

# Chapter 4: Symmetry in QM (09/05/2011)

## Symmetries in Classical Mechanics (1)

$$L(q, \dot{q}) \rightarrow L'(q + \delta q)$$

Graduate

$$\delta L = \frac{\partial L}{\partial q} \delta q + \frac{\partial L}{\partial \dot{q}} \delta \dot{q}$$

$$= \frac{\partial L}{\partial q} \delta q + \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}} \delta \dot{q} \right) - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}} \right) \delta q$$

$$= \left[ \frac{\partial L}{\partial q} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}} \right) \right] \delta q + \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}} \delta \dot{q} \right)$$

$$\int \delta L dt = \int \left[ \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}} \delta \dot{q} \right) \right] dt + \left. \frac{\partial L}{\partial \dot{q}} \delta \dot{q} \right|_{t=t_1}^{t=t_2}$$

"  $\leftarrow E-L$  equation

$$\text{if } \frac{\partial L}{\partial \dot{q}} = 0 \text{ then } \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}} \right) = 0$$

cyclic coordinate:  $P = \frac{\partial L}{\partial \dot{q}}$  is conserved.

Symmetry in QM.

$\mathcal{S}$ : symmetry operator.

~~Def~~

$$\mathcal{S} = 1 + \frac{i}{\hbar} \mathbf{E} \mathbf{G}.$$

$$\mathcal{S}^\dagger H \mathcal{S} = H. \text{ invariant}$$

$$H\mathcal{S} = \mathcal{S}H \rightarrow [H, \mathcal{S}] = 0.$$

$$\Leftrightarrow [H, G] = 0.$$

$$\rightarrow \frac{dG}{dt} = 0.$$

Heisenberg eq. of motion

Degeneracy

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

$$H|\psi\rangle = \mathcal{S}H|\psi\rangle = \mathcal{S}E_n|\psi\rangle \\ = E_n|\psi\rangle$$

$\therefore |\psi\rangle$  &  $\mathcal{S}|\psi\rangle$  are degenerate.

$\left( \text{if } \langle n | \mathcal{S} | n \rangle \neq 0 \right)$

$$[J, H] = 0$$

then

$$\text{Example. } [\mathbf{Q}(\mathbf{R}), H] = 0 \Rightarrow [\mathbf{J}^2, H] = 0$$

## 4.2 Discrete symmetries

Parity  $|\alpha\rangle \rightarrow \pi|\alpha\rangle$  ( $\vec{x} \rightarrow -\vec{x}$ )

$$\langle \alpha | \pi^+ \xrightarrow{\uparrow} \vec{x} \pi^- | \alpha \rangle = - \langle \alpha | \vec{x}^- | \alpha \rangle$$

$$\begin{aligned}\pi^+ \vec{x}^- \pi^- &= -\vec{x}^- \\ \vec{x}^- \pi^- &= -\pi^- \vec{x}^- \\ \{ \vec{x}^-, \pi^- \} &= 0.\end{aligned}$$

Suppose

$$\pi^- |\vec{x}'\rangle = e^{i\delta} |-\vec{x}'\rangle$$

$$\begin{aligned}\vec{x}^- \pi^- |\vec{x}'\rangle &= -\pi^- \vec{x}^- |\vec{x}'\rangle \\ &= -\pi^- (\vec{x}') |-\vec{x}'\rangle \\ &= (-\vec{x}') \pi^- |\vec{x}'\rangle.\end{aligned}$$

$e^{i\delta} = 1$   
convention

$$\therefore \pi^- |\vec{x}'\rangle = \underbrace{e^{i\delta} |-\vec{x}'\rangle}_{\text{unitary}} \quad (\text{arbitrary phase})$$

$$\pi^2 = 1$$

$$\pi^+ \pi^- |\vec{x}'\rangle = \pi^+ |-\vec{x}'\rangle = |\vec{x}'\rangle$$

$$\begin{aligned}\therefore \quad &\left[ \begin{array}{l} \pi^2 = 1 \\ \pi^+ \pi^- = 1 \end{array} \right] \text{ unitary} \\ &\Rightarrow \pi^+ = \pi^- \Rightarrow \text{Hermitian.}\end{aligned}$$

