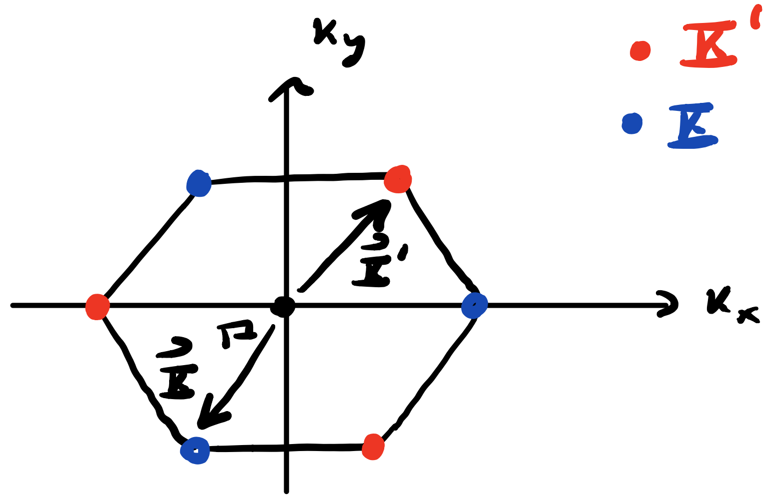
Mistake: $\Theta = \underline{K}$ was too naïve.

We forgot to act w/ Θ on the valley d.o.f.

Indeed, valley ~ momentum.

TR inverts momentum.

How does TR act on valley?



Momentum near K valley:

$$\vec{k} = \vec{K} + \vec{q} \quad (q \text{ small})$$

Momentum near K' valley:

$$\vec{k} = \vec{K}' + \vec{q} \quad (q \text{ small})$$

$\vec{k}$ = momentum measured from Γ.

Under TR, $\vec{k} \to -\vec{k}$.

Then,

(i) $\vec{k} = \vec{K} + \vec{q}$ (near K)

$$\Big\downarrow \text{TR}$$

$-\vec{k} = -\vec{K} - \vec{q} = \vec{K}' - \vec{q}$

(near K')

(ii) $\vec{k} = \vec{K}' + \vec{q}$ (near K')

$$\Big\downarrow \text{TR}$$

$-\vec{k} = -\vec{K}' - \vec{q} = \vec{K} - \vec{q}$

(near K)

So, TR flips valley and takes $\vec{q} \to -\vec{q}$.

To take this into account,

$\Theta = \tau^x \widehat{K}$ ← complex conjugation

Graphene has TRS

$$\Leftrightarrow h_{eff}(\vec{q}) = \tau^x \, h_{eff}(-\vec{q})^* \, \tau^x$$

$$\Leftrightarrow \quad v(\tau^z \sigma^x q_x + \sigma^y q_y)$$

$$= v\, \tau^x (-\tau^z \sigma^x q_x + \sigma^y q_y) \tau^x$$

$$= v\, (\tau^z \sigma^x q_x + \sigma^y q_y) \quad \checkmark$$

$\tau^x \tau^z \tau^x = -\tau^z$

3.3 Symmetries (II): space inversion

$\vec{r} \to -\vec{r}$

* Inversion operator: Π

$$\Pi \underbrace{\vec{r}}_{\substack{\uparrow \\ \text{position} \\ \text{operator}}} \Pi^{-1} = -\vec{r} \quad (1)$$

$$\Pi \underbrace{\vec{p}}_{\substack{\uparrow \\ \text{momentum} \\ \text{operator}}} \Pi^{-1} = -\vec{p} \quad (2)$$

(1) and (2) :

$$\Pi \, [x, p_x] \, \Pi^{-1} = [x, p_x]$$

Since $[x, p_x] = i\hbar$,

$$\Pi \, i \, \Pi^{-1} = i$$

$\Rightarrow$ Π is unitary $\quad (\Pi^{-1} = \Pi^{+})$

* $\boxed{\Pi^2 = \mathbb{1}}$ irrespective of spin of particles.

* A crystal has space inversion symmetry (SIS)

$\Leftrightarrow$ $[\mathcal{H}, \Pi] = 0$.

