$\boxed{\text{Time reversal}}$

In classical Mechanics,

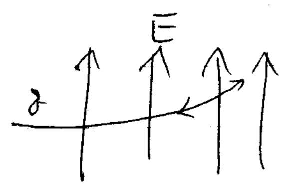
$\vec{F} = m\vec{a}$, $\vec{r}(t) \Rightarrow \vec{r}(-t)$ physically allowed?

In the $\vec{E}$ field

$$m\frac{d^2\vec{r}}{dt^2} = q\vec{E}(\vec{r}) \qquad \text{is time reversal inv.}$$

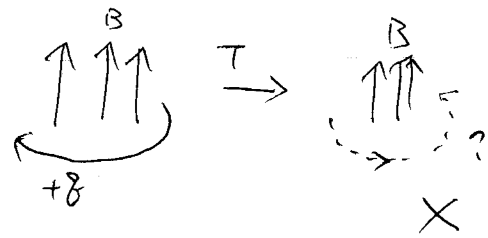
$(-)^2 = +$ $\qquad \vec{E} = -\vec{\nabla}\phi$ no time depend

$\Rightarrow \tau = -t, \quad \vec{r}(-t) = \vec{r}(\tau)$



However, in the presence of $\vec{B}$ field

$$m\underbrace{\frac{d^2\vec{r}}{dt^2}}_{(-)^2} = \frac{q}{c}\underbrace{\frac{d\vec{r}}{dt}}_{(-)}\times\vec{B}(\vec{r}) \qquad \text{doesn't seem to hold}$$



Need to consider the whole system which includes the sources to produce $\vec{E}$ & $\vec{B}$

$\rho \to \rho \qquad \vec{J} \to -\vec{J}$

$\Rightarrow \vec{E} \to \vec{E} \quad , \quad \vec{B} \to -\vec{B}$

Schrödinger Eq & Time reversal

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + q\phi(\vec{r})\right]\psi(\vec{r},t)$$

$\psi(\vec{r},-t)$ is not a solution. LHS change sign but RHS does not. But $\psi^*(\vec{r},-t)$ is a solution.

In magnetic field

$$i\hbar\frac{\partial}{\partial t}\psi = \frac{1}{2m}\left[-i\hbar\vec{\nabla} - \frac{q}{c}\vec{A}(\vec{r})\right]^2\psi$$

is invariant under

$$\psi \to \psi^*(\vec{r},-t)$$
$$\vec{A} \to -\vec{A}$$

Time reversal operator Θ

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H |\psi(t)\rangle$$

write $|\psi_r(t)\rangle = \Theta |\psi(-t)\rangle$, the time reversal state

Θ is a mapping from kets into other kets.

It doesn't involve time by itself. This is clear when $t=0$

$$|\psi_r(0)\rangle = \Theta |\psi(0)\rangle$$

* Postulates for Θ

① prob. conserved $\Rightarrow$ $\Theta^\dagger \Theta = \mathbb{1}$

② reproduce CM $\Rightarrow$ $\Theta \hat{r} \Theta^\dagger = \hat{r}$ Eq (1)

$\Theta \hat{p} \Theta^\dagger = -\hat{p}$ (2)

$\Theta \hat{L} \Theta^\dagger = -\hat{L}$

we assume the same happen for spin $\Theta \vec{S} \Theta^\dagger = -\vec{S}$ $\Bigg\}$ $\Theta \vec{J} \Theta^\dagger = -\vec{J}$

However, Θ can <u>NOT</u> be unitary !!

From Eqs (1),(2), it can't be achived by any unitary operator for $[r_i, p_j] = i\hbar \delta_{ij}$ to hold

$$\Theta [r_i, p_j] \Theta^\dagger = -[r_i, p_i] = -i\hbar \delta_{ij} = \Theta (i\hbar \delta_{ij}) \Theta^\dagger$$

if $\Theta\Theta^\dagger = 1$, $\Rightarrow$ Θ must be antilinear!!

If $\langle a|b\rangle = 0$ & $|\psi\rangle = \alpha|a\rangle + \beta|b\rangle$

If an operator Q represents a symmetry

① $Q|a\rangle$ and $Q|b\rangle$ are still orthogonal to each other.

② Q doesnot change the outcome of any measurement.

$$|\langle\psi|Q^\dagger Q|\psi'\rangle|^2 = |\langle\psi|\psi'\rangle|^2$$

two solutions.

either $\langle\psi|Q^\dagger Q|\psi'\rangle = \langle\psi|\psi'\rangle \Rightarrow$ Q is unitary (Q_u)

or $\langle\psi|Q^\dagger Q|\psi'\rangle = \langle\psi|\psi'\rangle^* = \langle\psi'|\psi\rangle \Rightarrow$ Q is antiunitary (Q_A)

and $Q|\psi\rangle = \alpha^* Q|a\rangle + \beta^* Q|b\rangle$

Any anti-unitary operator can be defined by the product

$$Q_A = Q_u K$$

K is the complex conjugation operator

$$K[\alpha|a\rangle + \beta|b\rangle] = \alpha^* K|a\rangle + \beta^* K|b\rangle$$

and $K^2 = 1$

Actually, odd number product of anti unitary $\Rightarrow$ antiunitary

even " $\Rightarrow$ unitary

Assume Q : a complete set of commuting observables

n : collective set of quantum numbers corresponding to Q.

