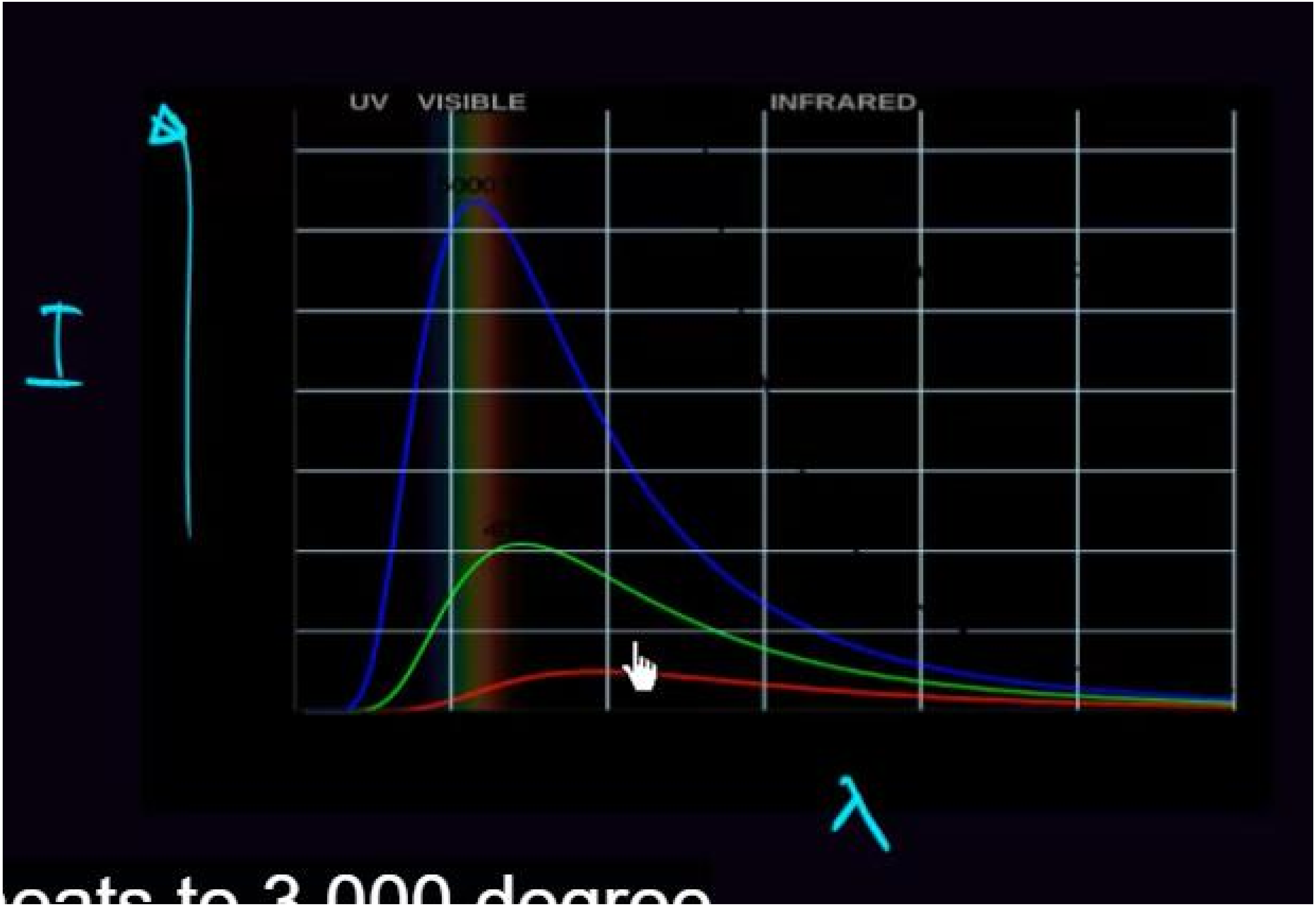
The Schrödinger Equation

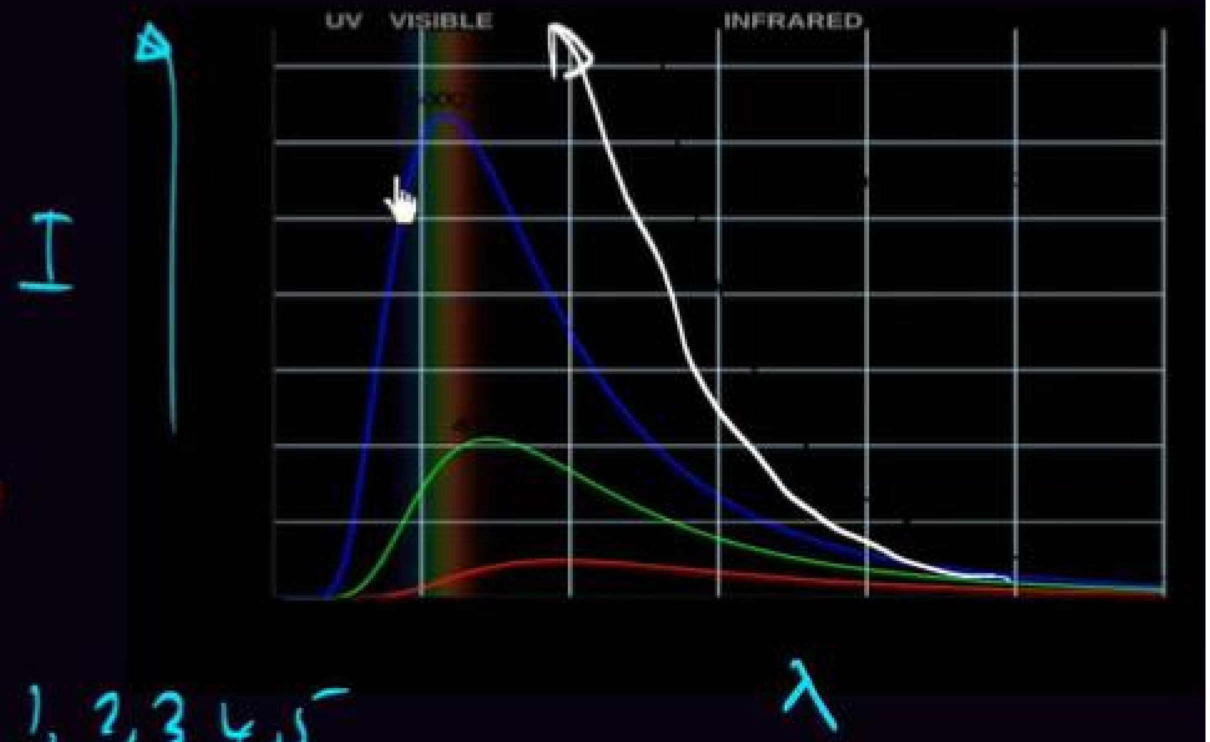
$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi = E\Psi$$


