E. Expectation Value and Uncertainty, What do they really mean?

- This is related to measurement**s** (the "s" in measurements is important)
- Measurement: $\begin{cases} \text{What to measure } (\hat{A})? \\ \text{What is the state (wavefunction) before measurement is made?} \end{cases}$

∴ We need 2 pieces of information

Operator $\hat{A}$ (corresponding to quantity to be measured)

$\Psi(x,y,z;t)$ OR $\psi(x,y,z)$ at the time of measurement

($\Psi(x,t)$ OR $\psi(x)$) (1D)

Let's learn from the only situation we know so far

$|\psi(x)|^2 dx$ = prob. of finding the particle in $x \to x+dx$

(Born) [saved "at time t (of measurement)" for simplicity]

<u>What is the mean position $\langle x \rangle$?</u>

Operationally, $\langle x \rangle = \int_{-\infty}^{\infty} x \, |\psi(x)|^2 dx$ (following Born's interpretation)

Suggesting a form of $\langle x \rangle = \int_{-\infty}^{\infty} x \, \psi^*(x) \, \psi(x) dx$

$$= \int_{-\infty}^{\infty} \psi^*(x) \, x \, \psi(x) dx$$

Finally $$\langle x \rangle = \int_{-\infty}^{\infty} \psi^*(x)\ \hat{x}\ \psi(x)\, dx \qquad (1)$$

Mean OR Expectation Value

RHS: $\left\{ \begin{array}{l} \hat{x} \quad \text{(which is } \hat{A} \text{ for position)} \\ \psi(x) \end{array} \right\}$ Need 2 pieces of information

<u>Postulate of QM (an extension of (1))</u>

- Measure A (thus $\hat{A}$) on a state (wavefunction) $\psi(x)$

Operationally, $$\langle A \rangle = \int_{-\infty}^{\infty} \psi^*(x)\ \hat{A}\ \psi(x)\, dx$$

Mean OR Expectation Value

Key Point

If a system is in a state described by a <u>normalized</u> wave function Ψ, then the expectation value of the quantity corresponding to $\hat{A}$ is given by

$$\langle A \rangle = \int_{-\infty}^{\infty} \Psi^* \hat{A} \Psi \, d^3r \qquad (3D)$$

If Ψ is <u>not normalized</u>,

$$\langle A \rangle = \frac{\int_{-\infty}^{\infty} \Psi^* \hat{A} \Psi \, d^3r}{\int_{-\infty}^{\infty} \Psi^* \Psi \, d^3r} = \frac{\int_{-\infty}^{\infty} \Psi^* \hat{A} \Psi \, d^3r}{\int_{-\infty}^{\infty} |\Psi|^2 \, d^3r}$$

Examples (Operational)

- Position: $\hat{x}$, States: 1D Box energy eigenfunctions $\psi_n(x)$

$$\langle x\rangle = \int_{-\infty}^{\infty} \psi_n^*(x)\, \hat{x}\, \psi_n(x) dx = \frac{2}{a} \underbrace{\int_0^a x \sin^2 \frac{n\pi x}{a} dx}_{\frac{a^2}{4} \text{ (Ex.)}} = \frac{a}{2} \text{ (for all } n)$$

[Makes Sense! $|\psi_n(x)|^2$ is symmetric about $\frac{a}{2}$]

- Momentum: $\hat{p} = \frac{\hbar}{i}\frac{d}{dx}$, States: $\psi_n(x)$ for 1D Box

$$\langle p\rangle = \int_{-\infty}^{\infty} \psi_n^*(x) \underbrace{\frac{\hbar}{i}\frac{d}{dx}}_{\hat{p}} \psi_n(x)\, dx = \frac{2}{a} \cdot \frac{n\pi}{a} \int_0^a \sin\frac{n\pi x}{a} \cos\frac{n\pi x}{a} dx \overset{\text{Why?}}{=} 0$$

(for all n)

Important Concept: What do $\langle x \rangle$, $\langle p \rangle$, $\langle A \rangle$ really mean?

- Measure A (thus $\hat{A}$), state: $\psi(x)$
- Why are we talking about the mean or average or expectation value?

Key idea: Measurements made on systems (prepared) in the same state

- Consider 1 million systems (e.g. an atom in its ground state) in the same state $\psi(x)$.

