Phys 491
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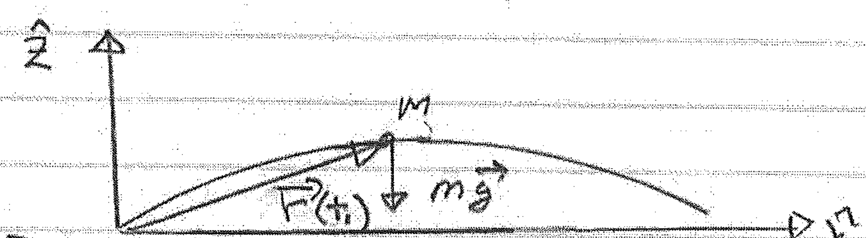
Fall 2021

Lecture #1 Basic Concepts

Classical mechanics uses force to calculate trajectory $\vec{r}(t)$.

example - projectile motion, no friction.



$$\vec{F} = \frac{d}{dt}\vec{p} = -mg\hat{z} \quad \text{solve for } x(t), z(t)$$
$$\vec{r}(t) = \hat{x}\, x(t) + \hat{z}\, z(t)$$

In quantum mechanics (QM) we cannot determine a trajectory in principle. Quantum systems (eg. electron) subject to Heisenberg uncertainty principle which limits our knowledge of canonically conjugate variables such as x, p_x:

$$\Delta x \, \Delta p_x \gtrsim \hbar$$

$$\hbar c = 197 \text{ eV}\cdot\text{nm} = 197 \text{ MeV-fm}$$

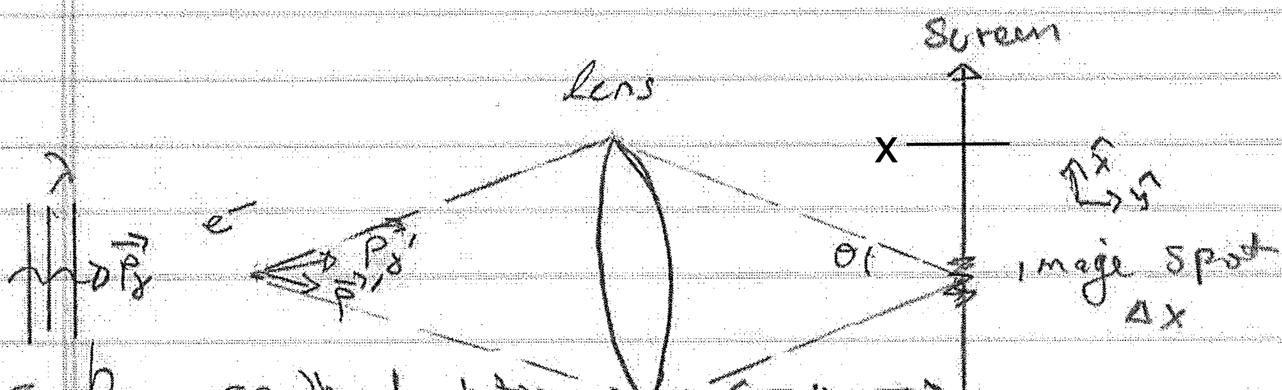
Bohr "complimentarity" - there is never an experimental conflict with the uncertainty principle.

Wave particle duality : QM object propagates as wave, interacts as particle.

de Broglie wavelength

$$\lambda = \frac{h}{p} \quad \text{(holds for relativistic } p\text{)}$$

uncertainty illustrated by Heisenberg microscope thought experiment, imaging electron



$P_\gamma = \frac{h}{\lambda}$ scattered photon imparts momentum $\vec{p}'$ to electron

p_x conserved

diameter of lens L, $\sin\theta \approx \tan\theta = \frac{X}{L}$

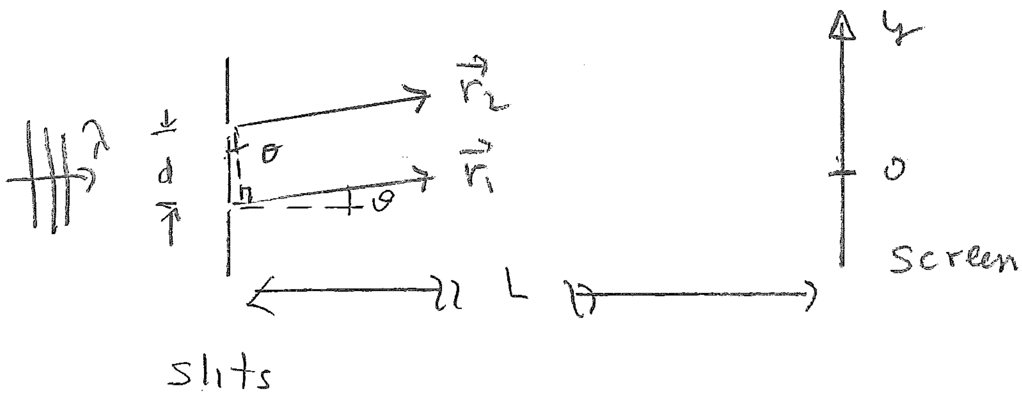
resolving power of lens $\Delta x \sim \frac{\lambda}{\sin\theta}$