Show that  $\{\vec{\pi}, \vec{p}\} = 0$

$$\{(\vec{\pi}, \vec{L}) = 0, \vec{L} = \vec{x} \times \vec{p}\}$$



parity & rotation  
commute

$$[R(\text{parity}), R(\text{rotation})] = 0.$$

$$[\vec{\pi}, \delta(R)] = 0.$$

$\Rightarrow$  generalization

$$[\vec{\pi}, \vec{J}] = 0$$

$\vec{x}, \vec{p}$  : polar vector.  $\{\vec{\pi}, \vec{x}\} = 0$

$\vec{L}, \vec{J}$  : axial vector.  $[\vec{\pi}, \vec{L}] = 0$

$\vec{x} \cdot \vec{p}$  : scalar  $\{\vec{\pi}, \vec{x} \cdot \vec{p}\} = 0$

$\vec{L} \cdot \vec{s}$  : pseudoscalar  $[\vec{\pi}, \vec{L} \cdot \vec{s}] = 0$

## Wavefunctions under Parity

$$\psi(x) = \langle x | \alpha \rangle$$

recall  $\begin{cases} \pi^+ = \pi \\ \pi(x) = (-x) \end{cases} \rightarrow \langle -x | = \langle x | \pi^+ = \langle x | \pi$

$$\therefore \langle -x | \alpha \rangle$$

$$\psi_\alpha(-x) = \langle -x | \alpha \rangle = \langle x | \pi | \alpha \rangle$$

$$\pi^2 = 1$$

if  $|\alpha\rangle$  is an eigenket of  $\pi$

$$\text{then } \pi|\alpha\rangle = \lambda|\alpha\rangle.$$

$$\pi^2|\alpha\rangle = \lambda^2|\alpha\rangle = |\alpha\rangle$$

$$\lambda^2 = 1 \rightarrow \lambda = \pm 1.$$

$$\psi_\alpha(-x) = \langle x | \pi | \alpha \rangle = \pm \langle x | \alpha \rangle.$$

+ : even parity

- : odd parity

- $\{\vec{\pi}, \vec{p}\} = 0$  ( $\vec{p}$  is a vector)
  - $\vec{\pi}\vec{p} \neq \vec{p}\vec{\pi} \Rightarrow$  no common eigenket.
  - $\Rightarrow |\vec{p}\rangle$  is not an eigenket of  $\vec{\pi}$ .