State:	$\psi(x)$	$\psi(x)$		$\psi(x)$		$\psi(x)$	[same state when measurement is made]
	●	●	...	●	...	●	
System	1	2	...	n		1,000,000	

[Measure A $\Rightarrow$ an operator $\hat{A}$ $\Rightarrow$ Eigenvalue problem $\hat{A}\phi_i = a_i \phi_i$

Outcome of <u>a</u> measurement must be one of $\{a_1, \cdots, a_i, \cdots\}$]

- Take System 1 and measure A : result is $a^{(1)}$ [one eigenvalue of $\hat{A}$]
  (then <u>throw the system away</u>, i.e. don't do measurement on it again!)
- Take System 2 and measure A : result is $a^{(2)}$ [one eigenvalue of $\hat{A}$]

⋮ ⋮

- Take System 1,000,000 and measure A : result is $a^{(1M)}$ [one eigenvalue of $\hat{A}$]

$\therefore$ Total 1,000,000 results (data), each one is an eigenvalue of $\hat{A}$

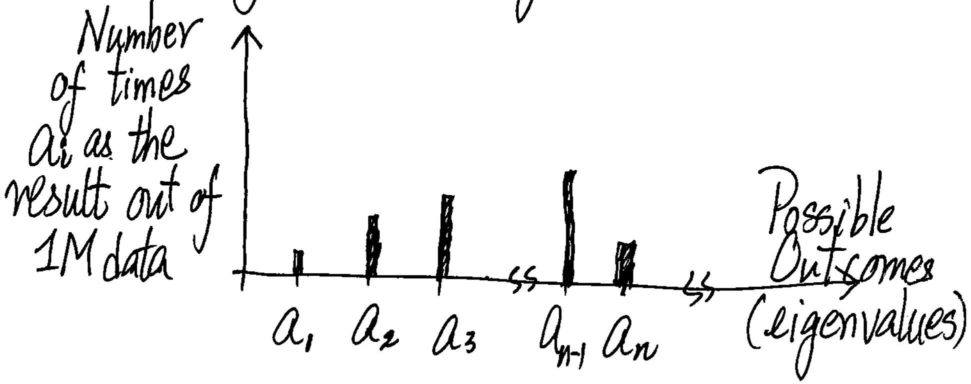
Key Points (up to here): Measurements on $\underbrace{\text{identically prepared systems}}_{\text{Same state}}$

State: $\psi(x)$ $\psi(x)$ ... $\psi(x)$ ... $\psi(x)$ [same state when measurement is made]

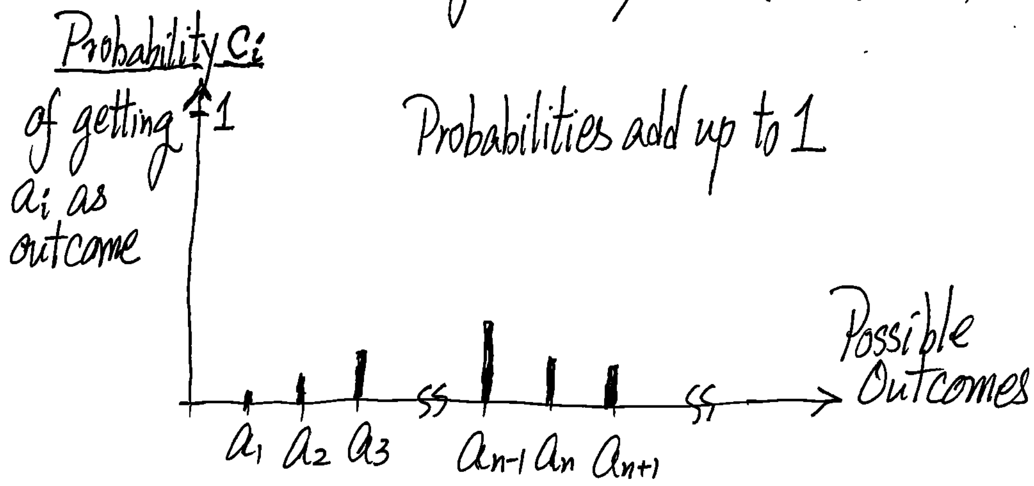
System: 1 2 ... n ... 1,000,000

Outcome: $\underbrace{a^{(1)} \quad a^{(2)} \quad \cdots \quad a^{(n)} \quad \cdots \quad a^{(1M)}}_{\text{Each is an eigenvalue of } \hat{A}}$

Data Analysis: Histogram



Divide y-axis by 1M (total data)



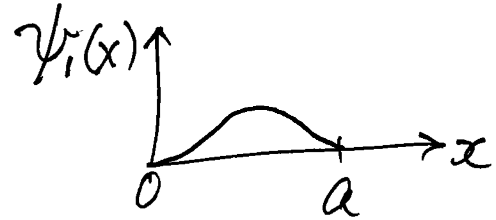
Question: What is $\underbrace{\text{the mean OR average}}_{}$ of the results?

