$$\langle \vec{X} \rangle \equiv \int_{\text{over All space}} \vec{X} \underbrace{|\Psi(\vec{x},t)|^2}_{\rho(\vec{x},t)} d^3X$$

"Expectation Value"

$$\int_{\text{All space}} \rho(\vec{x},t)\, d^3x = 1 \qquad \frac{\partial \rho(\vec{x},t)}{\partial t} + \vec{\nabla}\cdot\vec{J} = 0$$

$$\vec{J} = -\frac{i\hbar}{2m}\left[\Psi^*(\vec{x},t)\vec{\nabla}\Psi(\vec{x},t) - \left(\vec{\nabla}\Psi^*(\vec{x},t)\right)\Psi(\vec{x},t)\right]$$

"$\vec{J} = \rho\vec{v}$" In E&M

$$\frac{d\langle \vec{x}\rangle}{dt} = \int \vec{x}\frac{\partial}{\partial t}\rho(\vec{x},t)\, d^3x$$

$$= -\int \vec{x}\,(\vec{\nabla}\cdot\vec{J})\, d^3x$$

$$\frac{d\langle x_i\rangle}{dt} = -\int x_i\, \partial_j J_j\, d^3x = -\int\left[\partial_j(x_i J_j) + J_j(\partial_j x_i)\right] d^3x$$

Units:

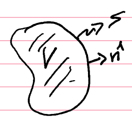
Comment, $\int \rho(\vec{x},t)\, d^3x = 1 \Rightarrow [\rho(\vec{x},t)] = [1/L^3]$

$$[\Psi(\vec{x},t)] = \left[\frac{1}{L^{3/2}}\right] \Rightarrow \lim_{|\vec{x}|\to\infty} \Psi(\vec{x},t) =$$

$$[\vec{\nabla}\Psi] = \left[\frac{1}{L^{5/2}}\right]$$

$\int_V \partial_j(x_i J_j)\, d^3X$ Has the form: $\int_V \vec{\nabla} f(\vec{x},t)\, d^3x = \int_S f(\vec{x},t)\,\hat{n}\, ds$

$$= \int_S (x_i J_j)\,\hat{n}\, ds \rightarrow 0$$



$$\therefore \frac{d\langle x_i\rangle}{dt} = \int J_j(\partial_j x_i)\, d^3x \qquad \partial_j x_i = \frac{\partial}{\partial x_j}x_i = \delta_{ij}$$

$$\int J_i\, d^3x \text{ "="} \int \rho v_i\, d^3x = \langle v_i\rangle$$

$$\frac{d\langle x_i\rangle}{dt} = \int J_i\, d^3x$$

$$= -\frac{i\hbar}{2m}\int\left[\Psi^*\partial_i\Psi - (\partial_i\Psi^*)\Psi\right] d^3x$$

$$\int(\partial_i\Psi^*)\Psi\, d^3x = \int\left(\cancelto{0}{\partial_i(\Psi^*\Psi)} - \Psi^*\partial_i\Psi\right) d^3x$$

$$\frac{d\langle x_i\rangle}{dt} = -\frac{i\hbar}{m}\int \Psi^*\partial_i\Psi\, d^3x$$

$$= \frac{1}{m}\int \Psi^*(-i\hbar\partial_i)\Psi\, d^3x$$

$$\frac{d\langle \hat{x}_i\rangle}{dt} = \langle v_i\rangle = \left\langle \frac{\hat{P}_i}{m}\right\rangle = \frac{1}{m}\langle \hat{P}_i\rangle$$

"Ehrenfest Theorem"

"Identify" $\hat{P}_i \equiv -i\hbar\partial_i \rightarrow \boxed{\hat{\vec{P}} \equiv -i\hbar\vec{\nabla}}$

$$\langle \hat{\vec{P}}\rangle = \int\left(\Psi^*(\vec{x},t)\,\hat{\vec{P}}\,\Psi(\vec{x},t)\right) d^3x$$

$$[\hat{q}_i, \hat{P}_j] = i\hbar\,\delta_{ij}$$

Abraham Pais:

"Subtle is the Lord"

"Inward Bound"

$$\langle \hat{\vec{P}} \rangle = \int \left(\Psi^*(\vec{x},t)\, \hat{\vec{P}}\, \Psi(\vec{x},t) \right) d^3x$$

In general,

$$\langle \hat{Q} \rangle \equiv \int \Psi^*(\vec{x},t)\, \hat{Q}\, \Psi(\vec{x},t)\, d^3x \quad \Big\} \text{ "Expectation Value"}$$

↳ "Any operator"

Principle of Q.M.: To each dynamical variable in classical Mechanics there corresponds an operator in Q.M.