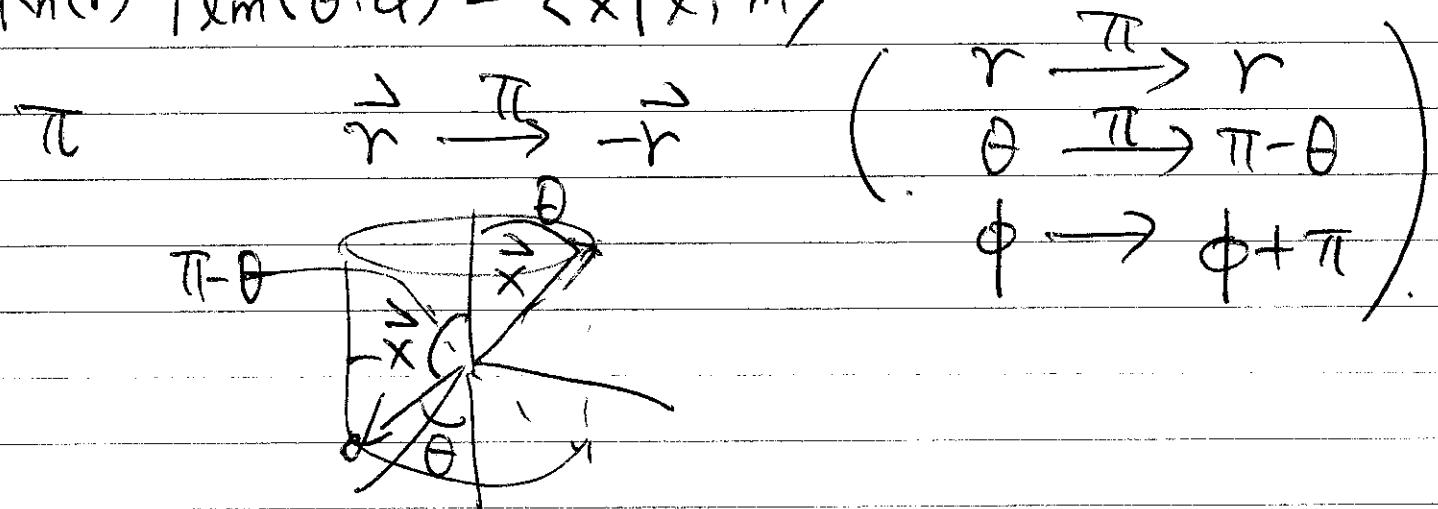
plane wave

$$\psi_\alpha(x) = e^{+\frac{i}{\hbar} \vec{p} \cdot \vec{x}} = \langle \vec{x} | \vec{p} \rangle$$

$$\begin{aligned} \psi_\alpha(-x) &= \langle -\vec{x} | \vec{p} \rangle = \langle \vec{x} | \pi \vec{l} \vec{p} \rangle = \langle \vec{x} | -\vec{p} \rangle \\ &= e^{-\frac{i}{\hbar} \vec{p} \cdot \vec{x}} \end{aligned}$$

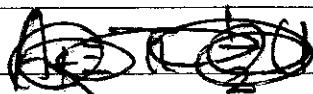
- $[\vec{\pi}, \vec{L}] = 0$  ( $\vec{L}$  is an axial vector)
  - $\vec{\pi}\vec{L} = \vec{L}\vec{\pi} \Rightarrow$  common eigenket.
  - $\Rightarrow |\vec{l}, m\rangle$

$$R_n(r)Y_{lm}(\theta, \phi) = \langle \vec{x} | \vec{l}, m \rangle$$



Theorem) If ~~suppose~~  $[H, \pi] = 0$ . & nondegenerate  
 $\& H|n\rangle = E_n|n\rangle$ ,  
then  $|n\rangle$  is an parity eigenket.

Note that  $\pi^+ = \pi$ ;  $\pi^2 = 1$ .



$$A = a + b\pi \quad \& \quad a \neq b \text{ are complex #.}$$

~~Suppose~~  $[A, \pi] = 0$

$$\pi A = a\pi + b$$

$$A\pi = a + b\pi = b\pi + a$$

$$\pi A|n\rangle = \pi(a\pi + b)|n\rangle$$

$$= (a + b\pi)|n\rangle = a|n\rangle + b(\pi|n\rangle)$$

$$\frac{1}{2}(f(x) + f(-x)) \Rightarrow \text{even}$$

$$\frac{1}{2}(f(x) - f(-x)). \Rightarrow \text{odd} \quad \text{for any } f(x)$$

$$\frac{1}{2}(\langle x|\alpha\rangle + \langle -x|\alpha\rangle) = \frac{1}{2}(\langle x|\alpha\rangle + \langle x|\pi|\alpha\rangle)$$

$$= \langle x| \frac{1}{2}(|\alpha\rangle + \pi|\alpha\rangle)$$

$$= \langle x| \frac{\frac{1}{2}(1+\pi)}{2} |\alpha\rangle$$

$$\frac{1}{2}(\langle x|\alpha\rangle - \langle -x|\alpha\rangle) = \langle x| \frac{\frac{1}{2}(1-\pi)}{2} |\alpha\rangle$$

$$|\alpha\rangle \rightarrow |n\rangle$$

Therefore,

$$\frac{1}{2}(1+\pi)|\alpha\rangle ; \text{ even parity}$$

$$\frac{1}{2}(1-\pi)|\alpha\rangle ; \text{ odd parity.}$$

$$H \frac{1}{2}(1+\pi)|\alpha\rangle = \frac{1}{2}(1+\pi)H|\alpha\rangle \quad \textcircled{*}$$

$$= \frac{1}{2}(1+\pi)E_n|n\rangle$$

$$= E_n \left[ \frac{1}{2}(1+\pi)|n\rangle \right]$$

$\therefore \frac{1}{2}(1+\pi)|n\rangle$  and  $|n\rangle$  ~~have~~ are degenerate.

