POSTULATE

$\boxed{\text{IN Q.M. ALL OBSERVABLES (DYNAMICAL VARIABLES) ARE ASSOCIATED WITH LINEAR OPERATORS}}$

$$\hat{A}(c_1\psi_1 + c_2\psi_2) = c_1\hat{A}\psi_1 + c_2\hat{A}\psi_2$$

EXAMPLES $\hat{H}$ IS LINEAR $\Rightarrow$ SUPERPOSITION

POSITION: $\hat{x}\,\psi(x,t) = x\,\psi(x,t)$

MOMENTUM: $\hat{p}\,\psi(x,t) = -i\hbar\,\partial_x \psi(x,t)$

3D: $\hat{\vec{x}} = \vec{x}$, $\hat{\vec{p}} = -i\hbar\left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right) = -i\hbar\vec{\nabla}$

$\boxed{\text{OPERATOR POSTULATE: RULE TO TRANSLATE A CLASSICAL OBSERVABLE INTO A Q.M. ONE}}$

3D: CLASSICAL QUANTUM

$$A(\vec{x},\vec{p}) \longrightarrow \hat{A}(\vec{x}, -i\hbar\vec{\nabla})$$

[NOTE THERE EXIST Q.M. OBSERVABLES WITHOUT CLASSICAL COUNTERPART $\rightarrow$ SPIN]

EXAMPLES: 1) $E = H(\vec{x},\vec{p}) = \frac{\vec{p}^{\,2}}{2m} + V(\vec{x}) \Rightarrow \hat{H} = -\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{x})$

2) ANGULAR MOMENTUM:

$$L_x = y p_z - z p_y \Rightarrow \hat{L}_x = y\hat{p}_z - z\hat{p}_y = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$

WHAT DO OPERATORS DO FOR A LIVING?

- THEY ACT ON WAVEFUNCTIONS TO PRODUCE NEW ONES : $\Psi(x,t) \Rightarrow \chi(x,t) = \hat{A}\,\Psi(x,t)$

  DIFF. OPERATOR

- SOMETIMES THEY CAN BE MATRICES (SEE LATER)

- SOMETIMES THEY COMMUTE, SOMETIMES THEY DON'T : (NEED TO LEARN TO CHECK)

  COMMUTATOR: $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$

  - MOMENTUM OPERATORS COMMUTE WITH EACH OTHER $[\hat{p}_x, \hat{p}_y] = 0$

  - VERY IMPORTANT

$$[x, \hat{p}_x] = i\hbar$$

PROOF: THAT'S HOW IT'S DONE IN GENERAL: ACT ON WAVE FUNCTION

$$[x, \hat{p}_x]\,\psi(x) = -i\hbar\left(x\frac{\partial\psi}{\partial x} - \frac{\partial}{\partial x}(x\psi)\right)$$

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

$$= i\hbar\,\psi$$

TRUE FOR ALL $\psi \Rightarrow$

OPERATOR EQN. $\boxed{[x, \hat{p}_x] = i\hbar}$

- NIFTIER METHOD (USING THIS RESULT)

USE LEIBNIZ RULE FOR OPERATORS

$$[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}]$$

$$[\hat{A}\hat{B}, \hat{C}] = [\hat{A}, \hat{C}]\hat{B} + \hat{A}[\hat{B}, \hat{C}]$$

<u>EX1)</u> $[x^2, \hat{p}_x] = [\underset{\hat{A}}{x}\,\underset{\hat{B}}{x}, \underset{\hat{C}}{\hat{p}_x}] = [x, \hat{p}_x]x + x[x, \hat{p}_x] = \underline{\underline{2i\hbar x}}$

(TRY THE OTHER WAY ....)

