COMPATIBLE OBSERVABLES
(= COMMUTING OBSERVABLES)

- GENERALISED UNCERTAINTY PRINCIPLE (HEISENBERG)

$$\Delta A \, \Delta B \geq \frac{1}{2} \left| \langle [\hat{A}, \hat{B}] \rangle \right|$$

IMPLIES THAT 2 OBSERVABLES $\hat{A}, \hat{B}$ CAN ONLY BE MEASURED SIMULTANEOUSLY TO 100% IF

$$[\hat{A}, \hat{B}] = 0$$

$$\Rightarrow \Delta A \, \Delta B \geq 0$$

- NOTE $\Delta A = 0$ IMPLIES ψ IS EIGENSTATE OF $\hat{A}$
  $\Delta B = 0$ —— " —— $\hat{B}$

Q: UNDER WHICH CONDITION DO WE HAVE SIMULTANEOUS EIGENSTATES?

DEF $\hat{A}, \hat{B}$ ARE COMPATIBLE OBSERVABLES IF

$\exists$ A COMPLETE SET OF EIGENSTATES ψ_n SUCH THAT EACH ψ_n IS EIGENSTATE OF $\hat{A}$ AND OF $\hat{B}$ (SIMULTANEOUS EIGENSTATES)

$$\hat{A} \psi_n = a_n \psi_n \quad \& \quad \hat{B} \psi_n = b_n \psi_n$$

$$\hat{A} \hat{B} \psi_n = \hat{A} (b_n \psi_n) = a_n b_n \psi_n = b_n a_n \psi_n = \hat{B} \hat{A} \psi_n$$

$$\Rightarrow [\hat{A}, \hat{B}] \psi_n = 0$$

ψ_n "COMPLETE SET"

$\Rightarrow$ most general state $\psi = \sum c_n \psi_n$

$$\Rightarrow \quad [\hat{A}, \hat{B}]\,\psi = 0 \qquad \text{FOR ANY } \psi$$

$$\Rightarrow \quad \boxed{[\hat{A}, \hat{B}] = 0}$$

IF $\exists$ SIMULTANEOUS EIGENSTATES = COMPATIBLE OBSERVABLES
$\Rightarrow$ COMMUTING OPERATORS

CONVERSE ALSO TRUE (WILL ONLY PROVE CASE OF NON-DEGENERATE EIGENVALUES, BUT RESULT IS TRUE ALSO FOR DEGENERATE EIGENVALUES)

ASSUME $[\hat{A}, \hat{B}] = 0$

$$\hat{A}\,\psi_n = a_n \psi_n \qquad \text{(NON-DEGENERATE)}$$

$$\Rightarrow \hat{A}(\hat{B}\psi_n) = \hat{B}\underbrace{\hat{A}\psi_n}_{a_n\psi_n} = a_n(\hat{B}\psi_n)$$

$\Rightarrow \hat{B}\psi_n$ ALSO EIGENSTATE OF $\hat{A}$ WITH EIGENVALUE a_n, NON-DEGENERACY $\Rightarrow$

$\hat{B}\psi_n$ PROPORTIONAL TO ψ_n

$$\hat{B}\psi_n = b_n \psi_n$$

PROPORTIONALITY CONST.

SO IF $[\hat{A}, \hat{B}] = 0 \Rightarrow$ THERE EXISTS A COMPLETE SET OF SIMULTANEOUS EIGENFUNCTIONS

SUMMARY

$$\boxed{[\hat{A}, \hat{B}] = 0 \Leftrightarrow \text{COMPLETE SET OF SIMULTANEOUS EIGENSTATES } (\hat{A}, \hat{B} \text{ COMPATIBLE})}$$

COMMENTS

- SOMETIMES THERE ARE MORE THAN 2 COMPATIBLE OBSERVABLES

- COMPLETE SET OF COMMUTING/COMPATIBLE OBSERVABLES

$\equiv$ LARGEST SET OF COMMUTING OPERATORS

$\rightarrow$ EIGENVALUES OF THESE OPERATORS ~~LABEL~~ SPECIFY EIGENSTATES COMPLETELY!

E.G HYDROGEN ATOM (IGNORING SPIN)

$\hat{H} \leftrightarrow E_n$ DEGENERACY $= n^2$

n: PRINCIPAL QUANTUM NUMBER

COMPLETE SET OF OPERATORS

$$\{\hat{H}, \hat{\vec{L}}^2, \hat{L}_z\}$$

EIGENVALUES: E_n $\quad \hbar^2 l(l+1)$ $\quad \hbar m$

EIGENSTATE: $\Psi_{nlm}(\vec{x},t) = R_{nl}(r) Y_{lm}(\theta,\varphi) e^{-iE_n t/\hbar}$

- OPERATORS THAT COMMUTE WITH $\hat{H}$ ARE RELATED TO SYMMETRIES!

