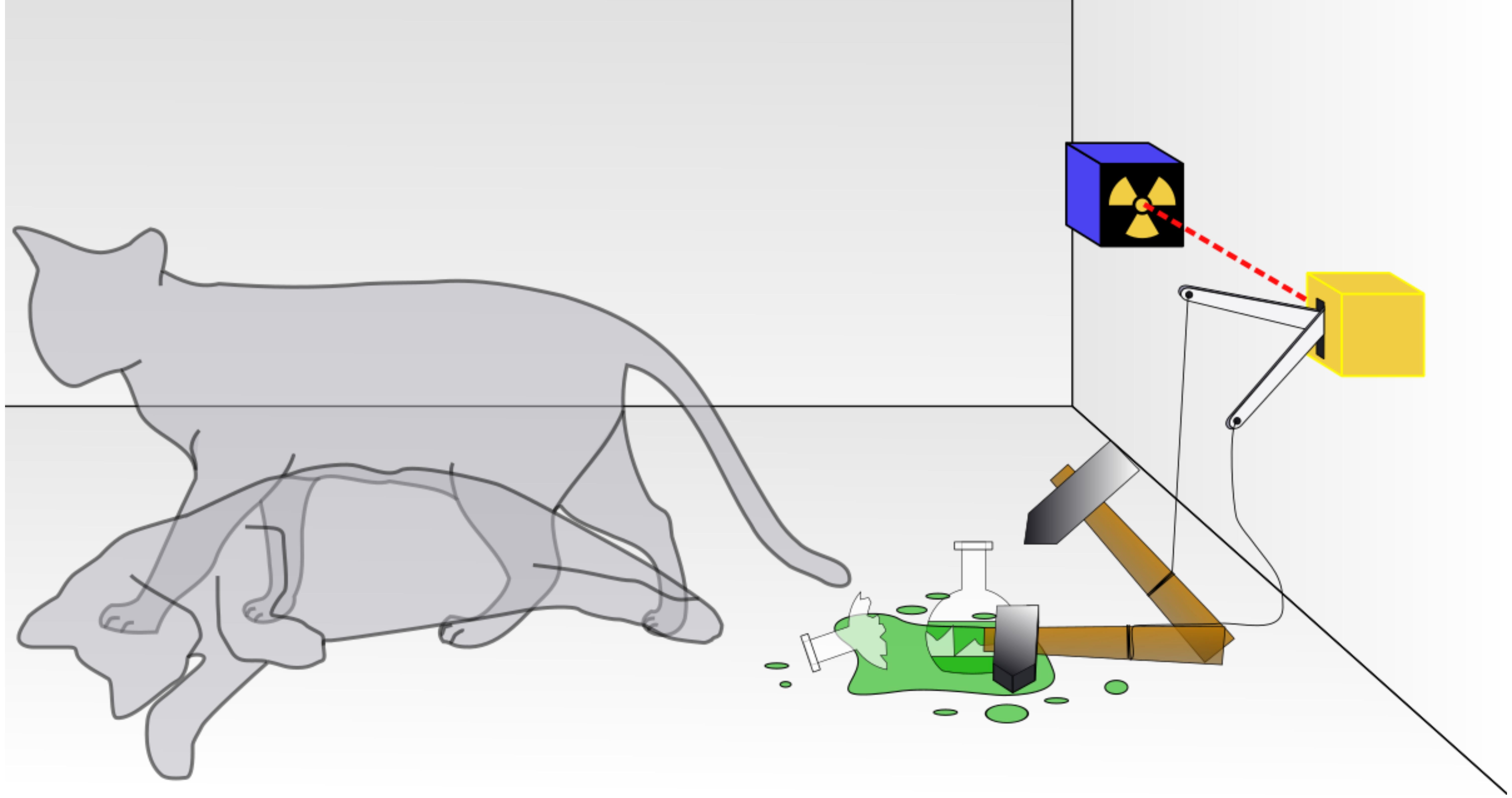


Lecture 06

Expectation values and Operators

Classical Domain

Different approaches $F = Ma$

Lagrangian and Hamiltonian dynamics

Hamiltonian Approach $\dot{x} = \frac{\partial H}{\partial p_i}, \quad \dot{p} = -\frac{\partial H}{\partial x_i}$