<u>EX2)</u> $[\underset{\hat{A}}{x^2}, \underset{\hat{B}\hat{C}}{\hat{p}_x^2}] = [x^2, \hat{p}_x]\hat{p}_x + \hat{p}_x[x^2, \hat{p}_x]$

$$= 2i\hbar(x\hat{p}_x + \hat{p}_x x)$$

<u>SIMPLIFY:</u> $[x, \hat{p}_x] = i\hbar = x\hat{p}_x - \hat{p}_x x \Rightarrow \hat{p}_x x = x\hat{p}_x - i\hbar$

$$\Rightarrow [x^2, \hat{p}_x^2] = 2i\hbar(x\hat{p}_x + x\hat{p}_x - i\hbar)$$

$$= \underline{\underline{4i\hbar\, x\hat{p}_x + 2\hbar^2}}$$

APPLICATION OF COMMUTATORS

HEISENBERG'S GENERALISED UNCERTAINTY PRINCIPLE: MEASURE TWO OBSERVABLES $\hat{A}, \hat{B}$ SIMULTANEOUSLY: $\Rightarrow$ UNCERTAINTIES

$$\Delta A = \sqrt{\langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2}, \quad \Delta B = \sqrt{\langle \hat{B}^2 \rangle - \langle \hat{B} \rangle^2}$$

FOR A GIVEN STATE WE HAVE LOWER BOUND ON THE UNCERTAINTY PRODUCT

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

$$\langle [\hat{A}, \hat{B}] \rangle = \int \Psi^* [\hat{A}, \hat{B}] \Psi \, dx$$

depends in general on time and state Ψ

EX $\hat{A} = x, \quad \hat{B} = \hat{p}_x$

$$[\hat{A}, \hat{B}] = [x, \hat{p}_x] = i\hbar$$ (IN THIS CASE THIS IS A NUMBER)

$$\langle [\hat{A}, \hat{B}] \rangle = i\hbar \int \Psi^* \Psi \, dx = i\hbar$$

IN THIS CASE INDEPENDENT OF TIME AND Ψ.

SO $\Delta x \, \Delta p_x \geq \hbar/2$

ALSO $\Delta y \, \Delta p_y \geq \frac{\hbar}{2}$

$$\Delta z \, \Delta p_z \geq \frac{\hbar}{2}$$

- IF TWO OBSERVABLES DO NOT COMMUTE $[\hat{A},\hat{B}]\neq 0$ WE CANNOT MEASURE THEM SIMULTANEOUSLY TO ARBITRARY PRECISION (NOTHING WRONG WITH EXPERIMENT!)

- WE ALSO SAY x AND $\hat{p}_x$ ARE COMPLIMENTARY PROPERTIES OF PARTICLE

  - IN PRINCIPLE WE CAN MEASURE POSITION TO ARBITRARY PRECISION $(\Delta x=0)$, BUT THEN WE KNOW NOTHING ABOUT MOMENTUM $\Delta p_x=\infty$

- COMMUTATORS RELATIONS HAVE MANY MORE APPLICATIONS AND IMPLICATIONS (SEE LATER IN COURSE)

  EX IF $[\hat{A},\hat{B}]=0$, THEN THERE EXIST SIMULTANEOUS EIGENSTATES

  $$\hat{A}\psi=a\psi \quad \text{AND} \quad \hat{B}\psi=b\psi$$

  - CAN MEASURE $\hat{A}$ AND $\hat{B}$ IN PRINCIPLE WITH ARBITRARY PRECISION!

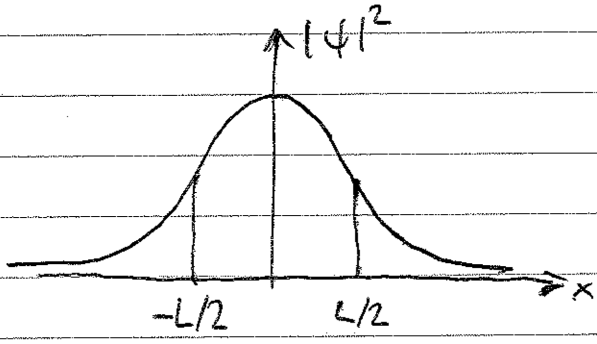
MINIMUM UNCERTAINTY WAVEFUNCTION

$$\psi(x) = \left(\frac{2}{\pi L^2}\right)^{1/4} e^{-x^2/L^2}$$

$$\langle \hat{x} \rangle = 0 \quad , \quad \langle \hat{x}^2 \rangle = \frac{L^2}{4} \Rightarrow \Delta x = \frac{L}{2}$$

$$\langle \hat{p}_x \rangle = 0 \quad , \quad \langle \hat{p}_x^2 \rangle = \frac{\hbar^2}{L^2} \Rightarrow \Delta p_x = \frac{\hbar}{L}$$

$$\Delta x \, \Delta p_x = \frac{\hbar}{2}$$ <u>FOR THIS PARTICULAR W.F.</u>



F.T. $$\Phi(p_x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} dx \, \psi(x) \, e^{-ip_x x/\hbar}$$

$$= \left(\frac{L^2}{\hbar^2 (2\pi)}\right)^{1/4} e^{-L^2 p_x^2/(4\hbar^2)}$$

$$\Delta p_x = \frac{\hbar}{L}$$

AN ASIDE: MOMENTUM WAVEFUNCTIONS AND MOMENTUM IN Q.M.