(the same energy  $E_n$ )

This contradicts to the assumption that.

~~Because~~  $|n\rangle$  is non-degenerate

Therefore,  $|n\rangle$  and  $\frac{1}{2}(1+\pi)|n\rangle$  are the

$$\frac{1}{2}(1+\pi)|n\rangle \propto |n\rangle$$

$$\Rightarrow \pi|n\rangle \propto |n\rangle.$$

same up to an overall factor.

$$\left( \pi \frac{1}{2}(1+\pi) = \frac{1}{2}(\pi + \pi^2) = \frac{1}{2}(\pi + 1) \right)$$

$$= \pm \left[ \frac{1}{2}(1 \pm \pi) \right].$$

$$\therefore \boxed{\pi|n\rangle = \pm |n\rangle}$$

(Example)

Simple harmonic oscillator

$|0\rangle$  ground state

$|1\rangle = a^\dagger |0\rangle$  first excited state

① Show that  $|0\rangle$  is even.

$$\langle x|0\rangle = \frac{1}{\sqrt{\pi x_0}} e^{-\frac{1}{2} \left(\frac{x}{x_0}\right)^2}$$

$$x_0 = \sqrt{\frac{\hbar}{m\omega}}$$

②  $\langle -x|0\rangle = \langle x|\cancel{\pi}|0\rangle = \langle x|0\rangle$ .

③  $|1\rangle = a^\dagger |0\rangle$ .

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left(x - \frac{iP}{m\omega}\right)$$

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}} |0\rangle$$

$$a = \sqrt{\frac{m\omega}{2\hbar}} \left(x + \frac{iP}{m\omega}\right)$$

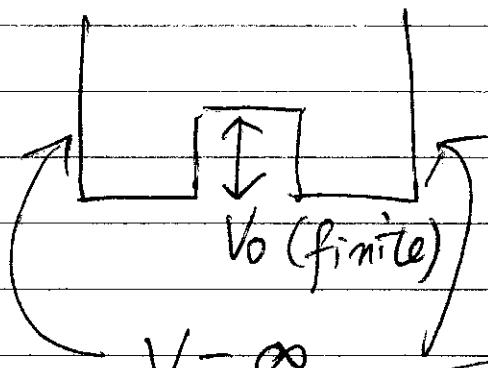
$$H = \hbar\omega(a^\dagger a + \frac{1}{2})$$

④  $\langle -x|1\rangle = \langle x|\pi|1\rangle$  at  $\pi|0\rangle = |0\rangle$

$$\begin{aligned} &= \langle x|\pi \left(x - \frac{iP}{m\omega}\right) |0\rangle \sqrt{\frac{m\omega}{2\hbar}} \\ &= \langle x|\pi \left(x - \frac{iP}{m\omega}\right) \pi^\dagger \pi |0\rangle \sqrt{\frac{m\omega}{2\hbar}} \\ -\langle x|1\rangle &= \langle x| \left[-\left(x - \frac{iP}{m\omega}\right)\right] \pi |0\rangle = -\langle x|a^\dagger |0\rangle \end{aligned}$$

odd

# Symmetrical Double-Well potential

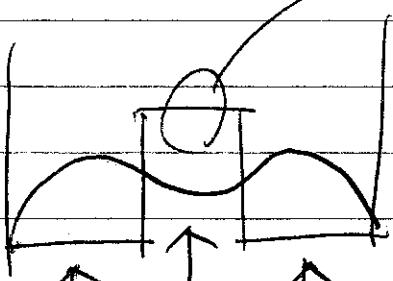


$$V(x) = V(-x)$$

$$[H, \pi] = 0$$

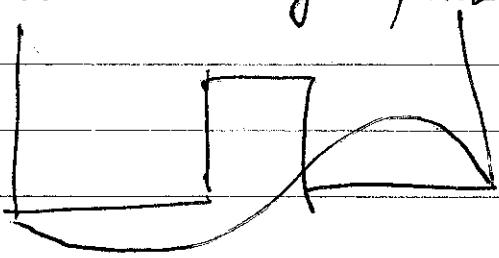
$$V = \infty$$

Classically forbidden.