uncertainty of position of e^- due to photon scattering

$$\Delta p_x \sim \left(\frac{h}{\lambda}\right)\sin\theta = h\left(\frac{1}{\Delta x \sin\theta}\right)\sin\theta$$

$$\boxed{\Delta x\, \Delta p_x \sim h}$$

Young's Double Slit

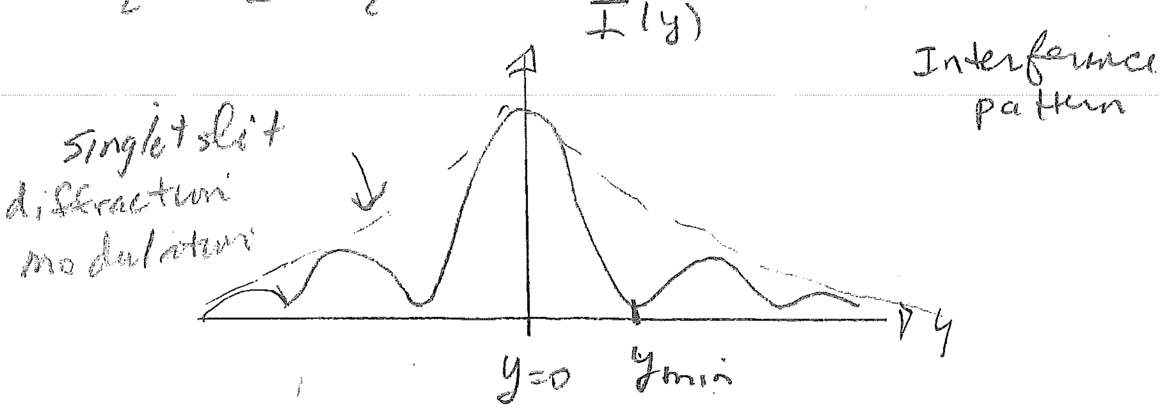


Huygen's principle: slits act as coherent source

path difference $\sin\theta\, d \equiv \Delta$; $\sin\theta \simeq \theta \simeq \tan\theta = \frac{y}{L}$

$r_1 \simeq L + \frac{1}{2}\Delta \qquad \Delta = \theta d = \frac{y}{L} d$

$r_2 \simeq L - \frac{1}{2}\Delta$



first minimum $\quad \Delta = \frac{\lambda}{2} = \theta d = \frac{y}{L} d$

$$y_{min} = \frac{L}{2}\left(\frac{\lambda}{d}\right)$$

3-0236 — 100 SHEETS — 5 SQUARES
3-0237 — 200 SHEETS — 5 SQUARES
3-0137 — 200 SHEETS — FILLER
COMET

Convenient to use complex amplitudes (since $L \gg d$ we ignore small differences in amplitudes, $|\vec{E}_1| \approx |\vec{E}_2| = E_0$)

$$E = \mathrm{Re}\, E_0\, e^{i(kr - \omega t)}$$

electric field amplitude

↑ real part

E_0 real

$$k = \frac{2\pi}{\lambda}\,;\ \omega = ck$$

$$E_1 + E_2 = E_0\, e^{-i\omega t}\, e^{ikL}\left(e^{ik\Delta/2} + e^{-ik\Delta/2}\right)$$

$$= 2E_0\, e^{i(kL - \omega t)} \cos\frac{k\Delta}{2}$$

Intensity on screen $I = |E_1 + E_2|^2$

$$= 4E_0^2 \cos^2\left(\frac{k\Delta}{2}\right)$$

$$\frac{k\Delta}{2} = \frac{2\pi}{\lambda}\left(\frac{1}{2}\right)\frac{y}{L}d = \frac{\pi}{\lambda}\frac{y}{L}d$$

first min $\quad \frac{k\Delta}{2} = \frac{\pi}{2} = \frac{\pi}{\lambda}\frac{y_{min}}{L}d$

$$y_{min} = \frac{L}{2}\left(\frac{\lambda}{d}\right)$$

EM wave is coherent superposition of photons, with

$$E = pc = hf = \frac{hc}{\lambda}$$

recall: ① black-body spectrum
② Photo-electric effect
Phy 330 ③ Compton scattering

EM energy, momentum quantized as photons
black-body spectrum due to photon gas in equilibrium at temperature T.