FOURIER TRANSFORM: $$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \Phi(p_x,t) \underbrace{e^{ip_x x/\hbar}} dp_x$$

MOM. W.F.

- DE BROGLIE W.F.
- EIGENFUNCTION OF $\hat{p}_x$

IN VERSE F.T.

$$\Phi(p_x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} dx\, e^{-ip_x x/\hbar}\, \Psi(x,t)$$

INTERPRETATION

$|\Phi(p_x,t)|^2 dp_x$ .. PROB. TO FIND PARTICLE WITH MOMENTUM BETWEEN p_x AND $p_x + dp_x$.

$$\int |\psi|^2 dx = 1 \iff \int |\Phi|^2 dp_x = 1$$ PARSEVAL'S THEOREM

WHY? CHECK DEFINITION OF $\hat{p}_x$ IN Q.M.

$$\langle \hat{p}_x \rangle = \int \Psi^* (-i\hbar\partial_x) \Psi \, dx$$

$$= \int dp_x \int dp_x' \int dx\, \Phi^*(p_x',t) e^{-ip_x' x/\hbar} (-i\hbar\, ip_x/\hbar)\, \Phi(p_x,t) e^{ip_x x/\hbar} \frac{1}{2\pi\hbar}$$

$$= \int dp_x \int dp_x' \underbrace{\int dx\, e^{ix(p_x - p_x')/\hbar}}_{2\pi\hbar\,\delta(p_x - p_x')} \Phi^*(p_x',t)\, p_x\, \Phi(p_x,t) \frac{1}{2\pi\hbar}$$

$$= \int dp_x\, p_x\, |\Phi(p_x,t)|^2$$

END LECT2 / WEEK2
2/10/2012

STATIONARY STATES & ENERGY EIGENSTATES

TDSE $\boxed{\hat{H}\,\Psi(x,t) = i\hbar \frac{\partial}{\partial t} \Psi(x,t)}$

POTENTIAL

$$\hat{H} = \frac{1}{2m}\left(\hat{p}_x^2\right) + V(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)$$

- ASSUME $V(x,t)$ IS <u>TIME INDEPENDENT</u> $\Rightarrow V(x)$
- THEN WE CAN MAKE ANSATZ OF SEPERATION OF VARIABLES

$$\Psi(x,t) = \psi(x)\, f(t)$$

TDSE $\rightarrow$ $\left(\hat{H}\,\psi(x)\right) f(t) = \psi(x)\left(i\hbar \frac{\partial}{\partial t} f\right)$

$$\Rightarrow \underbrace{\frac{1}{\psi(x)}\left(\hat{H}\,\psi(x)\right)}_{\text{depends only on } x} = \underbrace{\frac{1}{f(t)}\left(i\hbar \frac{\partial f(t)}{\partial t}\right)}_{\text{depends only on } t} = \underset{\text{const}}{E}$$

$$\Rightarrow \quad \hat{H}\,\psi(x) = E\,\psi(x) \quad \underline{\underline{\text{TISE}}}$$

$$i\hbar \frac{\partial f}{\partial t} = E\, f(t) \Rightarrow f = \underset{\text{const}}{C}\, e^{-iEt/\hbar}$$

SO $\boxed{\Psi_E(x,t) = e^{-iEt/\hbar}\,\psi(x)}$

ENERGY EIGENSTATE

IF SYSTEM IS IN THIS STATE, MEASUREMENT OF ENERGY ALWAYS GIVES RESULT E!