This is what $\langle A \rangle$ means physically (conceptually)

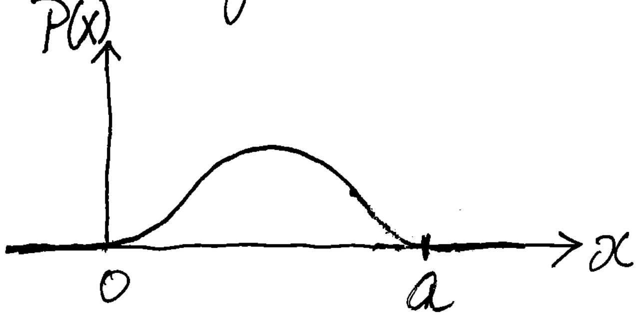
Operationally, it is given by $\langle A \rangle = \int_{-\infty}^{\infty} \psi^* \hat{A} \psi \, dx$

Example

- 1M copies of 1D box ground state



- Measure position once on each copy $\Rightarrow$ 1M data on position
- Result is a value $0 < x < a$ for each measurement
- Draw histogram (narrow binning) and then divide by 1M



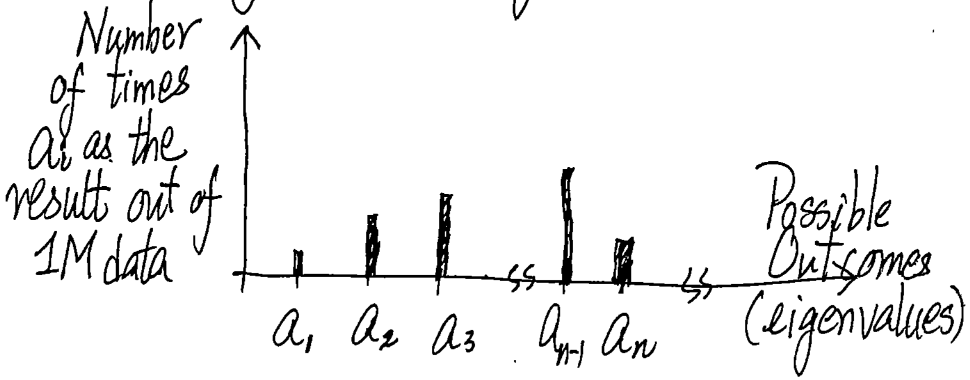
"experimental"

which is $|\psi_1(x)|^2 = \begin{cases} \frac{2}{a} \sin^2\left(\frac{\pi a}{X}\right) & \text{for } 0 < x < a \\ 0 & \text{for } X \leq 0 \ \& \ x \geq a \end{cases}$

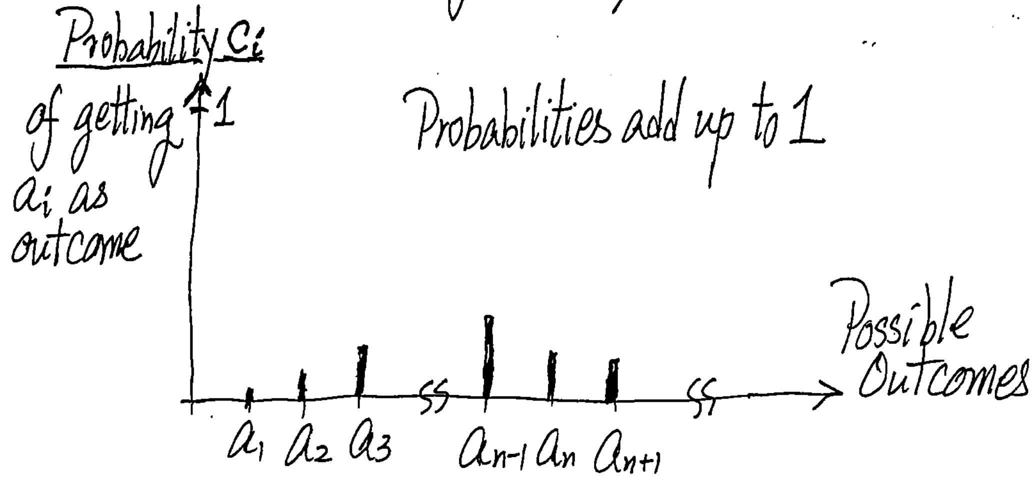
- With $\psi_i(x)$, we cannot predict outcome of a single measurement, but we can tell the probability density of every possible outcome