UV
VISIBLE
INFRARED
I
λ

$\Delta E = nh\nu$

frequency

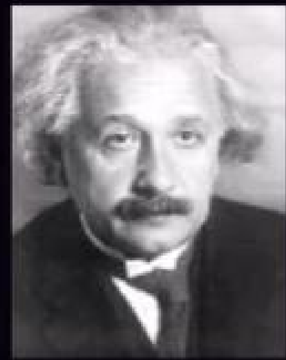
Plancks Constant

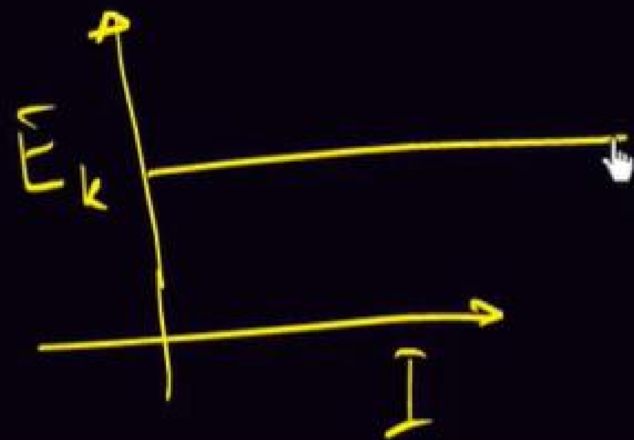


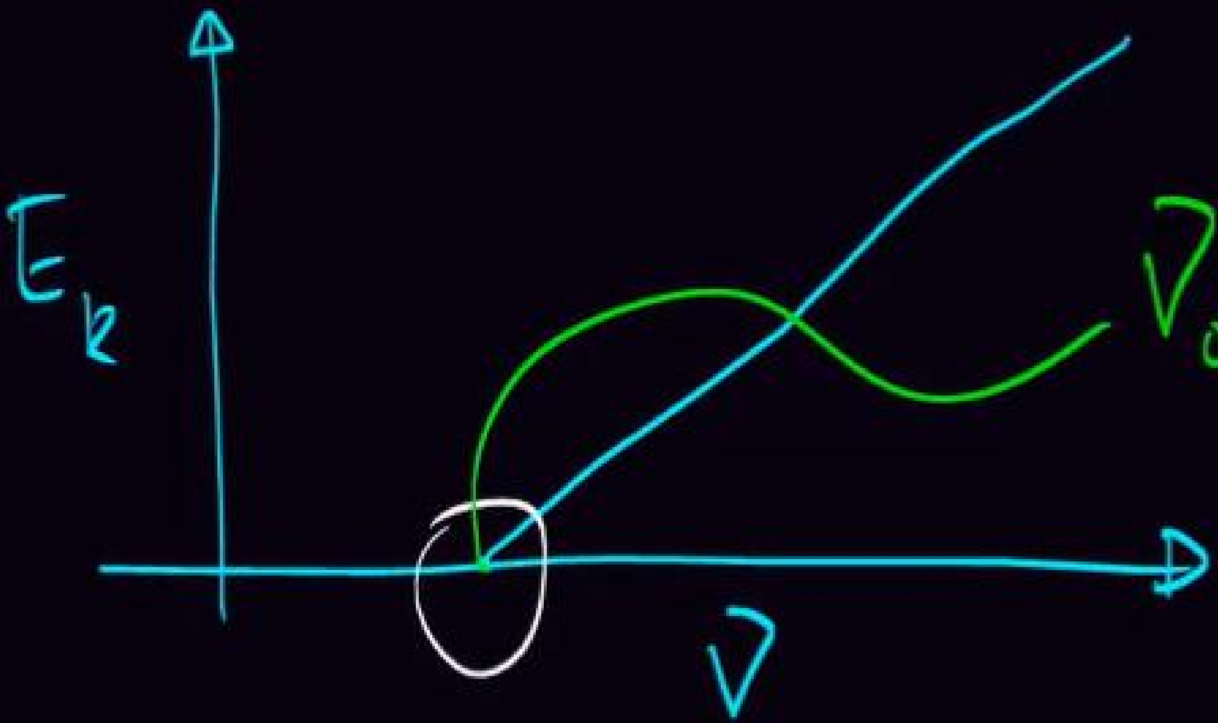
$n = 1, 2, 3, 4, 5$

Wave Particle Duality of Energy - Explanation of the Photoelectric Effect

$$\Delta E = h\nu$$







ν_0 – threshold frequency

$h\nu_0 = \Phi$

$E = h\nu$

$$h\nu = \Phi + E_k$$

$$E_k = h\nu - \Phi$$

$$E = h\nu = \frac{hc}{\lambda} \quad ; \quad E = mc^2$$

$$\frac{h\cancel{c}}{\lambda} = m\cancel{c}^{\,c}{}^2 \quad ; \quad \frac{h}{\lambda} = mc$$

momentum

What is the kinetic energy (J) of electrons emitted from K metal (threshold energy = 2.25eV) using incident radiation of (a) 3.5 eV and (b) 2.2 eV