$|n\rangle$: basis kets in this representation.

$K_Q^\dagger K_Q = K_Q K_Q^\dagger = \mathbb{1}$ $\quad$ K_Q : antilinear

$K_Q|n\rangle = |n\rangle$ $\quad$ (if K_Q were a linear operator $\Rightarrow K_Q = \mathbb{1}$
but it is antilinear, $\Rightarrow K_Q \neq \mathbb{1}$)

say $|\psi\rangle$ an arbitrary ket

$$|\psi\rangle = \sum_n c_n|n\rangle$$

$$K_Q|\psi\rangle = \sum_n \underbrace{c_n^*}_{\text{same as the wave function in the } Q \text{ representation}}|n\rangle$$

A spinless particle in 3D

$Q = \hat{\vec{r}}$, $|\vec{r}\rangle$: basis, $K_r |\vec{r}\rangle = |\vec{r}\rangle$

$$K_r|\psi\rangle = K_r \int d^3\vec{r}\, |\vec{r}\rangle\langle\vec{r}|\psi\rangle = K_r \int d^3\vec{r}\, |\vec{r}\rangle \psi(\vec{r})$$
$$= \int d^3 r\, |\vec{r}\rangle \psi^*(\vec{r})$$

$K_Q^2 = 1$, $\because$ $K_Q(K_Q|n\rangle) = K_Q|n\rangle = |n\rangle$

$\Rightarrow$ $K_Q = K_Q^+$ & $K_Q^+|n\rangle = |n\rangle$

Time reversed motion

Is $|\psi_r(t)\rangle$ a solution which satisfies Schrödinger Eq ?

H : time-independent

$$i\hbar\frac{\partial}{\partial t}|\psi_r(t)\rangle = i\hbar\frac{\partial}{\partial t}\,\theta|\psi(-t)\rangle = \theta\left(-i\hbar\frac{\partial}{\partial t}|\psi(-t)\rangle\right)$$

θ commutes with $\frac{\partial}{\partial t}$, θ is a Hilbert space operator

$\frac{\partial}{\partial t}$: a derivation with respect to a parameter that the state depends on.

write $\tau = -t$

$\Rightarrow$ $|\psi_r(t)\rangle = \theta|\psi(\tau)\rangle$

$$\Rightarrow i\hbar\frac{\partial}{\partial t}|\psi_r(t)\rangle = \theta\left[i\hbar\frac{\partial}{\partial \tau}|\psi(\tau)\rangle\right] = \theta H|\psi(\tau)\rangle$$
$$= (\theta H \theta^+)\theta|\psi(\tau)\rangle = (\theta H \theta^+)|\psi_r(t)\rangle$$

if $\theta H \theta^+ = H$, or $[\theta, H] = 0$

the time reversal motion satisfies the original Schrödinger Eq.

Another approach.

$$|\psi(t)\rangle = \exp\left[\frac{-itH}{\hbar}\right]|\psi(0)\rangle$$

$$\theta|\psi(t)\rangle = \theta\exp\left[\frac{-itH}{\hbar}\right]\theta^+\theta|\psi(0)\rangle = \exp\left[+\frac{itH}{\hbar}\right]\theta|\psi(0)\rangle$$

~~$|\psi_r(\tau)\rangle = \theta|\psi(-\tau)\rangle = \exp\left(\frac{-i\tau H}{\hbar}\theta\right)|\psi(\tau=0)\rangle$~~

$$\Rightarrow \quad |\psi_r(t)\rangle = \exp\left(\frac{-itH}{\hbar}\right) |\psi_r(0)\rangle$$

namely, $|\psi_r(t)\rangle$ is also a solution to the time-depend Schrödinger Eq.

Spinless ~~pa~~ system

$\mathcal{E} = \text{span}\{|\vec{r}\rangle\}$, Wave function $\psi(\vec{r})$

$\Theta = L K_r$, $\boxed{\begin{array}{l} K_r \hat{r} K_r^+ = \hat{r} \\ K_r \hat{p} K_r^+ = -\hat{p} \end{array}}$ we take $L = \mathbb{1}$

$$\psi(\vec{r}_1, \cdots \vec{r}_n) \xrightarrow{\Theta} \psi^*(\vec{r}_1, \cdots \vec{r}_n)$$

$$\because \langle r| K_r \hat{r} K_r^+ |\psi\rangle = \int d\vec{s}^3 \langle r| K_r \hat{r} K_r^+ |s\rangle\langle s|\psi\rangle$$