$\sinh$  or  $\cosh$ .

$$E_S < E_A$$

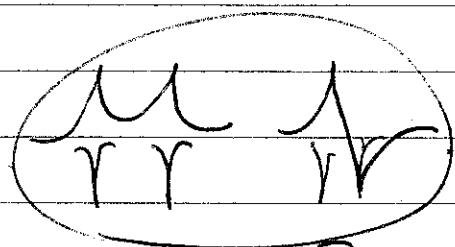


$\sin$  or  $\cos$ .

$$H|S\rangle = E_S |S\rangle$$

$$H|A\rangle = E_A |A\rangle$$

,  $\delta$ -function. double  $\delta$ .



Classically allowed.

$$\pi|A\rangle = -|A\rangle$$

$$|S\rangle, \pi|S\rangle = |S\rangle$$

Symmetric

$$|A\rangle$$

antisymmetric.

$$|R\rangle \equiv \frac{1}{\sqrt{2}}(|S\rangle + |A\rangle)$$

more probable  
on the right side

$$|L\rangle \equiv \frac{1}{\sqrt{2}}(|S\rangle - |A\rangle)$$

left.

$|R\rangle$  &  $|L\rangle$  : not eigenkets  
of  $\pi$  &  $H$ .

$$|\alpha(t=0)\rangle = |R\rangle$$

$$= \frac{1}{\sqrt{2}} (|S\rangle + |A\rangle)$$

$$|\alpha(t)\rangle = e^{-\frac{i}{\hbar}Ht} |\alpha(t=0)\rangle$$

$$= \frac{1}{\sqrt{2}} \left( e^{-\frac{i}{\hbar}E_{S,t}} |S\rangle + e^{-\frac{i}{\hbar}E_{A,t}} |A\rangle \right)$$

$$= \frac{1}{\sqrt{2}} e^{-\frac{i}{\hbar}E_{S,t}} \left( |S\rangle + e^{\frac{-i}{\hbar}(E_A - E_S)t} |A\rangle \right)$$

$$\omega = \frac{E_A - E_S}{\hbar}$$

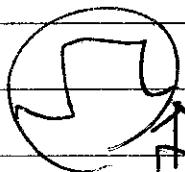
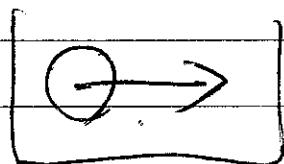
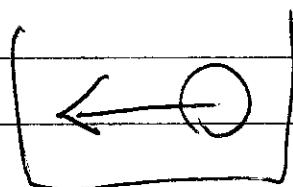
$$T = \frac{2\pi}{\omega}$$

$$\text{at } t=T(n+\frac{1}{2}) \quad \alpha \frac{1}{\sqrt{2}} (|S\rangle - |A\rangle) = |L\rangle$$

$\rightarrow$  os

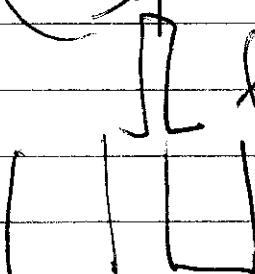
$$|R\rangle \leftrightarrow |L\rangle$$

oscillation?

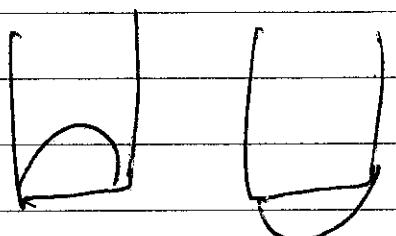
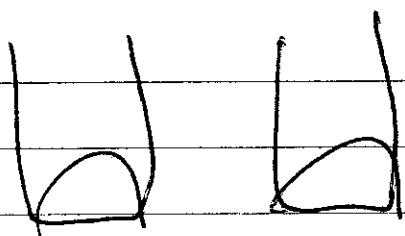


finite barrier  $\Rightarrow$  tunnelling.

\* as



higher  $\rightarrow$  two isolated infinite potential wells  
 $\rightarrow$  no tunnelling  
 $\rightarrow$  no oscillation.



