eg. #2 1g object with position ⑤

localized to $\Delta x \sim 10^{-6}$ m ~ 1/100 of human hair, wave packet doubles in $t \sim 10^{19}$s (> estimated age of universe)

** We will see later, measurement localizes wavefunction and then it spreads again.

Heisenberg Uncertainty Principle

A. Position & momentum $\Delta x \Delta p_x \gtrsim \hbar$

→ really a property of Fourier transforms

→ restrictions only on complementary pairs $\Delta x \Delta p_x$, $\Delta y \Delta p_y$, ...

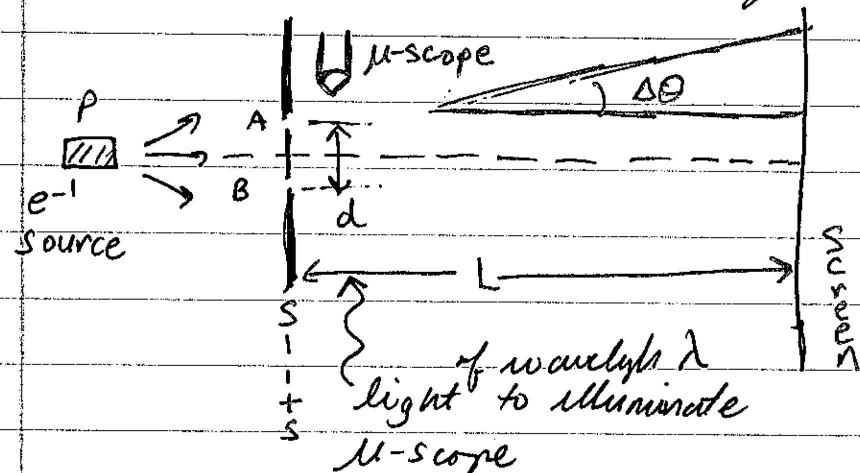
No restriction for different components

* → No restriction when measuring a single quantity

eg. measure x to accuracy Δa, then a has measure of p $\Delta p \gtrsim \frac{\hbar}{\Delta a}$

Consider the Heisenberg Microscope.

Eg. Double slit experiment with a microscope to determine which slit e^{-1} goes through.



- To resolve slits, need $\lambda < d$
  Momentum of photons (γ-rays) $P_\gamma = h/\lambda_\gamma$ must be larger than h/d

- The photon kicks the e^{-1}, causing an uncertainty in its momentum. $\Delta P_{e^{-1}} \sim h/\lambda_\gamma$

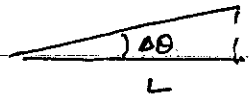
$$\Delta P_{e^{-1}} \sim \frac{h}{\lambda_\gamma} \gtrsim \frac{h}{d}$$

$$d\Delta P_{e^{-1}} \gtrsim h$$

- The deflection causes the trajectory of the e^{-1} to become uncertain by $\Delta\theta$

7

$$\Delta\theta \approx \frac{\Delta p_{e^{-1}}}{p_{e^{-1}}} = \frac{h}{pd} = \frac{\lambda_e}{d}$$ ← de Broglie wavelgh of e^{-1}



$\} L\Delta\theta$ ← uncertainty in position on the screen.

$$L\Delta\theta = \underbrace{\lambda_{e^{-1}}\frac{L}{d}}$$

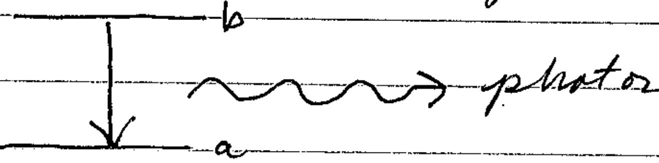
Comparable to the spacing on the screen between maxima

⟹ Thus, if you measure which slit e^{-1} goes through, you will not observe interference pattern!

B. Uncertainty in Energy & Time.

Like $\Delta p_x \Delta x \gtrsim \hbar$, we have $\Delta E \Delta t \gtrsim \hbar$

Consider two levels of an atom



- The time of emission is random from an excited atom and cannot be determined

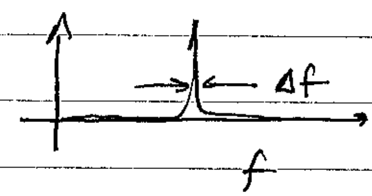
• We can calculate the probability of emission at a certain time.