* $$\mathcal{H} = \sum_{\vec{k}} \sum_{\sigma\sigma'} \sum_{\alpha\alpha'} c^{+}_{\vec{k}\alpha\sigma} h^{\alpha\alpha'}_{\sigma\sigma'}(\vec{k}) \, c_{\vec{k}\alpha'\sigma'}$$

σ, σ' : spin

α, α' : everything else

$$\text{SIS} \Leftrightarrow \quad \Pi \mathcal{H} \Pi^{-1} = \mathcal{H}$$

$$* \quad \Pi \mathcal{H} \Pi^{-1} = \sum_{\vec{k}} \sum_{\alpha\alpha'} \sum_{\sigma\sigma'}$$

$$\underbrace{\Pi \, c^{\dagger}_{\vec{k}\alpha\sigma} \, \Pi^{-1}}_{?} \; \underbrace{\Pi \, h^{\alpha\alpha'}_{\sigma\sigma'}(\vec{k}) \, \Pi^{-1}}_{?} \; \underbrace{\Pi \, c_{\vec{k}\alpha'\sigma'} \, \Pi^{-1}}_{?}$$

$$* \quad \Pi \, c_{j\sigma\alpha} \, \Pi^{-1}$$

$$= \sum_{\alpha'} \Pi_{\alpha\alpha'} c_{-j\sigma\alpha'}$$

$$(\vec{r}_j = - \vec{r}_{-j})$$

same as lecture 16

$$\Rightarrow \Pi \, c_{\vec{k}\sigma\alpha} \, \Pi^{-1} \overset{\checkmark}{=}$$

$$= \sum_{\alpha'} \Pi_{\alpha\alpha'} \, c_{-\vec{k},\sigma\alpha'}$$

$$* \quad \Pi \underbrace{h^{\alpha\alpha'}_{\sigma\sigma'}(\vec{k})}_{\text{a number}} \Pi^{-1} = h^{\alpha\alpha'}_{\sigma\sigma'}(\vec{k})$$

$$* \quad \Pi \mathcal{H} \Pi^{-1}$$

$$= \sum_{\vec{k}} c^{+}_{-\vec{k}} \, \Pi^{+} \underbrace{h(\vec{k})}_{\text{matrix}} \underbrace{\Pi}_{\text{matrix}} c_{-\vec{k}}$$

same as
Lecture 16

$$= \sum_{\vec{k}} c^{+}_{+\vec{k}} \, \Pi^{+} h(-\vec{k}) \, \Pi \, c_{\vec{k}}$$

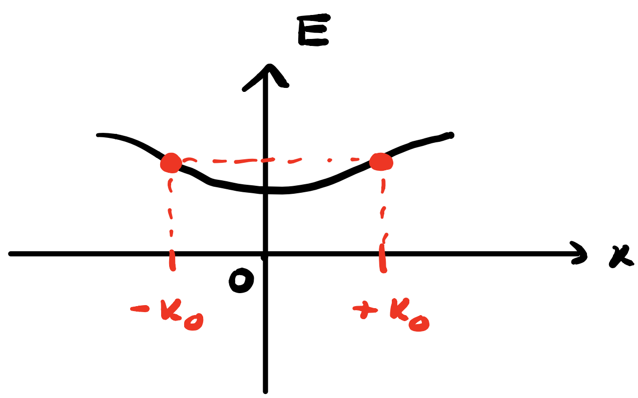
$$* \quad \Pi \mathcal{H} \Pi^{-1} = \mathcal{H} \Leftrightarrow$$

$$\boxed{h(\vec{k}) = \Pi^{+} h(-\vec{k}) \, \Pi}$$

condition for SIS.

* Implication for electronic structure:

In a crystal w/ SIS, if $|u_{\vec{k}}\rangle$ is an eigenstate of $h(\vec{k})$, then $\Pi\,|u_{\vec{k}}\rangle$ is an eigenstate of $h(-\vec{k})$, with same energy.



* In general,

$$h(\vec{k}) = \Pi^{-1}\, h(-\vec{k})\, \Pi$$

does not imply $[\,h(\vec{k}), \Pi\,] = 0$.

But, $[h(\vec{k}_{tr}), \Pi] = 0$.

