Time reversal (TR)

$$f(t) \longrightarrow f(-t) \rightarrow \text{time reversed counterpart.}$$
$$t' = -t$$

Classically: $v = \frac{dx(t)}{dt} \longrightarrow \quad \frac{dx(-t)}{dt} = \frac{dx(t')}{dt'}\frac{dt'}{dt} = v(-1) = -v$

Given $\{q_i, v_i\}$, its TR counterpart is $\{q_i, -v_i\}$

If energy is same then H must have TR symmetry.
(For example if H does not depend on odd power of $\dot{q}_i$)

Note that you can not go from one description to the other description unless you flip the force but TR does not flip force: $\frac{d^2x}{dt^2} \xrightarrow[TR]{} \frac{d^2x}{dt^2}$

So there are <u>discrete</u> snap shots.

TR symmetry $\rightarrow$ discrete symmetry.

In QM: motion $\longrightarrow \frac{1}{m}\langle\psi|\hat{p}|\psi\rangle$

$i\theta x \quad i\theta' x$

let $\psi = c_q e^{iqx} + c_{q'} e^{iq'x}$

$$\langle \psi | \hat{p} | \psi \rangle = |c_q|^2 q + |c_{q'}|^2 q'$$

$$\psi^* = c_q^* e^{-iqx} + c_{q'}^* e^{-iq'x}$$

$$\langle \psi^* | \hat{p} | \psi^* \rangle = |c_q|^2 (-q) + |c_{q'}|^2 (-q')$$

$\therefore$ $\langle \psi | \hat{p} | \psi \rangle$ and $\langle \psi^* | \hat{p} | \psi^* \rangle$ are motion reversed!

$\therefore$ In QM : motion reversal $\rightarrow$ Complex conjugation of space part.

We can see it more formally by going through TDSE.

TDSE :
$$i\hbar \frac{\partial}{\partial t} \psi(x,t) = H \psi(x,t)$$

$$\Rightarrow \langle \psi | \left(i\hbar \frac{\partial}{\partial t} \right) | \psi \rangle = E \quad \text{Real} \quad \text{— (4)}$$

$$|\psi(-t)\rangle = E$$

TR: $t \to -t$ in ψ : $\langle \psi(-t) | i\hbar \frac{\partial}{\partial t}$ ...

[Let $-t = t'$]

$\frac{\partial t'}{\partial t} \to -$ $\langle \psi(t') | i\hbar \frac{\partial}{\partial t'} | \psi(t') \rangle = E$ — (B)

t' can as well be set to t :

$\therefore \; -\langle \psi(t) | i\hbar \frac{\partial}{\partial t} | \psi(t) \rangle = E$ contradicts (A) !

However if we do complex conjugation of (B)

$\langle \psi^*(-t) | -i\hbar \frac{\partial}{\partial t} | \psi^*(-t) \rangle = E$

[$t' = -t$] $\Rightarrow$ $\langle \psi^*(t') | i\hbar \frac{\partial}{\partial (t')} | \psi^*(t') \rangle = E$

No contradiction with (A) 

$\therefore$ In QM $\xrightarrow{TR}$ (set t to $-t$) + Complex conjugation.

$\Rightarrow \psi(x, t) \xrightarrow[TR]{} \psi^*(x, -t)$

Note that we do this <u>only in wave function</u>.

NOT in operators. Because they are our measuring tools, and $\Psi(x,t)$ and $\Psi^*(x,-t)$ are two states of the same system. They could as well be the same state. Think of e^{iqx} with $q=0$.

Define TR operator as $\hat{\Theta}$ which does complex conjugation and converts t to $-t$ at all states.

Let us see how $\hat{\Theta}$ operates on Bloch states.

$$\hat{\Theta}\ \hat{H}\Psi_{qn} = E_{qn}\Theta\Psi_{qn}\ ] \quad \text{since } E_{qn} \text{ is real.}$$

$$\Rightarrow \hat{H}\hat{\Theta}\Psi_{qn} = E_{qn}\hat{\Theta}\Psi_{qn} \quad \text{since } \hat{H} \text{ is real.}$$

$$\Rightarrow [\hat{H}\ \hat{\Theta}] = 0 \Rightarrow \Psi_{qn} \text{ and } \hat{\Theta}\Psi_{qn} \text{ are degenerate!}$$

What is $\hat{\Theta}\Psi_{qn}$?

$\hat{\Theta}$ ... $\hat{\Theta}\ e^{iqx}$ ...

$$\hat{\Theta}\psi_{qn} = \hat{\Theta}e^{i\ldots}u_{q_n}(x)$$

$$= e^{-iqx}\underline{\hat{\Theta}u_{q_n}(x)} \quad ?$$

Recall,

$$\hat{H}_q u_q = E_q u_q$$

$$\hat{\Theta}\hat{H}_q u_q = E_q\hat{\Theta}u_q$$

$$\hat{\Theta}\hat{H}_q u_{qn} = \hat{\Theta}\left[\frac{(p+\hbar q)^2}{2m} + V\right]u_{qn}$$

$$= \hat{\Theta}\frac{1}{2m}\left[\hbar^2 q^2 - \hbar^2\frac{\partial}{\partial x^2} + 2i\hbar^2 q\frac{\partial}{\partial x} + V\right]u^*_{qn}$$