(a) $h\nu = \Phi + E_k$

$E_k = h\nu - \Phi$

$E_k = (3.5\,eV - 2.25\,eV) = 1.25\,eV$

$= 1.25 \times 1.602 \times 10^{-19}\,J = \boxed{2.0 \times 10^{-19}\,J}$

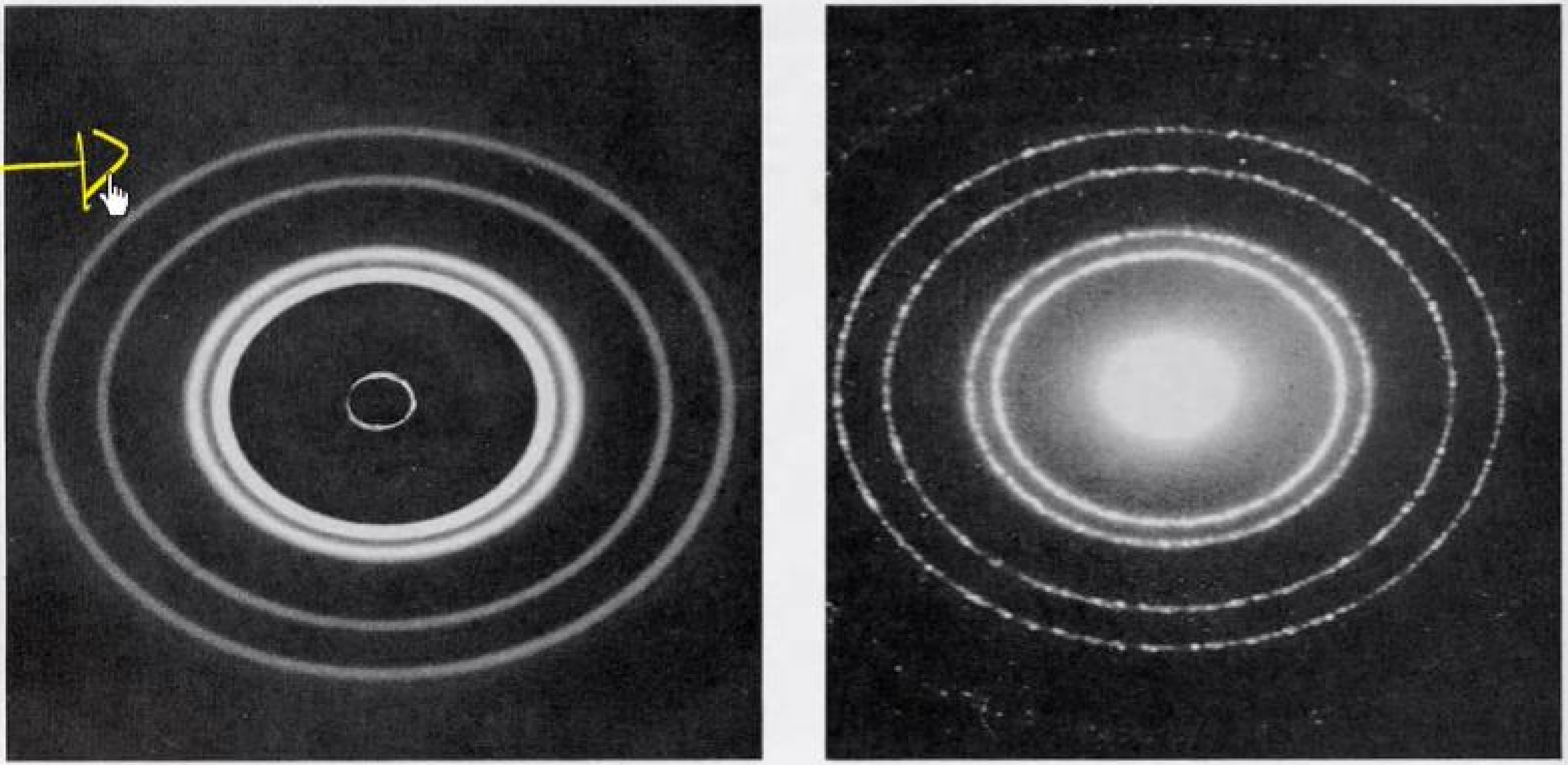
de Broglie's Postulate

$$mc = \frac{h}{\lambda} \quad ; \quad mv = \frac{h}{\lambda}$$

$$p = \frac{h}{\lambda} \quad \text{or} \quad \lambda = \frac{h}{p}$$

de Broglie

The diffraction pattern on the left was made by a beam of x rays passing through thin aluminum foil. The