Photons are intrinsically relativistic. Begin Q.M. with nonrelativistic particles (e.g. electron)

Electron bound in atom is non-relativistic:

α is fine structure constant
$\alpha^{-1} = 137.036\ldots$

atomic scale given by <u>Bohr radius</u>

$$a_0 = \frac{\hbar}{mc\alpha} \qquad m = \text{electron mass}$$

$$mc^2 = 511 \text{ keV}$$

$$a_0 = \frac{\hbar c}{mc^2\alpha} \cong \frac{200 \text{ eV.nm}}{\frac{1}{2}\times 10^6 \text{ eV}}(137) = 4(1.37)\times 10^{2+2-6}$$

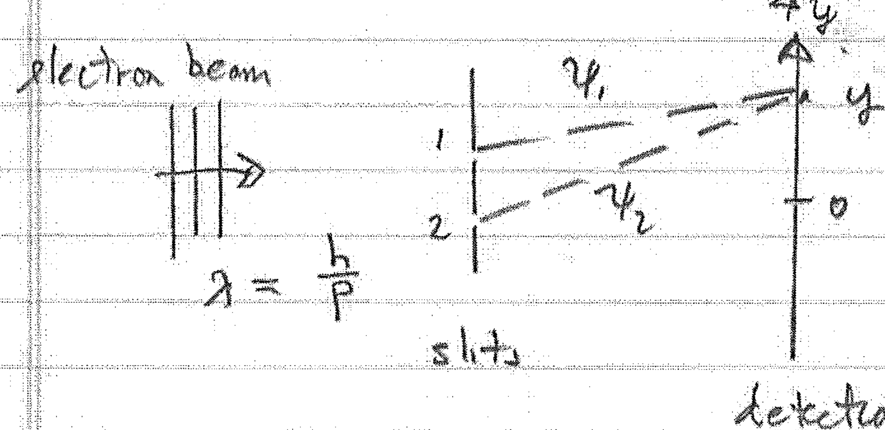
$$= 0.05 \text{ nm} = 0.5 \text{ Å} \quad (10^{-10} \text{ m})$$

from uncertainty relation

$$\Delta p \cong \frac{\hbar}{a_0} = mc\alpha = mc\beta\gamma$$

$$\frac{\beta}{\sqrt{1-\beta^2}} = \alpha \Rightarrow \frac{v}{c} = \alpha \quad \text{non-relativistic}$$

Interference of matter waves



ψ_i = amplitude to propagate from slit i to y

Probability to detect electron at y

$$P(y) = |\psi_1 + \psi_2|^2$$

Interference pattern develops as electrons are detected. In advance of detection, only probability is known.

Non-relativistic Schrödinger equation in 1D

$\psi(x,t)$ complex probability amplitude
"wave function"

$|\psi(x,t)|^2 dx$ probability to observe particle in interval $x, x+dx$ @ time t

Requirements for wave equation

① oscillatory solutions
② conserved propability
③ interference

plane wave $p = \hbar k$ $k = 2\pi/\lambda$
$E = \hbar\omega$ $\omega = 2\pi f$

$$\psi_k(x,t) = e^{i(kx-\omega t)}$$

constant phase condition $\frac{d}{dt}(kx - \omega t) = 0$

$$\frac{dx}{dt} = \frac{\omega}{k} = f\lambda$$ phase velocity
wave travels $+x$

to get ①,② equation must be first order in time

$$i\frac{\partial}{\partial t}\psi_k = -i^2\omega\psi_k = \omega\left(-\frac{1}{k^2}\right)\frac{\partial^2\psi_k}{\partial x^2}$$

$$i\frac{\partial}{\partial t}\psi_k = -\frac{\omega}{k^2}\frac{\partial^2\psi}{\partial x^2}$$

non-relativistic energy $\hbar\omega = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$

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

notation $i\ \frac{\partial\psi}{\partial t} \equiv \dot{\psi} \qquad \frac{\partial\psi}{\partial x} \equiv \psi'$

give each term dimention energy × ψ

$$i\hbar\dot{\psi} = -\frac{\hbar^2}{2m}\psi'' \quad \text{free particle equation}$$

<u>Eigenvalue equation</u>.