Concept of Phase Space and Dynamical variables $Q(x, p)$

Momentum , Kinetic energy, Angular Momentum , etc

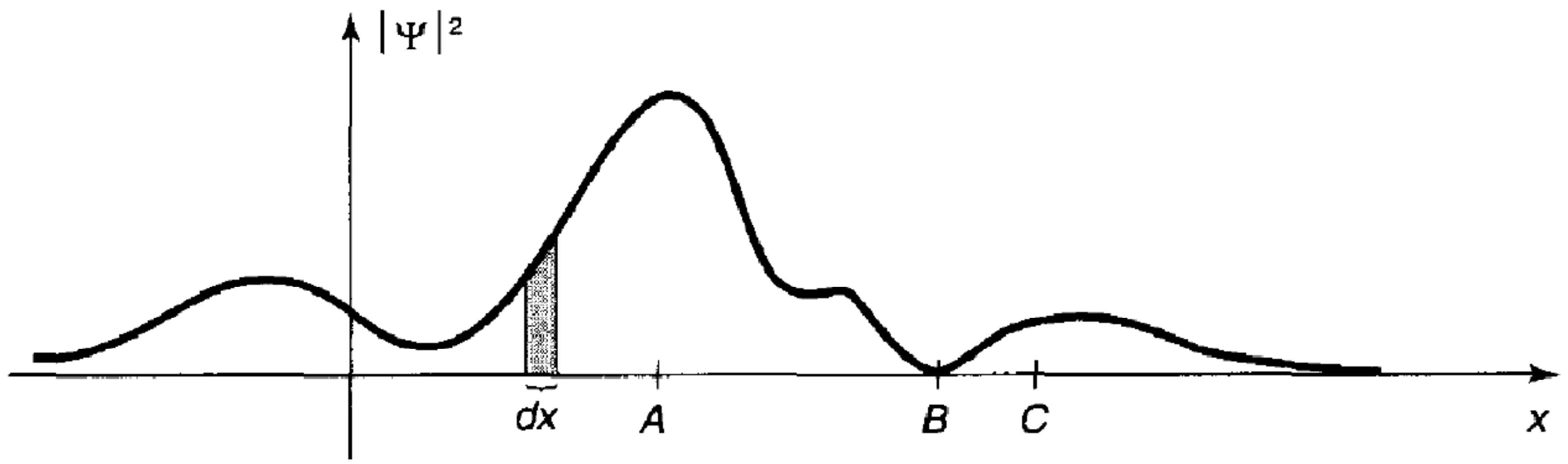
Classical Approach breaks down- *Uncertainty Principle comes in*

Wave Particle duality

Wave function and Schrodinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi. = H\psi$$

$$P(x, t)\, dx = |\Psi(x, t)|^2\, dx$$



How does Probability evolve with time

$$\frac{d}{dt}\int_{-\infty}^{+\infty}|\Psi(x,t)|^2\,dx = \int_{-\infty}^{+\infty}\frac{\partial}{\partial t}|\Psi(x,t)|^2\,dx.$$

$$\frac{\partial}{\partial t}|\Psi|^2 = \frac{\partial}{\partial t}(\Psi^*\Psi) = \Psi^*\frac{\partial\Psi}{\partial t} + \frac{\partial\Psi^*}{\partial t}\Psi$$

$$\frac{\partial\Psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2\Psi}{\partial x^2} - \frac{i}{\hbar}V\Psi, \qquad \frac{\partial\Psi^*}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2\Psi^*}{\partial x^2} + \frac{i}{\hbar}V\Psi^*$$

$$\frac{\partial}{\partial t}|\Psi|^2 = \frac{i\hbar}{2m}\left(\Psi^*\frac{\partial^2\Psi}{\partial x^2} - \frac{\partial^2\Psi^*}{\partial x^2}\Psi\right)$$

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

$$J(x,t) \equiv \frac{i\hbar}{2m}\left(\Psi\frac{\partial\Psi^*}{\partial x} - \Psi^*\frac{\partial\Psi}{\partial x}\right)$$

How does Probability evolve with time

$$\frac{d}{dt}\int_{-\infty}^{+\infty}|\Psi(x,t)|^2\,dx = \frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)\Bigg|_{-\infty}^{+\infty} = 0$$