diffraction pattern on the right was made by a beam of electrons passing through the same foil.



Tennis ball — mass 57 g — velocity

80 km h^{-1}. What is λ?

$$\lambda = \frac{h}{mv} = \frac{6.626 \times 10^{-34}\ \text{J s}}{57 \times 10^{-3}\ \text{kg} \times \frac{80 \times 10^{3}}{60 \times 60}\ \text{m s}^{-1}}$$

$$= \boxed{5.2 \times 10^{-34}\ \text{m}}$$

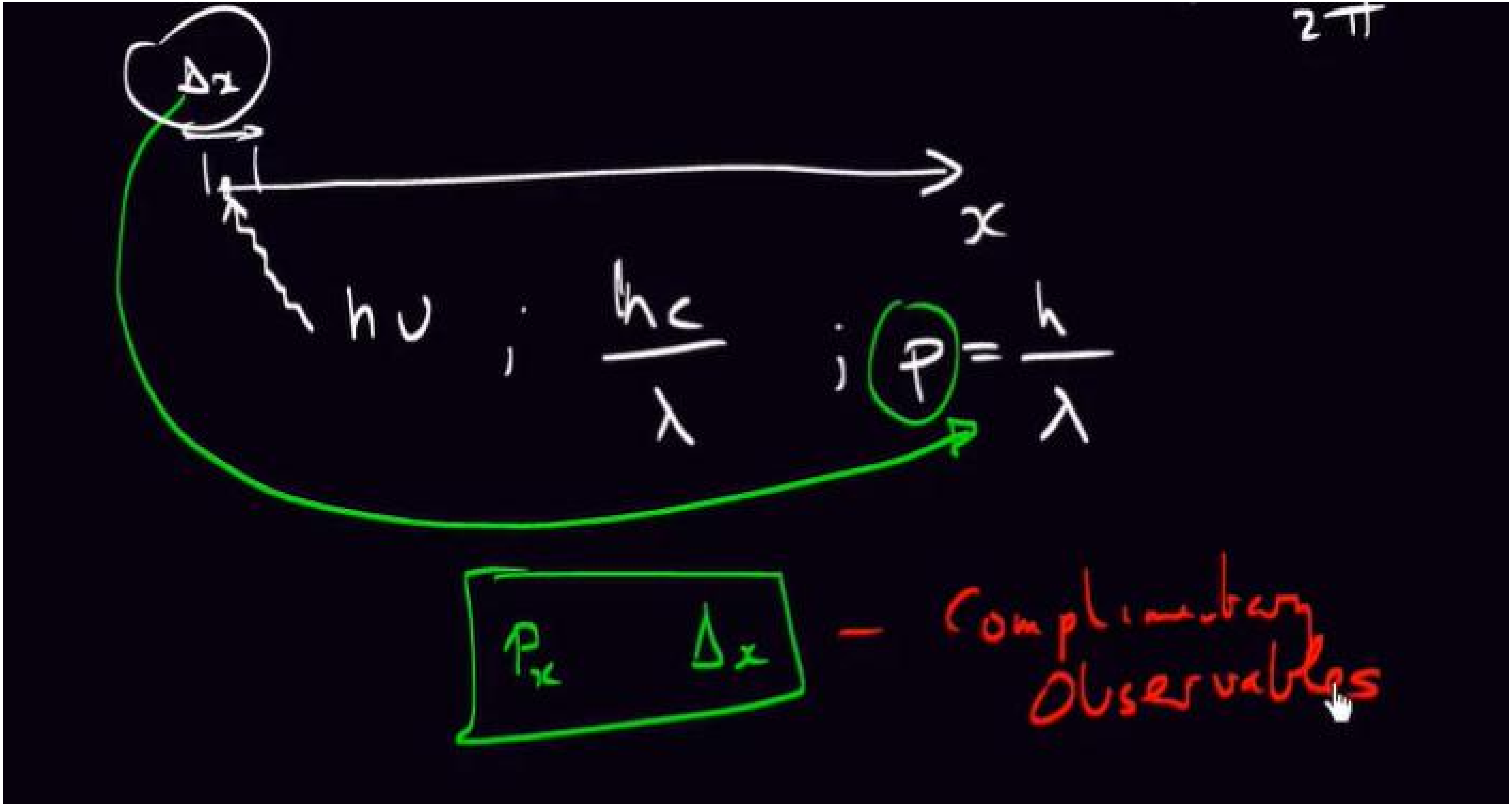
Electron — velocity $\longrightarrow$ $1.0 \times 10^{7}\ m\,s^{-1}$