$$= \frac{1}{2m}\left[\hbar^2 q^2 - \hbar^2\frac{\partial}{\partial x^2} - 2i\hbar^2 q\frac{\partial}{\partial x} + V\right]u^*_{qn}$$

$$= \left[\frac{(p-\hbar q)^2}{2m} + V\right]\hat{\Theta}u_{qn} \qquad \hookrightarrow \hat{\Theta}u_{qn}$$

$$\therefore \hat{\Theta}(\hat{H}_q u_q) = E_{qn} \hat{\Theta} u_q$$

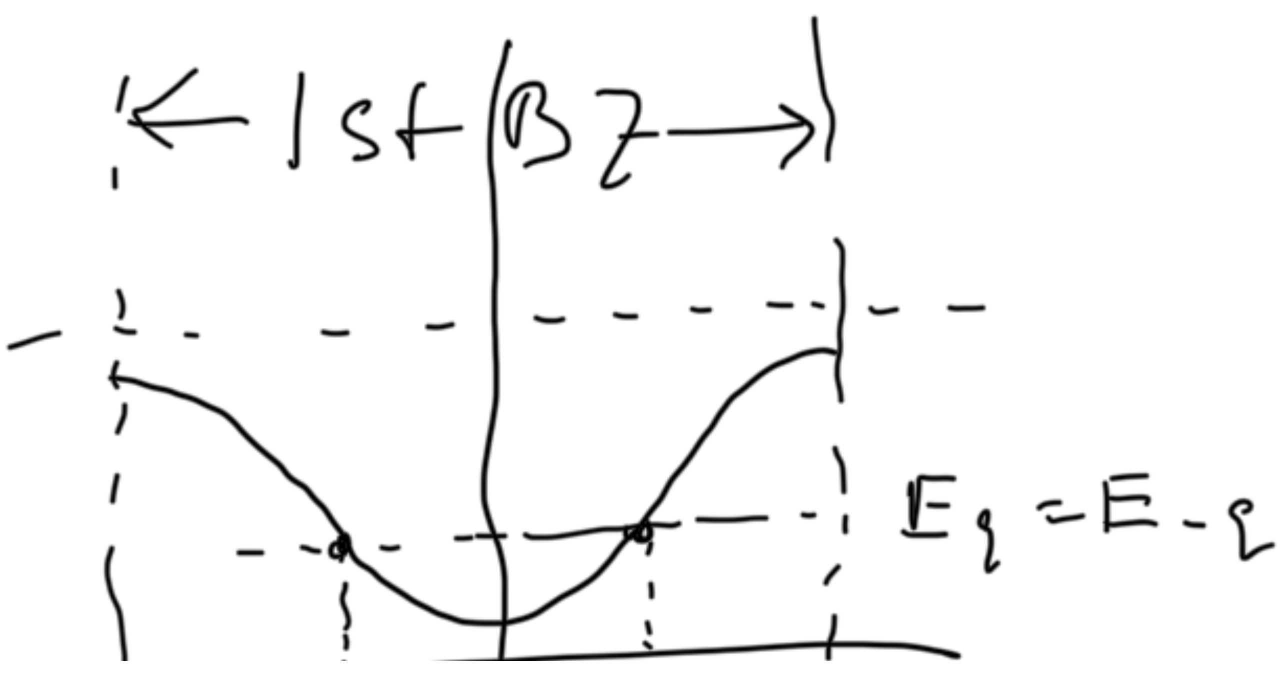
$$\Rightarrow \hat{H}_{-q} \hat{\Theta} u_{qn} = E_{qn} \hat{\Theta} u_{qn}$$

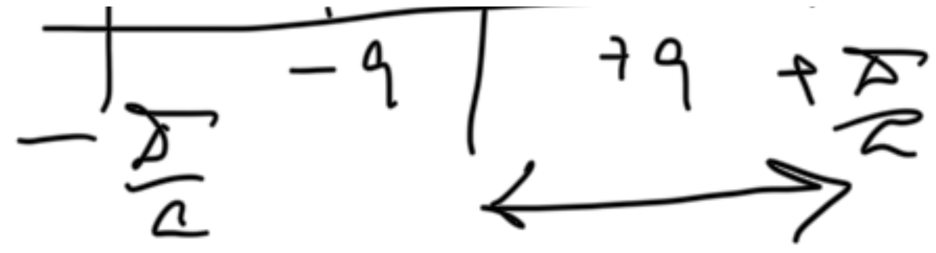
Compare with $\hat{H}_{-q} u_{-qn} = E_{-qn} u_{-qn}$

$$\Rightarrow \hat{\Theta} u_{qn} = u_{-qn} \text{ and } E_{qn} = E_{-qn}$$

$$\therefore \hat{\Theta} \Psi_{qn} = e^{-iqn} \hat{\Theta} u_{qn} = e^{-iqn} u_{-qn} = \Psi_{-qn}$$

$$\therefore [\hat{H}, \hat{\Theta}] = 0 \Rightarrow \hat{\Theta} \Psi_{qn} = \Psi_{-qn} \Rightarrow \Psi_{qn} \text{ and } \Psi_{-qn} \text{ degenerate!}$$





Irreducible BZ

If $[H,\hat{O}]=0$, it is sufficient to know $\{E_{qn}, \psi_{qn}\}$ of half of the 1st BZ.