(AND SYMMETRIES ARE RELATED TO CONSERVED QUANTITIES!)

EX1) SIMPLEST EXAMPLE PARITY

1D: $x \to -x$ (3D: $\vec{x} \to -\vec{x}$)

SYMMETRY: TRANSFORMATION OF COORDINATES THAT LEAVES $\hat{H}$ INVARIANT:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

$$x \to -x: \quad \frac{\partial}{\partial x} \to \frac{\partial}{\partial(-x)} = -\frac{\partial}{\partial x}$$

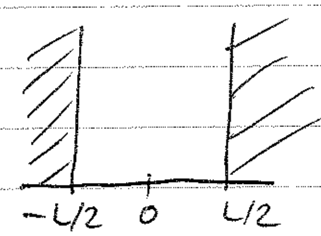
$$\frac{\partial^2}{\partial x^2} \to \frac{\partial^2}{\partial x^2} \ \checkmark$$

ALSO: $V(x) \to V(-x)$ SO NEED $V(x) = V(-x)$

THEN $\hat{H}(x) = \hat{H}(-x)$

EX: SHO $V(x) = \frac{m}{2}\omega^2 x^2$

INFINITE SQUARE WELL



$n = 1,3,5$ $\quad \psi_n = \sqrt{\frac{2}{L}}\cos\left(\frac{n\pi x}{L}\right) \quad \psi_n(x) = +\psi_n(-x)$

$n = 2,4,6$ $\quad \psi_n = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) \quad \psi_n(-x) = -\psi_n(x)$

PARITY OPERATOR $\quad \hat{P}\psi(x) = \psi(-x)$

$$[\hat{P}, \hat{H}(x)]\psi(x) = \hat{P}(\hat{H}(x)\psi(x)) - \hat{H}(x)\hat{P}\psi(x)$$

$$= \hat{H}(-x)\psi(-x) - \hat{H}(x)\psi(-x)$$

$$= 0 \quad \text{IF} \quad \hat{H}(x) = \hat{H}(-x)$$

SO $[\hat{P}, \hat{H}(x)] = 0$ IF $\hat{H}$ IS PARITY SYMM.!

SIMULTANEOUS EIGEN STATES

TISE: $\hat{H}(x)\,\psi_E(x) = E\,\psi_E(x)$

$x \to -x$: $\hat{H}(-x)\,\psi_E(-x) = E\,\psi_E(-x)$

$\hat{H}(x)\,\psi_E(-x) = E\,\psi_E(-x)$

2 SOLUTIONS WITH SAME EIGENVALUE

$\Rightarrow \quad \psi_E(-x) = \lambda\,\psi_E(x)$

$\xrightarrow{x \to -x} \quad \psi_E(x) = \lambda\,\psi_E(-x)$

$\Rightarrow \psi_E(x) = \lambda^2 \psi_E(x) \Rightarrow \lambda^2 = 1$

$\Rightarrow \boxed{\lambda = \pm 1}$ (POSSIBLE EIGENVALUES OF $\hat{P}$)

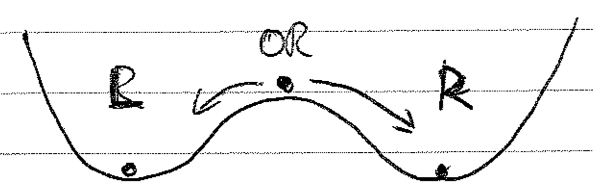
$\Rightarrow \boxed{\psi_E(-x) = \hat{P}\,\psi_E(x) = \pm\,\psi_E(x)}$

$\psi_E(x)$ <u>SIMULTANEOUS EIGENSTATE</u> OF $\hat{P}$ AND $\hat{H}$ IF POTENTIAL IS SYMMETRIC! $V(x) = V(-x)$

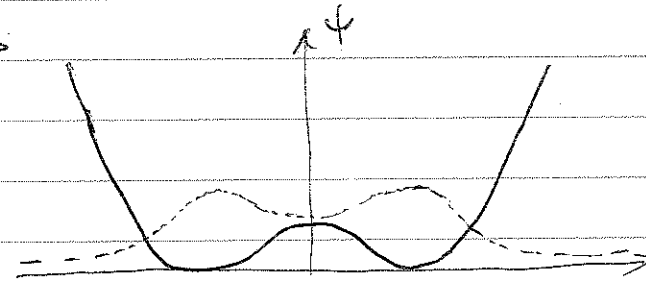
<u>EX</u> SHO: $\hat{P}\psi_n(x) = \psi_n(-x) = (-1)^n\,\psi_n(x)$, $n = 0,1,2,3,\ldots$

<u>COMMENTS</u> GROUNDSTATE ALWAYS PARITY EVEN ($\hat{P} = 1$) (NO NODES)

<u>PROFOUND CONSEQUENCES</u>



CLASSICAL GROUNDSTATE DEGENERATE!



