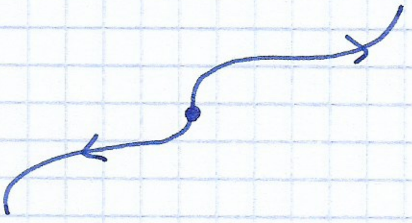
§5. Time reversal symmetry (TRS)

$$\boxed{t \longrightarrow t_T = -t}$$

In classical mechanics equation of motion is TRS. It is impossible to distinguish forward or backward time moving



$$\bar{r} \to \bar{r}_T = \bar{r}$$

$$\bar{p} \to \bar{p}_T = -\bar{p} \qquad \bar{p} = m\frac{d\bar{r}}{dt}$$

$$\dot{\bar{r}}_T(t) = \frac{d\bar{r}_T(t)}{dt} = \frac{d\bar{r}(-t)}{dt} = -\frac{d\bar{r}(-t)}{d(-t)} =$$

$$= -\dot{\bar{r}}(-t)$$

$$\bar{F} \to \bar{F}_T = \bar{F}$$

$$\bar{a}_T(t) = \ddot{\bar{r}}_T(t) = \ddot{\bar{r}}(-t) =$$

$$= \bar{a}(-t)$$

$$\bar{E} \to \bar{E}_T = \bar{E} \qquad \bar{F} = q\bar{E}$$

$$\bar{B} \to \bar{B}_T = -\bar{B} \qquad \bar{F} = q\bar{v} \times \bar{B}$$

How about TRS in quantum mechanics?

$$-\frac{\hbar^2}{2m}\bar{\nabla}^2\Psi(\bar{r},t)+V(\bar{r})\Psi(\bar{r},t)=i\hbar\frac{\partial\Psi(\bar{r},t)}{\partial t}$$

$$\updownarrow \qquad t \Rightarrow t_T=-t$$

$$-\frac{\hbar^2}{2m}\bar{\nabla}^2\Psi(\bar{r},t)+V(\bar{r})\Psi(\bar{r},-t)=-i\hbar\frac{\partial\Psi(\bar{r},-t)}{\partial t}$$

Formally, this is the same equation if we take the <u>complex conjugation</u>

$$-\frac{\hbar^2}{2m}\bar{\nabla}^2\Psi^*(\bar{r},t)+V(\bar{r})\Psi^*(r,-t)=i\hbar\frac{\partial\Psi^*(\bar{r},t)}{\partial t}$$

Therefore, if TRS is demanded we find that

$$\Psi(\bar{r},t)\longrightarrow\Psi^*(\bar{r},-t)$$

Let $\hat{U}=\hat{\Theta}$ for TR symmetry operator

$$\boxed{\hat{\Theta}\,\Psi(\bar{r},t)=\Psi^*(\bar{r},-t)}$$

<u>Fact</u>: $\hat{\Theta}$ is <u>antilinear</u> (antiunitary) operator.
(impossible to formulate a unique eigenvalue problem).

<u>proof</u>:

$$\begin{aligned}\hat{\Theta}(c_1\Psi_1(t)+c_2\Psi_2(t)) &=\\ &= c_1^*\Psi_1^*(-t)+c_2^*\Psi_2^*(-t)=\\ &= c_1^*(\hat{\Theta}\Psi_1(t))+c_2^*(\hat{\Theta}\Psi_2(t))\end{aligned}$$

□

<u>Note</u>: $\langle\hat{\Theta}\phi|\hat{\Theta}\Psi\rangle=\langle\Psi|\phi\rangle=\langle\phi|\Psi\rangle^*$

only $|\langle\Psi|\phi\rangle|$ is conserved!

Central properties of $\hat{\Theta}$ - antilinear operator

$$\hat{\Theta}\,\alpha|\psi\rangle = \Theta\,\alpha\,\Theta^{-1}\Theta|\psi\rangle = \alpha^*\,\Theta|\psi\rangle = \alpha^*|\hat{\Theta}\psi\rangle$$

$$\rightarrow \quad \boxed{\hat{\Theta}\,\alpha\,\hat{\Theta}^{-1} = \alpha^*} \qquad \alpha \in \mathbb{C}$$