Thus Schrodinger equation guaranties if a wave function is normalised at t=0, it will stay normalised for all time

$$P_{ab}(t) = \int_a^b |\Psi(x,t)|^2 dx \qquad \frac{dP_{ab}(t)}{dt} = \int_a^b \frac{\partial}{\partial t}|\Psi(x,t)|^2 dx$$

$$\frac{\partial}{\partial t}|\Psi(x,t)|^2 = \frac{i\hbar}{2m}(\Psi*\frac{\partial^2\Psi}{\partial x^2} - \Psi\frac{\partial^2\Psi*}{\partial x^2})$$

$$= \frac{\partial}{\partial x}[\frac{i\hbar}{2m}(\Psi*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi*}{\partial x})]$$

$$\frac{\partial}{\partial t}P_{ab}(t) = -\int_a^b \frac{\partial}{\partial x}J(x,t)dx$$

Expectation values and Operators

Measurements in Quantum Mechanics

$$< x > = \int_{\infty}^{\infty} x\,|\Psi(x,t)|^2\,dx$$

Momentum expectation

$$p = mv = m\frac{dx}{dt}$$

$$< p > = \frac{d < x >}{dt}$$

$$< p > = \frac{d}{dt}\int_{\infty}^{\infty} \Psi(x,t)^* x \Psi(x,t) dx$$

$$= m \int_{-\infty}^{\infty} dx \left(\frac{\partial \psi^*(x,t)}{\partial t} x\psi(x,t) + \psi^*(x,t) x \frac{\partial \psi(x,t)}{\partial t} \right)$$

Expectation values and Operators

$$\langle p \rangle = \frac{\hbar}{2i} \int_{-\infty}^{\infty} dx \left(\frac{\partial^2 \psi^*}{\partial x^2} x\psi - \psi^* x \frac{\partial^2 \psi}{\partial x^2} \right)$$

$$\frac{\partial^2 \psi^*}{\partial x^2} x\psi = \frac{\partial}{\partial x}\left[\frac{\partial \psi^*}{\partial x} x\psi\right] - \frac{\partial \psi^*}{\partial x}\psi - \frac{\partial \psi^*}{\partial x} x \frac{\partial \psi}{\partial x}$$

$$= \frac{\partial}{\partial x}\left[\frac{\partial \psi^*}{\partial x} x\psi\right] - \frac{\partial}{\partial x}(\psi^*\psi) + \psi^* \frac{\partial \psi}{\partial x} - \frac{\partial}{\partial x}\left[\psi^* x \frac{\partial \psi}{\partial x}\right] + \psi^* \frac{\partial \psi}{\partial x} + \psi^* x \frac{\partial^2 \psi}{\partial x^2}$$

$$\left(\frac{\partial^2 \psi^*}{\partial x^2} x\psi - \psi^* x \frac{\partial^2 \psi}{\partial x^2} \right) = \frac{\partial}{\partial x}\left(\frac{\partial \psi^*}{\partial x} x\psi - \psi^* x \frac{\partial \psi}{\partial x} - \psi^*\psi \right) + 2\psi^* \frac{\partial \psi}{\partial x}$$

$$\langle p \rangle = \int_{-\infty}^{\infty} dx\, \psi^*(x, t)\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\psi(x, t)$$

Expectation values and Operators

$$\langle x \rangle = \int_{-\infty}^{+\infty} \psi^* x \psi \, dx$$

$$\hat{p} \rightarrow -i\hbar \frac{\partial}{\partial x}$$

$$\langle Q(x, p) \rangle = \int \Psi^* Q\left(x, \frac{\hbar}{i}\frac{\partial}{\partial x}\right)\Psi \, dx.$$

$$T = \frac{1}{2}mv^2 = \frac{p^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

$$\langle T \rangle = \frac{-\hbar^2}{2m}\int \Psi^* \frac{\partial^2 \Psi}{\partial x^2} \, dx.$$

Operators and expectation values

$$dx/dt = \partial H/\partial p \text{ and } dp/dt = -\partial H/\partial x,$$

To every physically measurable quantity A, called an observable or dynamical variable, there corresponds a linear Hermitian operator $\hat{A}$ whose eigenvectors form a complete basis.