Sym

$\uparrow \downarrow \rightarrow$  degenerate!

antisym

~~IS~~ IS  
IA

~~IS~~

~~IS~~ energy eigenkets do not have to be eigenkets of  $\pi$ , because  $|s\rangle$  &  $|A\rangle$  are degenerate.

Parity-selection rule..

$$\pi(\alpha) = E_\alpha |\alpha\rangle$$

$$\pi(\beta) = E_\beta |\beta\rangle. \quad E_\alpha, E_\beta = \pm 1$$

$$\begin{aligned} \langle \beta | \vec{x} | \alpha \rangle &= \langle \beta | \pi^+ \vec{x} \pi^+ | \alpha \rangle = - \langle \beta | \vec{x} | \alpha \rangle \\ &= - \langle \pi(\beta) | \vec{x} | \alpha \rangle \end{aligned}$$

$$\begin{aligned} \langle \beta | \vec{x} | \alpha \rangle &= \langle \beta | \pi^+ \vec{x} \pi^2 | \alpha \rangle \\ &= (\pi | \beta \rangle)^+ (\pi^+ \vec{x} \pi^f) (\pi | \alpha \rangle) \\ &= \langle \beta | \pi^+ (-\vec{x}) \pi | \alpha \rangle = -E_\alpha E_\beta \langle \beta | \vec{x} | \alpha \rangle \end{aligned}$$

$$(1 + \epsilon_\alpha \epsilon_\beta) \langle \beta | \vec{x} | \alpha \rangle = 0$$

if  $1 + \epsilon_\alpha \epsilon_\beta \neq 0$ , then  $\langle \beta | \vec{x} | \alpha \rangle = 0$ .  
 $(\epsilon_\alpha \epsilon_\beta \neq -1)$

~~Wigner showed that~~

If  $[H, \pi] = 0$  and  $|n\rangle$  are nondegenerate,  
then  $\langle n | \vec{x} | n \rangle = 0$ .

no permanent electric dipole moment

Parity Non-conservation

$$\langle \vec{s} \rangle \cdot \vec{p} \Rightarrow \text{pseudo scalar}$$

electromagnetic interaction  $\Rightarrow [H, \pi] \neq 0$

However, weak interaction  
does not conserve parity.

(T.D. Lee & C.N. Yang).

#### 4.4 Time Reversal. $t \rightarrow -t$ .

$$m \frac{d^2 \vec{x}}{dt^2} = -\vec{\nabla} V$$

$$t \rightarrow -t$$

$$\left. \begin{aligned} m \frac{d^2 \vec{x}}{d(-t)^2} &= -\vec{\nabla} V \\ &= m \frac{d^2 \vec{x}}{dt^2} \end{aligned} \right\} \text{time-reversal invariant.}$$

If  $\vec{x}(t)$  is a solution,  
then  $\vec{x}(-t)$  is also a solution?

$$m \ddot{\vec{x}} + b \dot{\vec{x}} + k \vec{x} = 0.$$

$$\left( t \rightarrow -t : m \ddot{\vec{x}} - b \dot{\vec{x}} + k \vec{x} = 0. \text{ not invariant?} \right)$$

## Maxwell's equations

$$\left\{ \begin{array}{l} \nabla \cdot \vec{E} = \rho \\ \nabla \times \vec{B} - \frac{1}{c} \frac{\partial \vec{E}}{\partial t} = \frac{1}{c} \vec{J} \\ \nabla \times \vec{E} = - \frac{1}{c} \frac{\partial \vec{B}}{\partial t} \\ \nabla \cdot \vec{B} = 0 \end{array} \right. \quad \begin{array}{l} t \rightarrow -t \\ \nabla \cdot \vec{E} = \rho \\ -\nabla \times \vec{B} + \frac{1}{c} \frac{\partial \vec{E}}{\partial t} = -\frac{1}{c} \vec{J} \\ \nabla \times \vec{E} = - \frac{1}{c} \frac{\partial \vec{B}}{\partial t} \\ \nabla \cdot \vec{B} = 0 \end{array}$$