Consider two states

$$|\psi\rangle = \sum_n \psi_n|n\rangle \qquad \{|n\rangle\} \text{ - orthonormal basis}$$

$$|\phi\rangle = \sum_m \phi_m|m\rangle$$

$$\hat{\Theta}|\psi\rangle = \sum_n \hat{\Theta}\psi_n\hat{\Theta}^{-1}|\hat{\Theta}n\rangle$$

$$\hat{\Theta}|\phi\rangle = \sum_m \hat{\Theta}\phi_m\hat{\Theta}^{-1}|\hat{\Theta}m\rangle$$

$$\boxed{\langle\hat{\Theta}\phi|\hat{\Theta}\psi\rangle} = \sum_{nm}(\hat{\Theta}\phi_m\hat{\Theta}^{-1})^*(\hat{\Theta}\psi_n\hat{\Theta}^{-1})\underbrace{\langle\hat{\Theta}m|\hat{\Theta}n\rangle}_{=\langle m|n\rangle = \delta_{mn}} =$$

$$= \sum_n(\hat{\Theta}\phi_m\hat{\Theta}^{-1})^*(\hat{\Theta}\psi_n\hat{\Theta}^{-1}) = \sum_n \phi_n\psi_n^* = \langle\psi|\phi\rangle =$$

$$\boxed{= \langle\phi|\psi\rangle^*}$$

since ϕ_m and ψ_n are arbitrary

$$(\hat{\Theta}\psi_n\hat{\Theta}^{-1}) = \psi_n^*$$

$$(\hat{\Theta}\phi_n\hat{\Theta}^{-1}) = \phi_n^*$$

If $\hat{\Theta}$ is a symmetry operator

$$\hat{\Theta}\hat{H}\hat{\Theta}^{-1} = \hat{H} \leftrightarrow [\hat{\Theta},\hat{H}] = 0$$

Therefore,

$$\hat{H}|E\rangle = E|E\rangle \rightarrow \hat{\Theta}\hat{H}\hat{\Theta}^{-1}\hat{\Theta}|E\rangle = E\hat{\Theta}|E\rangle$$

but $E \in \mathbb{R}$

$$\hat{H}|\hat{\Theta}E\rangle = E|\hat{\Theta}E\rangle$$

So $|E\rangle$ and $|\hat{\Theta}E\rangle$ are degenerate unless $|E\rangle = c|\hat{\Theta}E\rangle$.

Observation : In the presence of a magnetic field the TRS is broken. $\bar{B} = \bar{\nabla} \times \bar{A}$

$$i\hbar \frac{\partial \Psi(\bar{r},t)}{\partial t} = \left[\frac{(-i\hbar\bar{\nabla} - e\bar{A})^2}{2m} + V(\bar{r}) \right] \Psi(\bar{r},t) \Big| \hat{\Theta}$$

$$i\hbar \frac{\partial \Psi^*(\bar{r},t)}{\partial (-t)} = \left[\frac{(i\hbar\bar{\nabla} - e\bar{A})^2}{2m} + V(\bar{r}) \right] \Psi^*(\bar{r},t)$$

It is not the same equation unless $\bar{A} = 0$

□

Elementary cases

$$\hat{\bar{R}}|\bar{r}\rangle = \bar{r}|\bar{r}\rangle \qquad \hat{\bar{P}}|\bar{p}\rangle = \bar{p}|\bar{p}\rangle$$

we demand (on classical intuition)

$$\boxed{\hat{\Theta}|\bar{r}\rangle = |\bar{r}\rangle}$$

$$\Rightarrow \hat{\Theta}\hat{\bar{R}}\hat{\Theta}^{-1}\hat{\Theta}|\bar{r}\rangle = \bar{r}\hat{\Theta}|\bar{r}\rangle$$

$$\hat{\Theta}\hat{\bar{R}}\hat{\Theta}^{-1}|\bar{r}\rangle = \bar{r}|\bar{r}\rangle$$

$$\Rightarrow \boxed{\hat{\Theta}\hat{\bar{R}}\hat{\Theta}^{-1} = \hat{\bar{R}}} \quad \text{(as)} \quad \bar{r} \to \bar{r}_T = \bar{r}$$

Consider $|\psi\rangle = \int d\bar{r}\, |\bar{r}\rangle\langle\bar{r}|\psi\rangle = \int d\bar{r}\, \psi(\bar{r})|\bar{r}\rangle$

$$\hat{\Theta}|\psi\rangle = \int d\bar{r}\, \psi^*(\bar{r})|\hat{\Theta}\bar{r}\rangle = \int d\bar{r}\, \psi^*(\bar{r})\,|\bar{r}\rangle$$

Hence, $\boxed{\langle\bar{r}|\hat{\Theta}\psi\rangle = \psi^*(\bar{r})}$

How does $\hat{\Theta}$ ~~and~~ act on $\hat{\bar{p}}$?