[This is exactly what we discussed in Ch. I]

Data Analysis: Histogram



Divide y-axis by 1M (total data)



Question: What is the "Spread" in the results?

Meaning: $\begin{cases} \text{Variance } \sigma^2 \text{ OR } (\Delta A)^2 \\ \text{Standard Deviation } \sigma \text{ OR } \underbrace{(\Delta A)}_{} \end{cases}$

this is the "uncertainty in A" properly defined in QM

<u>Variance</u> $(\Delta A)^2 \equiv \langle (A - \langle A \rangle)^2 \rangle$ where $\langle \cdots \rangle = \int_{-\infty}^{\infty} \psi^* (\hat{\cdots}) \psi \, dx$

$$= \underbrace{\langle A^2 \rangle}_{\substack{\text{expectation} \\ \text{value of } \hat{A}^2}} - \underbrace{\langle A \rangle^2}_{\text{square of mean}} \quad \text{(formula for calculation)}$$

<u>Uncertainty</u> in A formally defined (recall: there is <u>a state</u> in the discussion)

$$(\Delta A) = \sqrt{(\Delta A)^2} = \sqrt{(\langle A^2 \rangle - \langle A \rangle^2)}$$

i.e. calculate variance and take square root (operationally)

It quantifies the spread in measurement results (physical meaning)

Examples: $\psi_1(x) = \sqrt{\frac{2}{a}} \sin \frac{\pi x}{a}$ (Box ground state) $(0 < x < a)$

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} \psi_1^*(x)\, \hat{x}^2\, \psi_1(x)\, dx = \frac{2}{a}\int_0^a x^2 \sin^2\left(\frac{\pi x}{a}\right) dx$$

$$= \frac{a^2}{3} - \frac{a^2}{2\pi^2} \quad (\text{Ex.})$$

$$(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2 = \frac{a^2}{3} - \frac{a^2}{2\pi^2} - \frac{a^2}{4} = a^2\left[\frac{1}{12} - \frac{1}{2\pi^2}\right]$$

Δx = Uncertainty in x for the state $\psi_1 = a\left[\frac{1}{12} - \frac{1}{2\pi^2}\right]^{1/2}$

$$\langle p^2 \rangle = \frac{2}{a}\int_0^a \sin\frac{\pi x}{a} \underbrace{\left(-\hbar^2\right)\frac{d^2}{dx^2}}_{\hat{p}^2} \left(\sin\frac{\pi x}{a}\right) dx = \frac{\pi^2\hbar^2}{a^2} \quad (\text{Ex})$$

$$(\Delta p)^2 = \langle p^2 \rangle - \cancel{\langle p \rangle^2}^{\,0} = \frac{\pi^2\hbar^2}{a^2}$$

Δp = Uncertainty in p for the state ψ_1

$$= \sqrt{(\Delta p)^2} = \frac{\pi\hbar}{a}$$

Finally, what is $\Delta x \cdot \Delta p$ for the state ψ_1?

$$\Delta x \cdot \Delta p = \pi\hbar \cdot \left[\frac{1}{12} - \frac{1}{2\pi^2}\right]^{1/2} = \frac{\hbar}{2}\left[\frac{\pi^2}{3} - 2\right]^{1/2} = \frac{\hbar}{2} \cdot (1.134) > \frac{\hbar}{2}$$

The points are:

- There are formulas for $\langle A \rangle$, $\langle A^2 \rangle$, $(\Delta A)^2$, (ΔA)
- Given the state $\psi(x)$, these quantities can be evaluated
- Deeper: Physical Meaning is related to results of measurements on identically prepared systems