VARIANCE, ROOT-MEAN SQUARE, OPERATORS, EIGENFUNCTIONS, EIGENVALUES

$x_i - \langle x \rangle \quad \equiv \quad$ Deviation of i^{th} measurement from average value $\langle x \rangle$

$\langle x_i - \langle x \rangle \rangle \quad \equiv \quad$ Average deviation from average value $\langle x \rangle$

But for particle in a box, $\langle x_i - \langle x \rangle \rangle = 0$

$\left(x_i - \langle x \rangle\right)^2 \quad \equiv \quad$ Square of deviation of i^{th} measurement from average value $\langle x \rangle$

$\left\langle \left(x_i - \langle x \rangle\right)^2 \right\rangle \equiv \sigma_x^2 \quad \equiv \quad$ the Variance in x

Note $\boxed{\left\langle \left(x_i - \langle x \rangle\right)^2 \right\rangle = \langle x^2 \rangle - \langle x \rangle^2 = \sigma_x^2}$

The Root Mean Square (rms) or Standard Deviation is then

$$\boxed{\sigma_x = \left[\langle x^2 \rangle - \langle x \rangle^2\right]^{1/2}}$$

The uncertainty in the measurement of x, Δx, is then defined as

$$\boxed{\Delta x = \sigma_x}$$

σ_x for particle in a box

$$\sigma_x^2 = \int_0^a \psi^*(x) x^2 \psi(x) dx - \int_{-\infty}^{\infty} \psi^*(x) x \psi(x) dx$$
$$= \left(\frac{2}{a}\right)\int_0^a x^2 \sin^2\left(\frac{n\pi x}{a}\right) dx - \left[\left(\frac{2}{a}\right)\int_0^a x \sin^2\left(\frac{n\pi x}{a}\right) dx\right]^2$$

Evaluate integral by parts

$$\Rightarrow \qquad \sigma_x^2 = \left[\frac{a^2}{3} - \frac{a^2}{2(n\pi)^2}\right] - \left[\frac{a^2}{4}\right]$$

$$\sigma_x^2 = \frac{a^2}{4(n\pi)^2}\left[\frac{(n\pi)^2}{3} - 2\right]$$

$$\boxed{\Delta x = \sigma_x = \frac{a}{2(n\pi)}\left[\frac{(n\pi)^2}{3} - 2\right]^{1/2}}$$

Note that deviation increases with *a*, and depends weakly on *n*.

Now suppose we want to test the Heisenberg Uncertainty Principle for the particle in a box.

We need $\langle p \rangle$ and $\langle p^2 \rangle$ to get $\Delta p = \sigma_p = \left[\langle p^2 \rangle - \langle p \rangle^2\right]^{1/2}$

But do we write $\langle p \rangle = \int_{-\infty}^{\infty} \psi^*(x)\, p\psi(x) dx$?

what do we put in here??

We need the concept of an <u>OPERATOR</u>

$$\hat{A} f(x) = g(x)$$

<u>operator</u> acts on <u>function</u> to get a <u>new function</u>

e.g. $$\underbrace{\frac{d}{dx}}_{\text{operator}}\underbrace{\left(\frac{x^2}{3}\right)}_{\text{function}} = \underbrace{\left(\frac{2x}{3}\right)}_{\text{new function}}$$

Special Case

If $\hat{A}f\left(x\right) = a\, f\left(x\right)$

number (constant)

then $f\left(x\right)$ is called an eigenfunction of the operator

and is the eigenvalue.

This is called an eigenvalue problem (as in linear algebra).

Quantum mechanics is full of operators and eigenvalue problems!!

e.g. Schrödinger's equation:

$$\underbrace{\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V\left(x\right)\right]}_{\hat{H}\text{ operator (Hamiltonian)}} \psi\left(x\right) \quad = \quad E\ \psi\left(x\right)$$

Eigenfunction constant

or $\boxed{\hat{H}\psi = E\psi}$ with $\boxed{\hat{H}\left(x\right) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V\left(x\right)}$ (in 1D)

The Hamiltonian operator, acting on an eigenfunction, gives the energy.
i.e. the Hamiltonian is the energy operator

If $V\left(x\right) = 0$, then $E = \text{K.E.} = \dfrac{p^2}{2m}$

$$\therefore \qquad \hat{H} = \frac{\left(\hat{p}\right)^2}{2m} \qquad \Rightarrow \qquad \left(\hat{p}\right)^2 = -\hbar^2 \frac{d^2}{dx^2}$$

$\left(\hat{p}\right)^2$ means $\left(\hat{p}\right)\left(\hat{p}\right)$ i.e. the operator acts sequentially on the function

$$\left(\hat{p}\right)^2 f\left(x\right)=\left(\hat{p}\right)\left(\hat{p}\right)f\left(x\right)=\hat{p}\left[\hat{p}f\left(x\right)\right]=\hat{p}\left[g\left(x\right)\right]$$

$$\Rightarrow \qquad \left(\hat{p}\right)\left(\hat{p}\right)=\left(-i\hbar\frac{d}{dx}\right)\left(-i\hbar\frac{d}{dx}\right)=-\hbar^2\frac{d^2}{dx^2}$$

$$\therefore \quad \boxed{\hat{p}=-i\hbar\frac{d}{dx}}$$ Momentum operator (in 1D)

for Particle in a Box

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

Note *order* is now very important! Operator acts only on the function to its right.

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

$$=\int_0^a\left[\left(\frac{2}{a}\right)^{1/2}\sin\left(\frac{n\pi x}{a}\right)\right]\left(-i\hbar\frac{d}{dx}\right)\left[\left(\frac{2}{a}\right)^{1/2}\sin\left(\frac{n\pi x}{a}\right)\right]dx$$

$$=0$$

$$\left\langle p^2\right\rangle=\int_0^a\left[\left(\frac{2}{a}\right)^{1/2}\sin\left(\frac{n\pi x}{a}\right)\right]\left(-i\hbar\frac{d}{dx}\right)\left(-i\hbar\frac{d}{dx}\right)\left[\left(\frac{2}{a}\right)^{1/2}\sin\left(\frac{n\pi x}{a}\right)\right]dx$$

$$=\frac{2\hbar^2}{a}\int_0^a\sin\left(\frac{n\pi x}{a}\right)\left(\frac{n\pi}{a}\right)^2\sin\left(\frac{n\pi x}{a}\right)dx=\frac{2\hbar^2}{a}\left(\frac{n\pi}{a}\right)^2\int_0^a\sin^2\left(\frac{n\pi x}{a}\right)dx$$

$$=\frac{n^2\pi^2\hbar^2}{a^2}$$

Note $\left\langle p^2 \right\rangle = \dfrac{n^2 h^2}{4a^2} = 2m \dfrac{n^2 h^2}{8ma^2} = 2mE$ as expected

E = K.E. since *V*(*x*) = 0

$$\sigma_p^2 = \frac{n^2 \pi^2 \hbar^2}{a^2} = \left(\Delta p\right)^2$$

$$\Rightarrow \qquad \Delta x \Delta p = \frac{a}{2\left(n\pi\right)} \left[\frac{\left(n\pi\right)^2}{3} - 2 \right]^{1/2} \frac{n\pi\hbar}{a} = \frac{\hbar}{2} \underbrace{\left[\frac{\left(n\pi\right)^2}{3} - 2 \right]^{1/2}}_{\text{always} > 1}$$

$\therefore \qquad \Delta x \Delta p \geq \dfrac{\hbar}{2}$ as expected from Heisenberg Uncertainty Principle