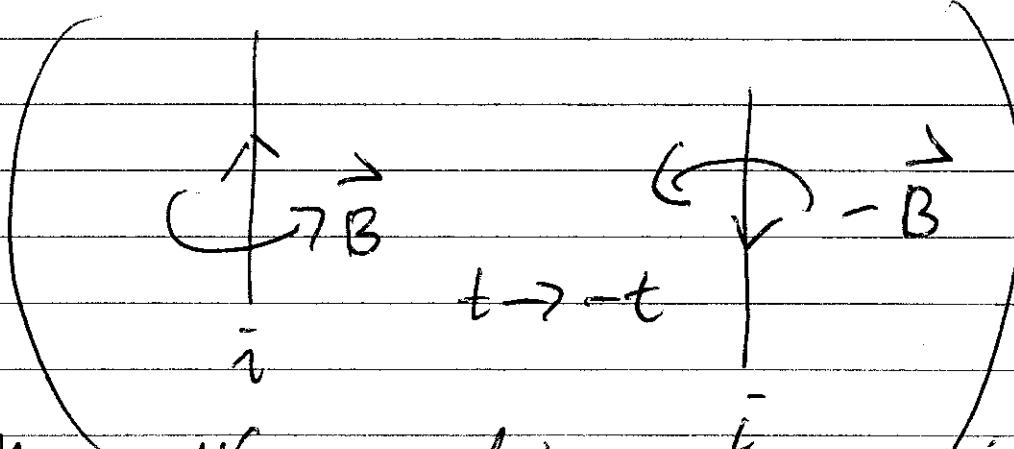
$e = |e|$   
 $qe = -e$

Lorentz force:  $\vec{F} = q(\vec{E} + \frac{v}{c} \times \vec{B})$ .

$$\begin{array}{l} \vec{E} = -\nabla \phi - \frac{1}{c} \frac{\partial \vec{A}}{\partial t} \\ \vec{B} = \nabla \times \vec{A} \end{array} \quad \begin{array}{l} (\vec{A} \propto \vec{J}) \\ \vec{F} = -q(\vec{E} + \frac{v}{c} \times \vec{B}) \end{array}$$

invariant

$$\left\{ \begin{array}{l} \phi \xrightarrow{T} \phi \\ A \xrightarrow{T} -A \end{array} \right\} \quad \begin{array}{l} E \rightarrow E \\ B \rightarrow -B \end{array} \quad \begin{array}{l} P \rightarrow P \\ J \rightarrow -J \\ v \rightarrow -v \end{array}$$



(Maxwell's equations are invariant under time reversal.)

Schrödinger equation

$$i\hbar \frac{\partial \psi(t, x)}{\partial t} = \left(-\frac{\hbar^2}{2m} \nabla^2 + V\right) \psi$$

$$-i\hbar \frac{\partial \psi^*(t, x)}{\partial t} = (\text{---}) \psi^*(t, x)$$

But

$$i\hbar \frac{\partial}{\partial t} \psi^*(-t, x) = (\text{"}) \psi^*(-t, x)$$

if  $\psi(t, \vec{x})$  is a solution,

then  $\psi^*(-t, \vec{x})$  is another solution.

$$e^{i(kx - \omega t)} \rightarrow [e^{i(kx + \omega t)}]^\ast e^{-i(-kx - \omega t)}$$

"Complex conjugate" is related  
to the time-reversed wavefunction

$$i\hbar \frac{\partial \psi(t,x)}{\partial t} = \left( -\frac{\hbar^2}{2m} \nabla^2 + V(x) \right) \psi(t,x)$$

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

complex conjugate

$$i\hbar \frac{\partial}{\partial t} \psi^*(-t,x) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(x) \right] \psi^*(-t,x).$$

$$\psi(t,x) = u_n(x) e^{-\frac{i}{\hbar} E_n t}$$

$$\psi^*(-t,x) = u_n^*(x) e^{-\frac{i}{\hbar} E_n t}$$

time reversal has something to do with  
the complex conjugation.

at  $t=0$

$$\psi(t=0, x) = u_n(x) = \langle x | \alpha \rangle$$

$$\psi^*(t=0, x) = u_n^*(x) = \langle \alpha | x \rangle = \langle x | \alpha \rangle^*$$