Are $|u_{\vec{k}_{tr}}\rangle$ and

$\Pi |u_{\vec{k}_{tr}}\rangle$

the same state? yes,

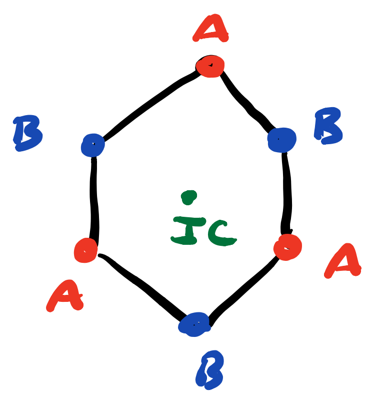
because $\Pi^2 = \mathbb{1}$.

$\rightarrow$ no Kramers degeneracy associated to SIS.

* Does graphene have SIS?

what's Π in graphene?

$\Pi \propto \tau^x$ (b/c $K \leftrightarrow K'$ under space inversion)



IC = inversion center.

(about which the graphene lattice is invariant under $\vec{r} \to -\vec{r}$)

Space inversion exchanges sublattices:

$A \leftrightarrow B$.

$\Pi \propto \sigma^x$

Then, $\Pi = \sigma^x \tau^x$

Graphene has SIS $\Leftrightarrow$

$$h_{eff}(\vec{q}) = \sigma^x \tau^x h_{eff}(-\vec{q}) \sigma^x \tau^x$$

check as an exercise that this is indeed satisfied for

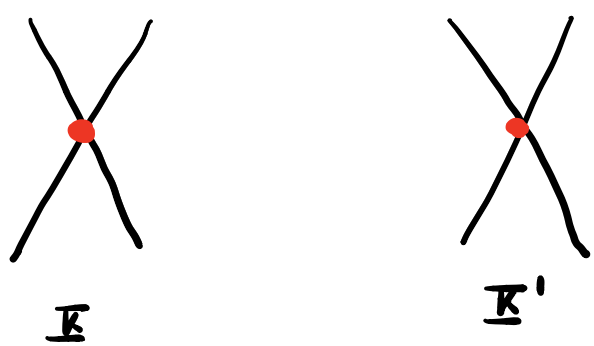
$$h_{eff}(\vec{q}) = v(\tau^z \sigma^x q_x + \sigma^y q_y)$$

(use
$$\sigma^x \sigma^y \sigma^x = -\sigma^y$$
$$\sigma^x \sigma^x \sigma^x = \sigma^x$$
$$\tau^x \tau^z \tau^x = -\tau^z$$
)

3.4 How to open a gap in graphene

Unperturbed graphene:

$$h_0(\vec{q}) = v(\tau^z \sigma^x q_x + \sigma^y q_y)$$



• Dirac points.

Consider perturbations that preserve translational symmetry of graphene (diagonal in $\vec{q}$ and diagonal in valley index).

Then, the most general perturbation :

$$\delta h(\vec{q}) = u_0 + \vec{u} \cdot \vec{\sigma} + \left(w_0 + \vec{w} \cdot \vec{\sigma} \right) \tau^z$$