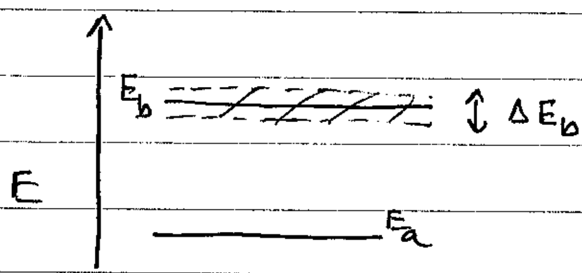
→ over a large # of atoms, this determines the lifetime of the state τ_b

Now, the wavefunction describing the atom in state b must be negligible outside of $\Delta t \gtrsim \tau_b$

Thus, the energy of the excited state is uncertain, and given by

$$\Delta E_b = \frac{h}{\tau_b} \longrightarrow \text{Natural linewidth}$$





• If E_a is the ground state, $\tau \to \infty$, $\Delta E = 0$

This level is <u>sharp</u>

$$f_{ab} = \frac{E_b - E_a}{h}$$

$$\Delta f = \Delta E_b / h$$

Absorption of Radiation by Atoms (9)

<u>Typically</u>, atomic recoil causes λ of emitted light to be different from absorption frequency.

However, radiation emitted from one atom <u>can be</u> absorbed by another atom b/c

linewidth > frequency change due to recoil

<u>Except</u>: Energy levels of nuclei are such that linewidth < frequency change due to recoil

<u>Thus</u>: γ rays emitted by one nucleus cannot in general be absorbed by another except when the nuclei are in a <u>crystal</u> and every once in a while the entire crystal recoils! The mass of the crystal is large and recoil frequency shift is negligible.

This resonant absorption is called the Mössbauer effect!
(Mössbauer) $\Longrightarrow$ Useful for spectroscopy of nuclei

The Schrödinger Equation

Requirements:

- linear, superposition holds
- should agree with classical physics (in proper limit)
- all time dependence should be determined once we know the wave function at a particular time!

*

Thus, we have $\frac{\partial \psi}{\partial t}$ and not $\frac{\partial^2 \psi}{\partial t^2}$

$\downarrow$

would need to specify ψ and $\frac{\partial \psi}{\partial t}$ at some t for a unique solution!

Recall: 1-D free (non-relativistic particle)

E $\quad \vec{P} = P_x \hat{X}$

m

Plane wave description: $\psi(x,t) = Ae^{i(kx-\omega t)}$

$= Ae^{i(P_x X - Et)/\hbar}$

$$E = \frac{P_x^2}{2m}$$

$$\Rightarrow \hbar\omega = \frac{(\hbar k)^2}{2m}$$

$$\Rightarrow \omega = \frac{\hbar k^2}{2m}$$

Note: $$\frac{\partial}{\partial t}\psi(x,t) = A(-i\omega)e^{i(kx-\omega t)}$$

$$= -i\omega\psi = \frac{-i}{\hbar}E\psi$$

$$\frac{\partial^2}{\partial x^2}\psi(x,t) = -k^2 A e^{i(kx-\omega t)} = \frac{-p_x^2}{\hbar^2}\psi$$

$$= \frac{-2Em}{\hbar^2}\psi$$

Thus, for a plane wave

$$\underbrace{i\hbar\frac{\partial}{\partial t}\psi(x,t) = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t)}$$

* Time dependent Schrödinger Eqn. for a free particle

* Operators (→ denote by (^)) are acting on ψ to return a value.

$$\hat{E} = i\hbar\frac{\partial}{\partial t} \qquad \hat{p}_x = -i\hbar\frac{\partial}{\partial x}$$

energy operator momentum operator.

Extend to 3D. ③

$$\psi(\vec{r},t) = A e^{i(\vec{k}\cdot\vec{r} - \omega t)}$$
$$= A e^{i(\vec{p}\cdot\vec{r} - Et)/\hbar}$$

$$i\hbar \frac{\partial}{\partial t}\psi(\vec{r},t) = \frac{-\hbar^2}{2m}\nabla^2 \psi(\vec{r},t)$$

Laplacian operator

$$\hat{E} = i\hbar\frac{\partial}{\partial t}$$

$$\hat{P} = -i\hbar\vec{\nabla}$$

Define kinetic energy operator $\hat{T} = \frac{\hat{p}^2}{2m}$

$$= \frac{-\hbar^2}{2m}\nabla^2$$

* Now, if the free particle feels a force (external) $\vec{F}(\vec{r},t)$ which can be derived from a potential,

$$\vec{F}(\vec{r},t) = -\vec{\nabla}V(\vec{r},t)$$

scalar potential.