$$= \int d\vec{s}^3 \langle r| K_r \hat{r} \langle\psi|s\rangle |s\rangle$$

$$= \int d^3 s \langle r| K_r \underbrace{\vec{s}}_{} \underbrace{\langle\psi|s\rangle}_{\text{both are c-\#}} |s\rangle$$

$$= \int d^3 s \langle s|\psi\rangle \vec{s} \langle r|s\rangle = \vec{r}\,\psi(\vec{r})$$

or

$$\psi(\vec{r}) \xrightarrow{K^+} \psi^*(\vec{r}) \xrightarrow{\hat{r}} \hat{r}\psi^*(\vec{r}) \xrightarrow{K} \vec{r}\psi(\vec{r})$$

similarly

$$\psi(\vec{r}) \xrightarrow{K^+} \psi^*(\vec{r}) \xrightarrow{\hat{p}} -i\hbar\vec{\nabla}\psi^*(\vec{r}) \xrightarrow{K} +i\hbar\vec{\nabla}\psi(\vec{r})$$

Energy eigenstates

$H|\psi\rangle = E|\psi\rangle$, suppose $[\Theta, H] = 0$

$$H(\Theta|\psi\rangle) = \Theta H|\psi\rangle = E(\Theta|\psi\rangle)$$

If the original eigenstate is nondegenerate

$\Theta|\psi\rangle = c|\psi\rangle$, c: const, in fact a phase factor $|c|^2 = 1$

$$\Rightarrow \quad \Theta|\psi\rangle = e^{i\alpha}|\psi\rangle$$

Multiplying the above by $e^{-\frac{i\alpha}{2}}$

$$e^{-\frac{i\alpha}{2}}\,\theta|\psi\rangle = \theta\underbrace{e^{\frac{i\alpha}{2}}|\psi\rangle}_{|\phi\rangle} = \underbrace{e^{\frac{i\alpha}{2}}|\psi\rangle}_{|\phi\rangle}$$

$\Rightarrow \quad \theta|\phi\rangle = |\phi\rangle$

$\Rightarrow$ Nondegenerate energy eigenstates of $[\theta, H]=0$ can always be chosen to be eigenstate of Θ

☆ Reality of Energy eigenfunctions in spinless system

3D, spinless, kinetic + potential Hamiltonian

$\Rightarrow \quad \psi^*(\vec{r}) = e^{i\alpha}\psi(\vec{r})$

define a new W.F.

$$\phi(\vec{r}) = e^{\frac{i\alpha}{2}}\psi(r) \quad \text{so} \quad \phi(r) = \phi^*(r)$$

$\Rightarrow$ Nondegenerate energy eigenfunction in a spinless, $\frac{p^2}{2m}+V(r)$ system is always proportional to a <u>REAL</u> eigenfunction.

Time reversal and spin

$\mathcal{E} = \text{span}\{|s\,m\rangle, \quad m = \underbrace{-s, -s+1, \cdots s}_{(2s+1)\text{-dim ket space}}\}$

$\theta\,\vec{S}\,\theta^+ = -\vec{S}$

$\theta\,\hat{S_z}\,\theta^+ = -\hat{S_z}$

$\Rightarrow S_z(\theta|sm\rangle) = -\theta S_z|sm\rangle = -m\hbar\,(\theta|sm\rangle)$

Since the eigenkets of $\vec{S_z}$ are nondegenerate

$\Rightarrow \quad \theta|sm\rangle = C_m\,|s,-m\rangle \qquad C_m$ is a phase factor

$$\Theta S_\pm \Theta^+ = \Theta (S_x \mp i S_y)\Theta^+ = -S_x \mp i S_y = -S_\mp$$

$$S_+ \Theta|sm\rangle = -\Theta S_- |sm\rangle = -\hbar \sqrt{s(s+1)-m(m-1)}\ \Theta|s, m-1\rangle$$
$$= -\hbar\, C_{m-1} \sqrt{s(s+1)-m(m-1)}\ |s, -m+1\rangle$$

$$\text{L.H.S.} = C_m S_+ |s, -m\rangle$$
$$= \hbar\, C_m \sqrt{s(s+1)-(-m)(-m+1)}\ |s, -m+1\rangle$$
$$= \hbar\, C_m \sqrt{s(s+1)-m(m-1)}\ |s, -m+1\rangle$$

$$\Rightarrow \quad C_m = -C_{m-1}$$

or $\quad C_m = C_{-s}(-1)^{m+s} = C_{-s}(i)^{2m+2s}$

$$\Rightarrow \quad \Theta|sm\rangle = \eta\,(i)^{2m}|s, -m\rangle, \qquad \eta = C_{-s}\, i^{2s}$$

can be absorbed into the definition of Θ or $|s,-s\rangle$

$$\Rightarrow \quad \boxed{\Theta|sm\rangle = (i)^{2m}|s\, -m\rangle}$$