where

$$u_i , w_i \in \mathbb{R}$$

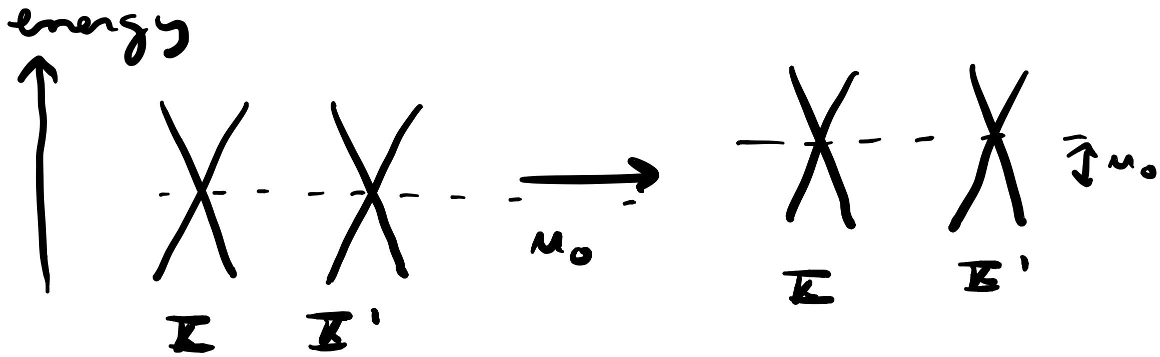
$$i = 0, x, y, z$$

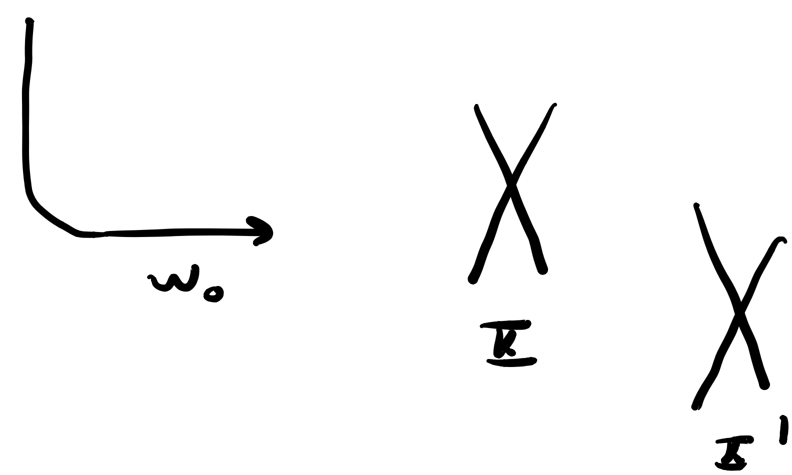
$$u_i = u_i(\vec{q})$$

$$w_i = w_i(\vec{q})$$

* Which terms open a gap at Dirac points?

(i) u_0, w_0 : shift of Dirac points w/o opening gap.





(ii) $u_x(\vec{q})$:

shifts position of Dirac point. No gap.

$$h_0 + \delta h =$$

$$= \begin{cases} v\left[\sigma^x\left(q_x + \frac{u_x}{v}\right) + \sigma^y q_y\right] & (K) \\ v\left[\sigma^x\left(-q_x + \frac{u_x}{v}\right) + \sigma^y q_y\right] & (K') \end{cases}$$

Unperturbed Dirac points are at $q_x = 0$, $q_y = 0$.

Perturbed Dirac points are at

$$q_x + \frac{u_x}{v} = 0, \quad q_y = 0 \quad (K)$$

$$q_x - \frac{u_x}{v} = 0, \quad q_y = 0 \quad (K')$$

(iii) similarly, u_y, w_x and w_y shift Dirac points but do not open gaps.

(iv) u_z, w_z : these open gaps.

$$h = \begin{cases} v(\sigma^x q_x + \sigma^y q_y) + m_K \sigma^z & (K) \\ v(-\sigma^x q_x + \sigma^y q_y) + m_{K'} \sigma^z & (K') \end{cases}$$