$$\hat{A}|\psi(t)\rangle = a_n|\psi_n\rangle,$$

$$f(\vec{r}, \vec{p}) \quad \longrightarrow \quad F(\hat{\vec{R}}, \hat{\vec{P}}) = f(\hat{\vec{R}}, -i\hbar\vec{\nabla}),$$

$$H = \frac{1}{2m}\vec{p}^{\,2} + V(\vec{r}, t)$$

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\hat{\vec{R}}, t),$$

Operators and expectation values

Symbol	Physical quantity	Operator
$f(x)$	Any function of x—the position x, the potential energy $V(x)$, etc.	$f(x)$
p_x	x component of momentum	$\frac{\hbar}{i}\frac{\partial}{\partial x}$
p_y	y component of momentum	$\frac{\hbar}{i}\frac{\partial}{\partial y}$
p_z	z component of momentum	$\frac{\hbar}{i}\frac{\partial}{\partial z}$

Operators and expectation values

Symbol	Physical quantity	Operator
E	Hamiltonian (time independent)	$\frac{p_{op}^2}{2m} + V(x)$
E	Hamiltonian (time dependent)	$i\hbar \frac{\partial}{\partial t}$
E_k	Kinetic energy	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$
L_z	z component of angular momentum	$-i\hbar \frac{\partial}{\partial \phi}$

Expectation values of p and p^2 for ground state of Infinite well

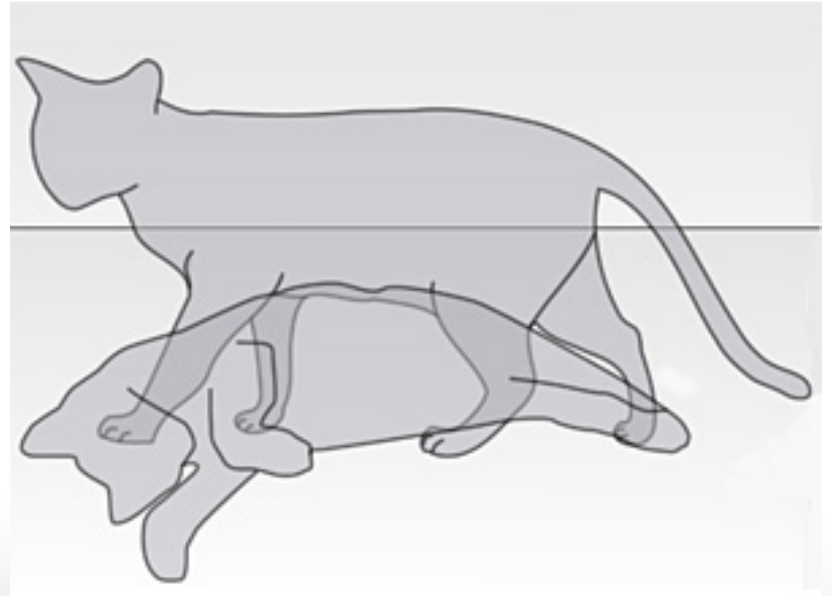
$$\langle p \rangle = \int_0^L \left(\sqrt{\frac{2}{L}} \sin \frac{nx}{L}\right)\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\left(\sqrt{\frac{2}{L}} \sin \frac{nx}{L}\right) dx$$

$$= \frac{\hbar}{i}\frac{2}{L}\frac{\pi}{L}\int_0^L \sin\frac{\pi x}{L}\cos\frac{\pi x}{L}\, dx = 0$$

$$\frac{\hbar}{i}\frac{\partial}{\partial x}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\psi = -\hbar^2\frac{\partial^2\psi}{\partial x^2} = -\hbar^2\left(-\frac{\pi^2}{L^2}\sqrt{\frac{2}{L}}\sin\frac{\pi x}{L}\right)$$

$$= +\frac{\hbar^2\pi^2}{L^2}\psi$$

$$\langle p^2 \rangle = \frac{\hbar^2\pi^2}{L^2}\int_0^L \psi^*\psi\, dx = \frac{\hbar^2\pi^2}{L^2}$$



Curiosity Kills the Cat

Lecture 06

Concluded