<u>UNIQUE $\hat{P} = +1$ GROUNDSTATE WAVEFUNCTION</u> $\psi(-x) = +\psi(x)$

ALSO $\frac{d}{dt}\langle \hat{P} \rangle = 0$ (SINCE $[\hat{H}, \hat{P}] = 0$) General proof later

$\langle \hat{P} \rangle$ FOR ~~[illegible]~~ SHO

$$\Psi(x,t) = \sum_{n=0}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar} \qquad \psi_n(-x) = (-1)^n \psi_n(x)$$

$$\hat{P}\Psi(x,t) = \sum_{n=0}^{\infty} (-1)^n c_n \psi_n(x) e^{-iE_n t/\hbar}$$

$$\langle \hat{P} \rangle = \int_{-\infty}^{+\infty} \Psi^*(x,t) \hat{P} \Psi(x,t) = \sum_{n=0,2,4..} (+1)|c_n|^2$$

ORTHONORMALITY

$$+ \sum_{n=1,3,5,..} (-1)|c_n|^2$$

$\langle \hat{P} \rangle$ INDEPENDENT OF TIME (BECAUSE $[\hat{H}, \hat{P}] = 0$)

SUMMARY: $V(-x) = V(x) \Rightarrow \hat{H}(-x) = \hat{H}(x)$

a) SIMULTANEOUS EIGENFUNCTIONS OF $\hat{H}$ AND $\hat{P}$ (EIGENVALUES ± 1)

b) $[\hat{P}, \hat{H}] = 0$

Q.M. in 3D CENTRAL POTENTIAL

$$\hat{P}: \vec{x} \to -\vec{x}$$

$$V(\vec{x}) = V(|\vec{x}|)$$

$$|\vec{x}| = \sqrt{x^2+y^2+z^2} \xrightarrow{\hat{P}: \vec{x} \to -\vec{x}} \sqrt{(-x)^2+(-y)^2+(-z)^2} = |\vec{x}|$$

PARITY SYMMETRIC

EX2) TRANSLATIONS : $x \to x + a$

$$\psi(x) \to \psi(x+a) = \psi(x) + a\frac{\partial}{\partial x}\psi(x) + \text{higher order in } a \text{ terms}$$

CHANGE OF $\psi(x)$: $\delta\psi(x) = \psi(x+a) - \psi(x) \cong a\frac{\partial}{\partial x}\psi(x)$

$$= \frac{a}{i\hbar}\hat{p}_x\psi(x)$$

$\downarrow$

MOMENTUM OPERATOR "GENERATES" TRANSLATIONS

IF $[\hat{H}, \hat{p}_x] = i\hbar\frac{\partial V}{\partial x} = 0$ (see HW2)

$\Rightarrow V = \text{const}$: $\hat{H}$ TRANSLATION INVARIANT

MOMENTUM CONSERVED (FREE PARTICLE)

$\Downarrow$

see later

EX3 $[\hat{H}, \hat{\vec{L}}] = 0 \Rightarrow$ ROTATION INVARIANCE

$\downarrow$

ANGULAR MOM. OPERATORS

$V(\vec{x}) = V(|\vec{x}|) = \frac{c}{|\vec{x}|}$ CENTRAL POTENTIAL

DEGENERACY (SOME COMMENTS)

- IN 1D SYSTEMS WE NEVER FIND DEGENERACIES (NON-TRIVIAL POTENTIAL $V(x)$)
- ENERGY EIGEN VALUES ARE DEGENERATE IF THERE ARE 2 OR MORE OPERATORS THAT COMMUTE WITH ~~EACH OTHER~~ $\hat{H}$ BUT NOT WITH EACH OTHER:

EX) E.G. THERE ARE 2 OPERATORS $\hat{A}, \hat{B}$ SUCH THAT

$\{\hat{H}, \hat{A}\}$ AND $\{\hat{H}, \hat{B}\}$ ARE COMPLETE SETS OF OPERATORS BUT $[\hat{A}, \hat{B}] \neq 0$