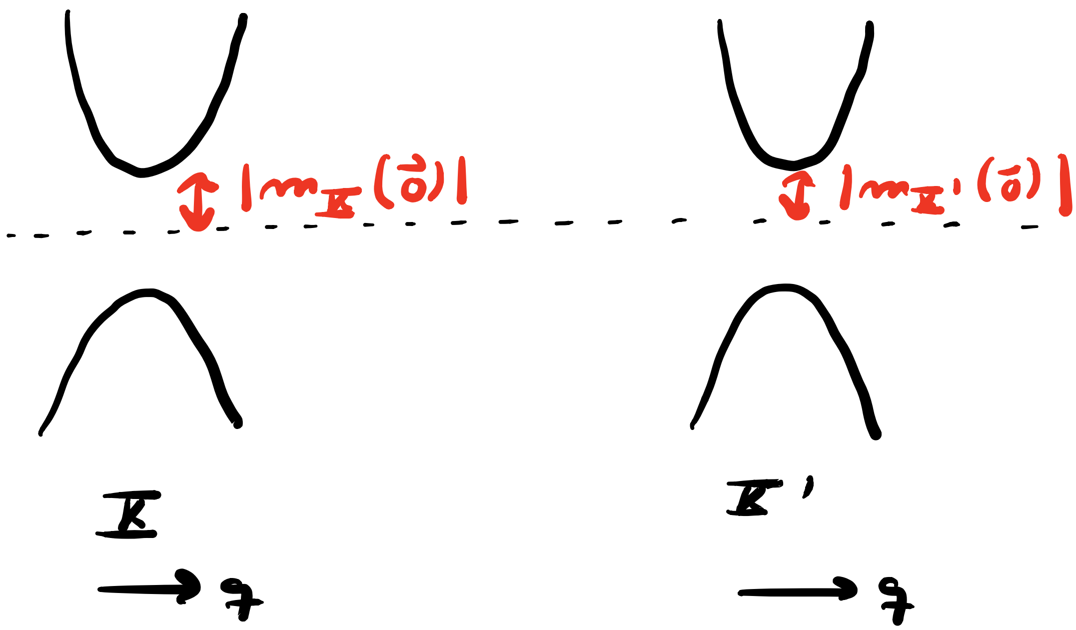
m_K and $m_{K'}$: mass terms

$$m_K = u_z + w_z$$

$$m_{K'} = u_z - w_z$$

$$E_{q,\pm}^{(K)} = \pm\sqrt{v^2(q_x^2+q_y^2)+m_K^2}$$

$$E_{q,\pm}^{(K')} = \pm\sqrt{v^2(q_x^2+q_y^2)+m_{K'}^2}$$



From here on, let's concentrate only on u_z and w_z.

$$\delta h(\vec{q}) = u_z(\vec{q})\,\sigma^z$$
$$+ w_z(\vec{q})\,\sigma^z \tau^z$$

$u_z(\vec{0})$: Semenoff mass

G. Semenoff, PRL 53, 2449 (1984)

$w_z(\vec{0})$: Haldane mass.

D. Haldane, PRL 61, 2015 (1988)

* TRS $\Leftrightarrow$ $h(\vec{q}) = \tau^x\, h(-\vec{q})^*\, \tau^x$

$\Leftrightarrow$ $\delta h(\vec{q}) = \tau^x\, \delta h(-\vec{q})^*\, \tau^x$

$$\Leftrightarrow \quad \begin{cases} u_z(\vec{q}) = u_z(-\vec{q}) \\ w_z(\vec{q}) = -w_z(-\vec{q}) \end{cases}$$

$\Rightarrow$ $w_z(\vec{0}) = 0$ $\rightarrow$ no Haldane mass.

Can still have a Semenoff mass.

* SIS $\Leftrightarrow$ $h(\vec{q}) = \tau^x \sigma^x h(-\vec{q}) \tau^x \sigma^x$

$\Leftrightarrow$ $\delta h(\vec{q}) = \tau^x \sigma^x \delta h(-\vec{q}) \tau^x \sigma^x$

$$\Leftrightarrow \quad \begin{cases} u_z(\vec{q}) = -u_z(-\vec{q}) \\ w_z(\vec{q}) = w_z(-\vec{q}) \end{cases}$$

$\Rightarrow$ $u_z(\vec{0}) = 0 \Rightarrow$ no Semenoff mass.

Can still have a Haldane mass.

* If <u>both</u> SIS and TRS are present:

$u_z = w_z = 0$ all $\vec{q}$.

$\Rightarrow$ no gap.

Need to break either SIS or TRS to gap graphene.

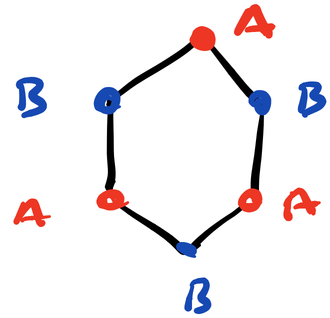
Break only SIS $\Rightarrow$ Semenoff mass

" only TRS $\Rightarrow$ Haldane "

* Physical origin of Semenoff mass?

$$\delta h = m_z(\vec{q})\,\sigma^z$$

Staggered potential (opposite sign for A and B sublattices). Realised if A and B are different atoms.



example: BN.

* Physical origin of Haldane mass?

Imaginary second neighbor hopping.

$$\delta h = i \sum_{\langle\langle i,j \rangle\rangle} \underbrace{t_2}_{\text{real}} c_i^{+} c_j + h.c.$$