- USUALLY THERE ARE MANY SOLUTIONS TO TISE LABEL THEM BY INDEX n

$$\hat{H}\,\psi_n(x) = E_n\,\psi_n(x)\,, \quad \Psi_n(x,t) = e^{-iE_nt/\hbar}\,\psi_n(x)$$

PROPERTIES

- E_n REAL (WILL PROVE THIS SHORTLY)
- $\Psi_n^*(x,t) = e^{+iE_nt/\hbar}\,\psi_n^*(x)$

$$P(x,t) = |\Psi_n|^2 = \Psi_n^*\,\Psi_n = \cancel{e^{iE_nt/\hbar}}\,\cancel{e^{-iE_nt/\hbar}}\,|\psi_n(x)|^2$$

TIME INDEPENDENT

$\Rightarrow$ "STATIONARY STATES"

- $\Psi = c_1\Psi_1 + c_2\Psi_2$ IN GENERAL NOT STATIONARY (INTERFERENCE TERM)

- $\psi_n(x)$ CAN BE CHOSEN TO BE REAL! (TISE IS A REAL EQN., UNLIKE TDSE)

- EXPECTATION VALUES ARE TIME INDEPENDENT (IF $\frac{\partial\hat{A}}{\partial t} = 0$)

$$\langle\hat{A}\rangle = \int_{-\infty}^{+\infty}\Psi_n^*\,\hat{A}\,\Psi_n\,dx = \underbrace{\int_{-\infty}^{+\infty}dx\,\psi_n^*(x)\,\hat{A}\,\psi_n(x)}_{\text{independent of time}}\,\cancel{e^{iE_nt/\hbar}}\,\cancel{e^{-iE_nt/\hbar}}$$

- $$\langle\hat{p}_x\rangle = -i\hbar\int_{-\infty}^{+\infty}\Psi_n^*\,\frac{\partial}{\partial x}\,\Psi_n(x,t) = -i\hbar\int_{-\infty}^{+\infty}\psi_n(x)\,\frac{\partial}{\partial x}\,\psi_n(x)$$

$$= -i\hbar\int_{-\infty}^{+\infty}dx\,\frac{1}{2}\,\frac{\partial}{\partial x}\left(\psi_n^2(x)\right) = -i\hbar\,\frac{1}{2}\,\psi_n^2(x)\Big|_{x=-\infty}^{+\infty}$$

USING $\psi_n^* = \psi_n$ $\qquad = \underline{0}$ (NORMALISABILITY)

EXPECTATION VALUE OF ENERGY

$$\langle \hat{H} \rangle = \langle E \rangle = \int_{-\infty}^{+\infty} \Psi_n^*(x,t) \underbrace{\hat{H}\, \Psi_n(x,t)}_{E_n \Psi_n(x,t)}$$

$$= E_n \underbrace{\int_{-\infty}^{+\infty} \Psi_n^* \Psi_n \, dx}_{=1} = E_n$$

ALSO $\hat{H}\hat{H}\, \Psi_n(x,t) = E_n^2\, \Psi_n(x,t)$

AND $\hat{H}^2 \psi_n = \hat{H}(\underbrace{\hat{H}\psi_n}_{E_n\psi_n}) = E_n \hat{H} \psi_n = E_n^2 \psi_n$

$$\Rightarrow \langle \hat{H}^2 \rangle = \langle E^2 \rangle = E_n^2$$

SO $\Delta E = \sqrt{\langle \hat{H}^2 \rangle - \langle \hat{H} \rangle} = 0$

- ENERGY UNCERTAINTY ZERO FOR $\Psi_n(x,t)$

- MEASUREMENT ALWAYS GIVES RESULT E_n

- FOR GENERAL STATE $\Psi = \sum c_n \Psi_n(x,t)$

$\Delta E \neq 0$

ORTHOGONALITY OF ENERGY EIGENSTATES

- MOST IMPORTANT PROPERTY OF ENERGY EIGENSTATES!
- ASSUME WE KNOW ALL $\psi_i(x)$ AND E_i FOR A GIVEN $\hat{H}$

(we will suppress x and t in the following)

CONSIDER QUANTITY

$$H_{ij} := \int_{-\infty}^{+\infty} \psi_i^* \underbrace{\hat{H}\psi_j}_{E_j\psi_j} dx = E_j \int_{-\infty}^{+\infty} \psi_i^* \psi_j dx \quad \text{(EXPR. 1)}$$

- IMPORTANT FACT: $\hat{H}$ IS SELF-ADJOINT (HERMITIAN)