operator $\hat{\theta}$ takes function → another function

$$\hat{\theta}\psi = \theta\psi$$

← eigenfunction

θ eigenvalue

same

for $\psi_k = \exp(+i(kx-\omega t))$

$$\hat{\theta} = i\hbar\frac{\partial}{\partial t} \rightarrow \theta = \hbar\omega = E \quad \text{energy}$$

$$\hat{\theta} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \rightarrow \theta = \frac{\hbar^2 k^2}{2m} = \frac{p^2}{2m} \quad \text{kinetic energy}$$

In QM, all observables are real eigenvalues.
Operators having real eigenvalues are called "hermitian"

To add interaction to equation, we require potential energy.

$$F_x = -\frac{\partial}{\partial x} V(x)$$

Schrödinger is then:

$$i\hbar \dot{\psi} = -\frac{\hbar^2}{2m} \psi'' + V(x)\,\psi$$

Dependence on potential has surprising physical consequences.

<u>Hamiltonian</u> (energy operator)

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)$$

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\,\psi$$

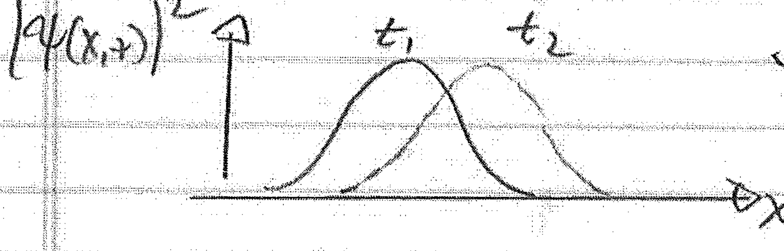
eigenfunctions of $\hat{H}$ energy eigenstates

$$\hat{H}\,\psi_E(x,t) = E\,\psi_E(x,t)$$

<u>Probability current</u>

normalizability

$$\int_{-\infty}^{\infty} |\psi|^2 dx = \text{const} \equiv 1$$



probability flow is conserved in Non relativistic QM

probability density $\rho(x,t) = |\psi(x,t)|^2 = \psi^*\psi$
P.D.F. probability density function

$\rho(x,t)\,\Delta x$ is probability to find particle $x,\ x+\Delta x$

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

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

Subtract, $V(x)$ assumed <u>real</u>

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

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

probability current density

$$j_x(x,t) \equiv \frac{\hbar}{2mi}\left(\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right)$$

$$= \frac{\hbar}{m}\,\mathrm{Im}\left(\psi^*\frac{\partial\psi}{\partial x}\right)$$

We have

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

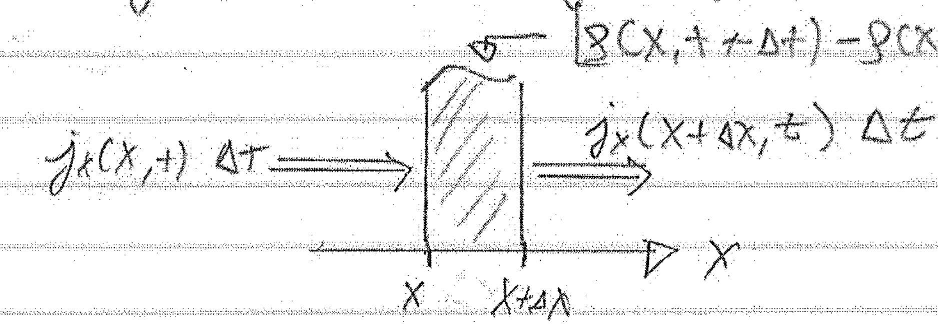
or $$\frac{\partial}{\partial t}\rho(x,t) + \frac{\partial}{\partial x} j_x(x,t) = 0$$

probability is conserved. Integrate to get

$$\frac{\partial}{\partial t}\int_{-\infty}^{+\infty} \rho(x,t)\, dt = j_x(x,t)\Big|_{-\infty}^{+\infty} = 0$$

if $\psi(x \to \pm\infty, t) = 0$

Schematically, in interval Δx, ρ changes due to flow in & out of region in time Δt



$$\left[\rho(x,t+\Delta t) - \rho(x,t)\right]\Delta x = -\left[j_x(x+\Delta x,t) - j_x(x,t)\right]\Delta t$$

$$\frac{\rho(x,t+\Delta t) - \rho(x,t)}{\Delta t} = -\frac{\left[j_x(x+\Delta x,t) - j_x(x,t)\right]}{\Delta x}$$

in limit
$\Delta x \to 0$
$\Delta t \to 0$

$$\frac{\partial \rho(x,t)}{\partial t} = -\frac{\partial}{\partial x} j_x(x,t)$$