$$\hat{V}(\vec{r},t)\psi(\vec{r},t) = V(\vec{r},t)\psi(\vec{r},t)$$

Then $\hat{E}\,\Psi(\vec{r},t) = \left[\frac{\hat{p}^2}{2m} + \hat{V}(\vec{r},t)\right]\Psi(\vec{r},t)$

$$i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t) = \Bigg[\underbrace{\frac{-\hbar^2}{2m}\nabla^2 + \hat{V}(\vec{r},t)}_{\hat{H}}\Bigg]\Psi(\vec{r},t)$$

* Proposed by Erwin Schrödinger in 1926

$\hat{H}$: Hamiltonian operator

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + \hat{V} = i\hbar\frac{\partial}{\partial t}$$

~ describes total energy, just like classical hamiltonian!

* Note: Like Newton's laws, cannot describe or derive from a guiding equation

→ just a statement of energy conservation.

Properties of physical operators include (5)

<u>Hermiticity</u>. What is a Hermitian operator?

(In mathematics, it is when an operator <u>equals</u> its adjoint).

Let's take a more practical route.

Start with probability conservation:

$$\int_V |\Psi(\vec{r},t)|^2 \, d\vec{r} = 1$$

V ~ volume where particle exists

$$\frac{\partial}{\partial t}\int_V \underbrace{|\Psi(\vec{r},t)|^2}_{\Psi^*\Psi} d\vec{r} = 0$$

$$= \int_V \Psi^*\left(\frac{\partial \Psi}{\partial t}\right) + \left(\frac{\partial \Psi^*}{\partial t}\right)\Psi \, d\vec{r}$$

Use Schrödinger equation and its conjugate.

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

and

<u>its conjugate</u> $-i\hbar \dfrac{\partial}{\partial t}\Psi^*(\vec{r},t) = [\hat{H}\Psi(\vec{r},t)]^*$

(*)

$$= \frac{1}{i\hbar} \int \left[\Psi^* (\hat{H}\Psi) - (\hat{H}\Psi)^* \Psi \right] d\vec{r} = 0$$ (6)

$$\Longrightarrow \int \Psi^* (\hat{H}\Psi)\, d\vec{r} = \int (\hat{H}\Psi)^* \Psi \, d\vec{r}$$

- This must hold true for all integrable functions Ψ and is thus a restriction on $\hat{H}$.

- Use definition $(\hat{A}\hat{B})^* = \hat{B}^* \hat{A}^*$
  Thus $(\hat{A}\Psi)^* = \Psi^* \hat{A}^*$

Thus $\hat{H} = \hat{H}^*$ The Hamiltonian is a Hermitian operator.

This will be important for distinguishing operators that correspond to <u>physical</u> properties.

<u>Probability current</u>

We can substitute into equation (*), assuming $V(\vec{r},t)$ is a real quantity.

$$\rightarrow \quad = \frac{i\hbar}{2m}\int_V \left[\psi^*(\nabla^2\psi) - (\nabla^2\psi^*)\psi\right] d\vec{r}$$

using standard vector identity:

$$= \frac{i\hbar}{2m}\int \vec{\nabla}\cdot\left[\psi^*(\vec{\nabla}\psi) - (\vec{\nabla}\psi^*)\psi\right] d\vec{r}$$

$$\equiv -\int_V \vec{\nabla}\cdot\vec{j}\, d\vec{r} \quad \text{where } \vec{j} = \frac{\hbar}{2mi}\left[\psi^*\vec{\nabla}\psi - (\nabla\psi^*)\psi\right]$$

What does $\vec{j}$ signify?

Use divergence Theorem $\int_V \vec{\nabla}\cdot\vec{A}\, d\vec{r}$ V ~ volume.

$= \int_S \vec{A}\cdot d\vec{s}$ S ~ surface

<u>Thus</u>:

$$\frac{\partial}{\partial t}\int_V \underbrace{|\psi(\vec{r},t)|^2 d\vec{r}}_{P(\vec{r},t)} = -\int_S \underbrace{\vec{j}}_{\text{probability current}}\cdot \underbrace{d\vec{s}}_{\text{area element}}$$

probability density

$$\Longrightarrow \frac{\partial}{\partial t}P(\vec{r},t) + \vec{\nabla}\cdot\vec{j}\,(\vec{r},t) = 0$$

(compare to charge & E+M)