THIS MEANS $\boxed{\int \psi_i^* \hat{H} \psi_j dx = \int (\hat{H}\psi_i)^* \psi_j dx}$

$$-\frac{\hbar^2}{2m}\left[\int_{-\infty}^{+\infty} \psi_i^* \frac{\partial^2}{\partial x^2}\psi_j dx\right] + \int_{-\infty}^{+\infty} \psi_i^* V(x) \psi_j dx$$

INTEGRATE BY PARTS

$$\cancel{\left[\psi_i^* \frac{\partial \psi_j}{\partial x}\right]_{-\infty}^{+\infty}} - \int_{-\infty}^{+\infty} \frac{\partial \psi_i^*}{\partial x}\frac{\partial \psi_j}{\partial x} dx$$

0 NORMALISABILITY

V(x) is real

$$-\cancel{\left[\frac{\partial \psi_i^*}{\partial x}\psi_j\right]_{-\infty}^{+\infty}} + \int \frac{\partial^2 \psi_i^*}{\partial x^2}\psi_j dx \qquad \int_{-\infty}^{+\infty} (V(x)\psi_i)^* \psi_j dx$$

0

$$= -\frac{\hbar^2}{2m}\int \frac{\partial^2 \psi_i^*}{\partial x^2}\psi_j dx + \int (V(x)\psi_i)^* \psi_j dx = \int_{-\infty}^{+\infty} (\hat{H}\psi_i)^* \psi_j dx$$

SO: $H_{ij} = \int_{-\infty}^{+\infty} (\underbrace{\underbrace{\hat{H}\psi_i}_{E_i\psi_i}}_{=E_i^*\psi_i^*})^* \psi_j \, dx = E_i^* \int_{-\infty}^{+\infty} \psi_i^* \psi_j \, dx$ EXPR2

$\Rightarrow$ EXPR1 $-$ EXPR2 $= 0$

$$\Rightarrow \boxed{(E_j - E_i^*) \int_{-\infty}^{+\infty} \psi_i^* \psi_j \, dx = 0}$$

WHAT CAN WE LEARN FROM THIS?

1) SET $i=j$: $\quad (E_i - E_i^*) \underbrace{\int_{-\infty}^{+\infty} |\psi_i|^2 dx}_{=1 \text{ (NORMALISED)}} = 0$

$\Rightarrow \quad E_i = E_i^*$

E_i IS REAL

2) SET $i \neq j$ (ASSUME ENERGY EIGENVALUES ARE NON-DEGENERATE I.E. FOR EVERY E_i THERE IS ONLY ONE EIGENSTATE ψ_i (ALWAYS TRUE IN 1D BUT NOT IN 3D)

$$i \neq j: \quad \underbrace{\left(E_j - E_i^*\right)}_{= E_j - E_i \neq 0} \int_{-\infty}^{+\infty} dx\, \psi_i^* \psi_j = 0$$

$$\Rightarrow \boxed{\int_{-\infty}^{+\infty} \psi_i^* \psi_j \, dx = 0}$$

- ENERGY EIGENSTATES ARE "ORTHOGONAL" FOR DIFFERENT EIGENVALUES

"THEY HAVE NOTHING IN COMMON"

IF SYSTEM IS PREPARED IN $\Psi = \Psi_i$ WE ALWAYS FIND E_i ENERGY MEASUREMENT NEVER E_j WITH $j \neq i$. HENCE THEY ARE "ORTHOGONAL"

- THIS GEOMETRIC INTERPRETATION OF INTEGRALS LIKE

$$\int \psi_i^* \psi_j \, dx \quad \text{AS} \quad \text{"DOT PRODUCTS"}$$

WILL DISCUSSED FURTHER LATER IN THE COURSE AND LEADS TO

- DIRAC'S BRA-KET NOTATION
- MATRIX QUANTUM MECHANICS

SUMMARY: E_i REAL FOR ALL i

$$\int_{-\infty}^{+\infty} \psi_i^* \psi_j \, dx = \delta_{ij} = \begin{cases} 1 & i = j \quad \text{NORMALISED} \\ 0 & i \neq j \quad \text{ORTHOGONAL} \end{cases}$$

$\Rightarrow$ ψ_i ARE "ORTHONORMAL"