$\{\hat{H}, \hat{A}\} \Rightarrow \psi_n$ SIMULTANEOUS EIGEN STATES

$\{\hat{H}, \hat{B}\} \Rightarrow \phi_n$ —— " ——

BUT SINCE $[\hat{A}, \hat{B}] \neq 0$

ψ_n, ϕ_n ARE NOT SIMULTANEOUS EIGEN STATES OF $\hat{A}$ AND $\hat{B}$

SO $\psi_n \neq \lambda \phi_n$

$\Rightarrow$ AT LEAST 2 DIFFERENT ENERGY EIGENSTATES WITH ENERGY E_n

- THE MORE SYMMETRY, THE MORE DEGENERACY
- EX Hydrogen $[\hat{H}, \hat{L}_x] = [\hat{H}, \hat{L}_y] = [\hat{H}, \hat{L}_z] = 0$

BUT $[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z, \ldots$

$\{\hat{H}, \hat{L}^2, \hat{L}_z\}$ COMPLETE SET OF COMPATIBLE OPERATORS

HEISENBERG'S EQUATION OF MOTION

- QUANTUM MECHANICAL EQUATIONS OF MOTION

Q: HOW DO Q.M. EXPECTATION VALUES CHANGE WITH TIME. THE RESULT WILL ALSO GIVE A Q.M. VERSION OF CONSERVATION LAWS WHICH ARE RELATED TO SYMMETRIES:

CONSIDER GENERAL STATE $\Psi(x,t)$ AND ANALYS THE TIME VARIATION OF $\langle \hat{A} \rangle = \int \Psi^* \hat{A} \Psi \, dx$ NAMELY

$$\frac{d}{dt}\langle \hat{A} \rangle :$$

$$\hat{H}\Psi = i\hbar \frac{\partial \Psi}{\partial t} \Rightarrow \frac{\partial \Psi}{\partial t} = \frac{1}{i\hbar}\hat{H}\Psi$$

$$\frac{\partial \Psi^*}{\partial t} = -\frac{1}{i\hbar}\hat{H}\Psi^* \quad : \hat{H} = \hat{H}^*$$

$$\frac{d\langle \hat{A} \rangle}{dt} = \frac{d}{dt}\int \Psi^*(x,t)\,\hat{A}\,\Psi(x,t)\,dx$$

$$= \int \frac{\partial \Psi^*}{\partial t}\hat{A}\Psi(x,t) + \int \Psi^* \frac{\partial \hat{A}}{\partial t}\Psi + \int \Psi^* \hat{A}\frac{\partial \Psi}{\partial t}$$

$$= \frac{1}{i\hbar}\left[-\int (\hat{H}\Psi)^* \hat{A}\Psi + \int \Psi^* \hat{A}\hat{H}\Psi\right] + \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle$$

HERMITICITY $\hat{H} = \hat{H}^\dagger$

$$= \frac{1}{i\hbar}\left[-\int \Psi^* \hat{H}\hat{A}\Psi + \int \Psi^* \hat{A}\hat{H}\Psi\right] + \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle$$

$$= \frac{i}{\hbar} \int \Psi^* [\hat{H}, \hat{A}] \Psi + \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle$$

SO

$$\boxed{\frac{d\langle \hat{A} \rangle}{dt} = \frac{i}{\hbar} \langle [\hat{H}, \hat{A}] \rangle + \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle}$$

HEISENBERG EQUATION OF MOTION

- USUALLY OPERATOR TIME INDEPENDENT $\frac{\partial \hat{A}}{\partial t} = 0$

$$\frac{d \langle \hat{A} \rangle}{dt} = \frac{i}{\hbar} \langle [\hat{H}, \hat{A}] \rangle$$

IF $[\hat{H}, \hat{A}] = 0$ THEN

$\langle \hat{A} \rangle$ <u>DOES NOT CHANGE WITH TIME</u>

$\Rightarrow$ <u>CONSERVED QUANTITY</u>

E.G. $[\hat{H}, \hat{\vec{p}}] = 0 \Rightarrow \hat{H}$ TRANSLATION INV.