Expectation Values

Average position $\langle \vec{r} \rangle = \int \vec{r} \underbrace{P(\vec{r},t)}_{\text{weight by probability}} d\vec{r}$

$$\underbrace{\langle \vec{r} \rangle}_{\text{expectation value}} = \int \hat{\Psi}^* \vec{r} \Psi \, d\vec{r}$$

equivalent to three different equations

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

$$\langle y \rangle = \int \Psi^*(\vec{r},t)\, y\, \Psi(\vec{r},t)\, d\vec{r}$$

$$\langle z \rangle = \int \Psi^*(\vec{r},t)\, z\, \Psi(\vec{r},t)\, d\vec{r}$$

More generally, given $f(\vec{r},t)$

$$\langle f(\vec{r},t) \rangle = \int f(\vec{r},t)\, P(\vec{r},t)\, d\vec{r}$$

generalize to operators.

$$= \int \Psi^*(\vec{r},t)\, \hat{f}(\vec{r},t)\, \Psi(\vec{r},t)\, d\vec{r}$$

Eg.

Potential Energy

$$\langle V(\vec{r},t)\rangle = \int \Psi^*(\vec{r},t)\,\hat{V}(\vec{r},t)\,\Psi(\vec{r},t)\,d\vec{r}$$

<u>Momentum</u>:

$$\langle \vec{p}\rangle = \int \Psi^*(\vec{r},t)\,\underbrace{\hat{p}}_{-i\hbar\vec{\nabla}}\,\Psi(\vec{r},t)\,d\vec{r}$$

$$= -i\hbar \int \Psi^*(\vec{r},t)\,\vec{\nabla}\,\Psi(\vec{r},t)\,d\vec{r}$$

<u>Note</u>: convince yourself $\hat{P}$ is Hermitian, even though it has an i!

For a general function of momentum $g(\vec{p},t)$

$$\langle g(\vec{p},t)\rangle = \int \Psi^*(\vec{r},t)\,\hat{g}(-i\hbar\vec{\nabla},t)\,\Psi(\vec{r},t)\,d\vec{r}$$

Thus, in general

$$\langle A\rangle = \int \Psi^*(\vec{r},t)\,\hat{A}\,\Psi(\vec{r},t)\,d\vec{r}$$

Hermitian operator associated with measurable quanti $\langle A\rangle$

Note: Operators act to the right $\longrightarrow$

* Not all operators formed by combining $\hat{r}, \hat{p}$ are Hermitian!

Consider $\widehat{xP_x}$ $\leftarrow$ which means "measure momentum, then 'position'"

$\underbrace{}_{\text{compound operation}}$

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

Integrate by parts:

$$\int u(x) v'(x)\, dx = u(x)V(x) - \int u'(x) V(x)\, dx$$

let $u = \psi^* x$, $V = \psi$

$$\langle x P_x \rangle = -i\hbar\, x \psi^*(x,t)\psi(x,t) \Big|_{-\infty}^{\infty} + i\hbar \int_{-\infty}^{\infty} \psi \left(\frac{\partial}{\partial x} [x \psi^*(x,t)] \right) dx$$

vanishes since $|\psi| \to 0$ as $|x| \to \infty$

Thus:

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

$$+ \; i\hbar \int_{-\infty}^{\infty} \psi^* \psi \, dx$$

$$= \langle x P_x \rangle^* + i\hbar$$

→ Not real! $\widehat{xP_x}$ not Hermitian

not well defined measurement

If you calculate $\langle P_x x \rangle = \langle P_x x \rangle^* - i\hbar$

<u>But</u>: $$\left\langle \frac{xP_x + P_x x}{2} \right\rangle = \left\langle \frac{xP_x + P_x x}{2} \right\rangle^*$$

→ real #, Hermitian operator

→ order matters in QM!

⇒ Operators, in general, do not commute! **

In this case, the order in which ⑤
you make a position + momentum measmt
matters! Recall
Heisenberg uncertainty

<u>Define:</u>

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

$= 0$ if $\hat{A}, \hat{B}$ "commute"

$\neq 0$ if $\hat{A}, \hat{B}$ <u>do not commute</u>

→ Basic meaning is that if

$\hat{A}, \hat{B}$ are Hermitian operators, and they commute, then you can measure them ~~in sequence~~.
both with <u>arbitrary</u> precision.

- $\hat{X}, \hat{P}_x$ <u>do not</u> commute, as shown above.

$[\hat{X}, \hat{P}_x] = (\hat{X}\hat{P}_x - \hat{P}_x\hat{X})$

act on ψ

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

$$= -i\hbar\, x \frac{\partial \psi}{\partial x} + i\hbar \left[\psi + x \frac{\partial \psi}{\partial x} \right] = i\hbar \psi$$

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

Canonical
commutation
relation