Note:

$$\int \Psi^*(\vec{x},t) \left(-i\hbar \vec{\nabla} \Psi(\vec{x},t) \right) d^3x = -i\hbar \int \Psi^* \vec{\nabla} \Psi \, d^3x$$

$$= i\hbar \int \left(\vec{\nabla} \Psi^* \right) \Psi \, d^3x$$

$$= \int \left(-i\hbar \vec{\nabla} \Psi(\vec{x},t) \right)^* \Psi(\vec{x},t)\, d^3x$$

$$\int \Psi^*(\vec{x},t)\, \hat{\vec{P}}\, \Psi(\vec{x},t) = \int \left(\hat{\vec{P}}\, \Psi(\vec{x},t) \right)^* \Psi(\vec{x},t)\, d^3x$$

Defn: Hermitian Operators:

If $\int \Psi^*(\vec{x},t)\, \hat{Q}\, \Psi(\vec{x},t) = \int \left(\hat{Q}\, \Psi^*(\vec{x},t) \right) \Psi(\vec{x},t)\, d^3x$ } Hermiticity

$\hat{Q} = \hat{Q}(\hat{x}, \hat{P})$

we say $\hat{Q}$ is Hermitian.

Principle of Q.M.: Observables of a system are represented by Hermitian Operators.

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Recall the TDSE:

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

$\Rightarrow$ "If Ψ is a soln so is Ψ^*"

$t \to -t$

$\Psi(\vec{x},-t) \to \Psi^*(\vec{x},t)$

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

$$\hat{H} \equiv \frac{\hat{P}^2}{2m} + V(\hat{x})$$

"Hamiltonian"

$\hat{H}$ is Hermitian

$$\hat{H}\, \Psi^*(\vec{x},t) = -i\hbar \frac{\partial}{\partial t} \Psi^*(\vec{x},t)$$

$$\xrightarrow{t \to -t} \hat{H}\, \Psi^*(\vec{x},-t) = i\hbar \frac{\partial \Psi^*(\vec{x},-t)}{\partial t}$$

$$\Psi(\vec{x},t) \xrightarrow{\text{time Reversal}} \Psi^*(\vec{x},-t)$$

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Classical Mechanics Mini-Review

Newton's 2nd Law can be written as Hamilton's Eqns:

$$H = T + V = \frac{P^2}{2m} + V(x) = H(P,x)$$

$$\frac{\partial H}{\partial P} = P/m = \dot{x} \qquad \frac{\partial H}{\partial x} = \frac{\partial V(x)}{\partial x} = -F = -\frac{\partial P}{\partial t}$$

$\frac{\partial H}{\partial p} = 1/m = \lambda \qquad \frac{\partial}{\partial x} - \frac{\partial}{\partial x} = \cdot \qquad \partial t$

$$H = H(p, q) \qquad \frac{\partial H}{\partial p_i} = \dot{q}_i \qquad \frac{\partial H}{\partial q_i} = -\dot{p}_i$$

for any observable $A = A(q, p, t)$

$$\frac{dA}{dt} = \frac{\partial A}{\partial t} + \frac{\partial A}{\partial q_i}\frac{\partial q_i}{\partial t} + \frac{\partial A}{\partial p_i}\frac{\partial p_i}{\partial t}$$

$$\frac{dA}{dt} = \frac{\partial A}{\partial t} + \frac{\partial A}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial H}{\partial q_i}$$

$$\boxed{\frac{dA}{dt} = \frac{\partial A}{\partial t} + \{A, H\}}$$

$$\{A, B\} \equiv \frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i}$$

"Poisson Bracket"

i.e. H governs the time Evolution of the system!!

$$\langle \hat{Q} \rangle = \int d^3x\, \Psi^*(\vec{x}, t)\, \hat{Q}\, \Psi(\vec{x}, t)$$

$$\frac{d\langle \hat{Q}\rangle}{dt} = \int d^3x \left[\frac{\partial \Psi^*}{\partial t} \hat{Q}\, \Psi(\vec{x}, t) + \Psi^*(\vec{x}, t) \frac{\partial \hat{Q}}{\partial t} \Psi(\vec{x}, t) + \Psi^* Q \frac{\partial}{\partial t}\Psi \right]$$

$$= \left\langle \frac{\partial \hat{Q}}{\partial t} \right\rangle + \frac{i}{\hbar} \int d^3x \left[(\hat{H}\Psi)^* Q \Psi - \Psi^* \hat{Q} \hat{H} \Psi \right]$$

$$= \left\langle \frac{\partial \hat{Q}}{\partial t} \right\rangle + \frac{i}{\hbar} \int d^3x\, \Psi^*(\vec{x}, t) \left[\hat{H}\hat{Q} - \hat{Q}\hat{H} \right] \Psi(\vec{x}, t)$$

$$= \left\langle \frac{\partial \hat{Q}}{\partial t} \right\rangle + \frac{i}{\hbar} \int d^3x\, \Psi^*(\vec{x}, t) \left[\hat{H}, \hat{Q} \right] \Psi(\vec{x}, t)$$

$$[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$$

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

"Heisenberg

Eqn of Motion" $\frac{i}{\hbar}[\hat{H}, \hat{Q}] \longleftrightarrow \{Q, H\}$