$$\langle\bar{r}|\bar{p}\rangle = \frac{e^{i\bar{p}\cdot\bar{r}/\hbar}}{(2\pi\hbar)^{3/2}}$$

$$\langle\hat{\Theta}\bar{r}|\hat{\Theta}\bar{p}\rangle = \langle\bar{p}|\bar{r}\rangle = \frac{e^{-i\bar{p}\cdot\bar{r}/\hbar}}{(2\pi\hbar)^{3/2}}$$

$$\parallel$$

$$\langle\bar{r}|\hat{\Theta}\bar{p}\rangle = \frac{e^{-i\bar{p}\cdot\bar{r}/\hbar}}{(2\pi\hbar)^{3/2}} = \langle\bar{r}|-\bar{p}\rangle$$

Hence $\boxed{\hat{\Theta}|\bar{p}\rangle = |-\bar{p}\rangle}$

or $\boxed{\hat{\Theta}\hat{\bar{p}}\hat{\Theta}^{-1} = -\hat{\bar{p}}}$

It is consistent with the commutator

$$[\hat{x}, \hat{p}] = i\hbar \qquad \text{dim} = 1$$

$$\hat{\Theta}\hat{x}\hat{\Theta}^{-1}\hat{\Theta}\hat{p}\hat{\Theta}^{-1} - \hat{\Theta}\hat{p}\hat{\Theta}^{-1}\hat{\Theta}\hat{x}\hat{\Theta}^{-1} = \hat{\Theta}i\hat{\Theta}^{-1}\hbar$$

$$-\hat{x}\hat{p} + \hat{p}\hat{x} = -i\hbar$$

Theorem

$$\boxed{\hat{\theta} = \hat{k}\,\hat{u}}$$

complex conjugation

unitary operator

Proof : Let $|\psi\rangle = \sum_n \psi_n |n\rangle$ orthonormal basis

$$\hat{\theta}|\psi\rangle = \sum_n \psi_n^* |\hat{\theta} n\rangle$$

but

$$\langle \hat{\theta} n|\hat{\theta}|m\rangle = \langle n|\hat{\theta}^+\hat{\theta}|m\rangle = \langle n|n\rangle = \delta_{nm}$$

therefore $|\hat{\theta} n\rangle = \sum_m U_{nm}|m\rangle$

unitary transformation

therefore

$$\hat{\theta}|\psi\rangle = \sum_{mn} \psi_n^+ U_{nm}|m\rangle =$$

$$= \hat{K} \sum_{mn} \psi_n U_{nm}^+ |m\rangle =$$

$$= \hat{K} \sum_{mn} \psi_n (U_{mn})^+ |m\rangle \qquad \Big| \langle k|$$

$$\langle k|\hat{\theta}|\psi\rangle = \hat{K} \sum_{mn} \psi_n (U_{mn})^+ \underbrace{\langle k|m\rangle}_{\delta_{km}} =$$

$$= \hat{K} \sum_n (U_{km})^+ \psi_n = \hat{K}\left[\hat{u}^+ \psi\right]_k$$

hence $\hat{\theta}|\psi\rangle = \hat{K}\hat{u}^+|\psi\rangle$

but $\hat{u}$ is unitary

and finally $\boxed{\hat{\theta} = \hat{k}\,\hat{u}}$

$\square$

we also write equivalently $\boxed{\hat{\theta} = \hat{u}\hat{K}}$

Theorem $\hat{\Theta}^2 = \pm \mathbb{1}$

proof $\hat{\Theta}^2 |\psi\rangle = c\,|\psi\rangle$ to get the same physics

so $(\hat{K}\hat{U})(\hat{K}\hat{U})|\psi\rangle = c\,|\psi\rangle$

$$\Big\downarrow$$

$$\hat{U}^* \hat{U}\, |\psi\rangle = c\,|\psi\rangle \qquad \forall |\psi\rangle$$

$$\Big\downarrow$$

$$\hat{U}^* \hat{U} = c \qquad \Big|\ \hat{U}^\dagger = \hat{U}^{-1}$$

$$\hat{U}^* = c\,\hat{U}^\dagger = c\,(\hat{U}^*)^T = c\,(c\,\hat{U}^\dagger)^\dagger = \boxed{c^2\,\hat{U}^*} \Rightarrow c^2 = 1 \rightarrow \boxed{c = \pm 1}$$

□

Kramers theorem $\boxed{\hat{\Theta}^2 = -\mathbb{1}}$ it cannot have an eigenvector

proof a.a.