$V(\vec{x}) = \text{const}$

$\Rightarrow \frac{d}{dt} \langle \hat{\vec{p}} \rangle = 0$ <u>MOMENTUM CONSERVED!</u>

OR $[\hat{H}, \hat{\vec{L}}] = 0 \Rightarrow \hat{H}$ ROTATION INVARIANT

$V(\vec{x}) = V(|\vec{x}|)$

$\Rightarrow \frac{d}{dt} \langle \hat{\vec{L}} \rangle = 0$ <u>ANGULAR MOMENTUM CONSERVED</u>

EHRENFEST'S THEOREM

- RELATION BETWEEN CLASSICAL (NEWTON) AND Q.M. EQUATIONS OF MOTION (HEISENBERG)

EHRENFEST'S FIRST RELATION: CHOOSE $\hat{A} = \hat{x}$

—||— SECOND —||— $\hat{A} = \hat{p}_x$

$\hat{A} = \hat{p}_x$: $[\hat{H}, \hat{p}_x]\psi(x) = [\frac{\hat{p}_x^2}{2m} + V(x), \hat{p}_x]\psi(x)$

$$= \frac{1}{2m}\underbrace{[\hat{p}_x^2, \hat{p}_x]}_{0}\psi(x) + (-i\hbar)[V(x), \frac{\partial}{\partial x}]\psi(x)$$

$$= (-i\hbar)\left\{\cancel{V(x)\frac{\partial\psi}{\partial x}} - \frac{\partial V}{\partial x}\psi(x) - \cancel{V(x)\frac{\partial\psi}{\partial x}}\right\}$$

$$= i\hbar\frac{\partial V}{\partial x}\psi(x) \Rightarrow [\hat{H}, \hat{p}_x] = i\hbar\frac{\partial V}{\partial x} \text{ (HW2)}$$

SO $\frac{d\langle\hat{p}_x\rangle}{dt} = \frac{i}{\hbar}i\hbar\langle\frac{\partial V}{\partial x}\rangle = -\langle\frac{\partial V}{\partial x}\rangle$ (II)

SIMILARLY FIRST EHRENFEST $\hat{A} = \hat{x}$ $\boxed{\frac{d}{dt}\langle\hat{x}\rangle = \frac{1}{m}\langle\hat{p}_x\rangle}$ (I)

- NOW (II) IS NOT QUITE AS EXPECTED

— NAIVE GUESS:

classical $\frac{dp_x}{dt} = -\frac{\partial V(x,t)}{\partial x}$

replace: $x \to \langle\hat{x}\rangle$, $p_x \to \langle\hat{p}_x\rangle$

$$\frac{d\langle\hat{p}_x\rangle}{dt} = -\frac{\partial V(\langle\hat{x}\rangle, t)}{\partial\langle\hat{x}\rangle}$$

Q UNDER WHICH CONDITION WOULD WE RECOVER THE NAIVE EXPECTATION?

$$\frac{d\langle\hat{p}_x\rangle}{dt} = -\left\langle \frac{\partial V}{\partial x} \right\rangle = \langle F_x \rangle$$

TAYLOR EXPAND F_x AROUND $x = \langle x \rangle$

$$F_x(x,t) \cong F_x(\langle x\rangle, t) + (x - \langle x\rangle)\frac{\partial F_x(\langle x\rangle, t)}{\partial x} + \frac{(x-\langle x\rangle)^2}{2}\frac{\partial^2 F(\langle x\rangle, t)}{\partial x^2}$$

NOW: $\langle x - \langle x\rangle\rangle = \langle x\rangle - \langle x\rangle = 0$

AND $\langle (x-\langle x\rangle)^2\rangle = \langle x^2 - 2x\langle x\rangle + \langle x\rangle^2\rangle$
$= \langle x^2\rangle - 2\langle x\rangle^2 + \langle x\rangle^2 = (\Delta x)^2$

$$\langle F_x(x,t)\rangle \cong \underbrace{F_x(\langle x\rangle, t)}_{\text{NAIVE EXPECTATION}} + \underbrace{\frac{(\Delta x)^2}{2}\frac{\partial^2 F(\langle x\rangle, t)}{\partial x^2}}_{\text{true quantum correction}}$$

NAIVE EXPECTATION
(FORCE AT "AVERAGE" POSITION OF PARTICLE)

true quantum correction that tests the "spread" of the particle Δx

$\Downarrow$

CAN BE NEGLECTED IF PARTICLE IS WELL LOCALISED (Δx small) AND THE FORCE VARIES SLOWLY WITH x!

$\Rightarrow$ UNDER THESE ASSUMPTIONS WE RECOVER CLASSICAL EQUATIONS (NEWTON II) FROM THE HEISENBERG EQUATIONS BY IDENTIFYING $x \Leftrightarrow \langle\hat{x}\rangle$ AND $p_x \Leftrightarrow \langle\hat{p}_x\rangle$