Let $\hat{\Theta}\,|\psi\rangle = \lambda\,|\psi\rangle$

Then $\hat{\Theta}^2\,|\psi\rangle = \hat{\Theta}\,\lambda\,|\psi\rangle = \lambda^*\,\hat{\Theta}\,|\psi\rangle = |\lambda|^2|\psi\rangle \neq -|\psi\rangle$

□

Thus what we have, are (at least) two degenerate states related by $\hat{\Theta}$

$$\boxed{\hat{\Theta}\,|\psi\rangle = |\chi\rangle \quad \text{and} \quad \hat{\Theta}\,|\chi\rangle = -|\psi\rangle}$$

This is called a Kramers' doublet

Fact: $|\psi\rangle$ and $|\hat{\Theta}\psi\rangle$ are orthogonal if $\hat{\Theta}^2 = -\mathbb{1}$

$$\langle\psi|\hat{\Theta}\psi\rangle = \langle\hat{\Theta}^2\psi|\hat{\Theta}\psi\rangle = -\langle\psi|\hat{\Theta}\psi\rangle = 0$$

therefore $|\psi\rangle$ and $|\hat{\Theta}\psi\rangle$ - orthogonal. □

E.g. for spinless particles

$E(\bar{k}) = E(-\bar{k})$ □

We have shown that

$$\hat{\Theta} = \underset{\substack{\uparrow \\ \text{unitary}}}{\hat{u}}\ \underset{\llcorner\ \text{complex conjugation}}{\hat{K}}$$

What is a representation for u?

It depends!

Case A - particles with spin zero

States are characterized by a single component wave functions

We had
$$\hat{\Theta}\,\hat{\bar{R}}\,\hat{\Theta}^{-1} = \hat{\bar{R}}$$

$$\hat{\Theta}\,\hat{\bar{p}}\,\hat{\Theta}^{-1} = -\hat{\bar{p}}$$

and $\bar{L} = \bar{r} \times \bar{p}$
$$\hat{\Theta}\,\hat{\bar{L}}\,\hat{\Theta}^{-1} = -\hat{\bar{L}}$$

In coordinate representation $\overset{\psi_\alpha(\bar{r})}{\vee}$, $\hat{\bar{p}} = -i\hbar\bar{\nabla}$,
$\hat{\bar{p}}$ - pure imaginary, so $\hat{u} = \mathbb{1}$

and $\boxed{\hat{\Theta} = \hat{K}}$

In momentum representation $\overbrace{\psi_\alpha(\bar{p}),}^{\bar{p}\text{ - multiplication}}$
$\hat{u}$ is such that $\hat{u}\,\psi_\alpha(\bar{p}) = \psi_\alpha(-\bar{p})$

unitary $\hat{u}$ transforms $\bar{p} \to -\bar{p}$

Case B | particle with a spin S

in coordinate representation

$$\hat{\Theta}\,\hat{\vec{S}}\,\hat{\Theta}^{-1} = -\hat{\vec{S}}$$

$$\hat{\Theta}\,\hat{\vec{J}}\,\hat{\Theta}^{-1} = -\vec{J}$$

We choose a set of spin matrices such that S_x and S_z are real and S_y is purely imaginary

$\hat{\vec{r}}$, $\hat{S}_x$, $\hat{S}_z$ - real operators

$\hat{\vec{p}}$, $\hat{\vec{L}}$, $\hat{S}_y$ - purely imaginary operators

We need $\hat{u}$ such that $\hat{u}$ commutes with $\hat{\vec{r}}$, $\hat{\vec{p}}$, $\hat{\vec{L}}$, $\hat{S}_y$ and obeys

$$\hat{S}_x \hat{u} = -\hat{u}\hat{S}_x$$

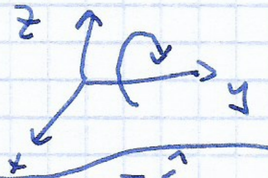
$$\hat{S}_z \hat{u} = -\hat{u}\hat{S}_z$$

If $\hat{u}$ is a function of S_y only we have

$$[\hat{\vec{r}}, \hat{u}] = [\hat{\vec{p}}, \hat{u}] = [\hat{\vec{L}}, \hat{u}] = [\hat{S}_y, \hat{u}] = 0$$

The choice $\boxed{\hat{u} = e^{-i\pi \frac{\hat{S}_y}{\hbar}}}$ satisfies this.

This is a rotation by $\varphi = \pi$ along y axis



Then $\hat{S}_x \to -\hat{S}_x$

$\hat{S}_z \to -\hat{S}_z$

$$\boxed{\hat{\Theta} = e^{-i\frac{\pi \hat{S}_y}{\hbar}}\,\hat{K}}$$

For spin $s = 1/2$ we get

$$\boxed{\hat{\Theta} = -i\,\sigma_y \hat{K}} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$