What is λ?

$$\lambda = \frac{h}{mv} = \frac{6.626 \times 10^{-34}\ Js}{9.11 \times 10^{-31}\ kg \times 1.0 \times 10^{7}\ m\,s^{-1}} = 7.3 \times 10^{-11}\ m$$

$$= 0.73 \times 10^{-10}\ m$$

$$\boxed{= 0.73\ \mathring{A}}$$


2π
Δx
x
hν ; hc/λ ; p = h/λ
P_x Δx
— Complimentary Observables

$$\boxed{p_x \quad \Delta x}$$ – complimentary observables

$$\Delta x \simeq \lambda \quad ; \quad \Delta p_x \simeq \frac{h}{\lambda}$$

$$\boxed{\Delta x \cdot \Delta p_x = h}$$

Heisenberg's Uncertainty Principle

"Impossible to know simultaneously both the position and the momentum of a particle with certainty"

$$\Delta x \cdot \Delta p_x \geq \frac{h}{4\pi}$$

$$\geq \frac{\hbar}{2}$$

$$\hbar = \frac{h}{2\pi}$$

$\times\ \psi(x)$

wavefunction

$$\boxed{\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V\right)}\psi(x) = E\psi(x)$$

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V\psi(x) = E\psi(x)}$$

Schrödingers Eqn. in 1-D.

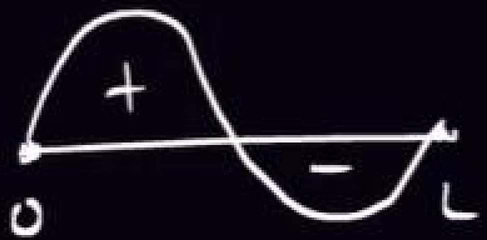
Hamiltonian $\equiv \hat{H}$

$$\hat{H}\psi(x) = E\psi(x)$$

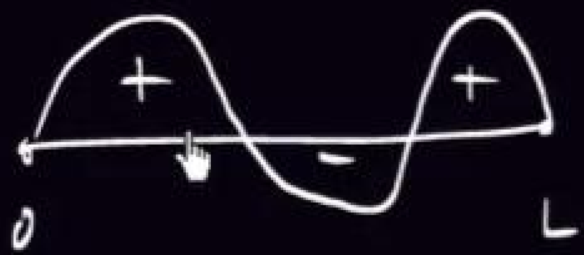
$$-\frac{\hbar^2}{2m}\underbrace{\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)}_{\nabla^2}\Psi(x,y,z)+V\Psi(x,y\,z)=E\Psi(x,y,z)$$

$$\boxed{-\frac{\hbar^2}{2m}\nabla^2\Psi+V\Psi=E\Psi}$$

$$\psi(x) = A \sin\left(\frac{\pi x}{L}\right) \quad n = 1$$



$$\psi(x) = A \sin\left(\frac{2\pi x}{L}\right) \quad n = 2$$

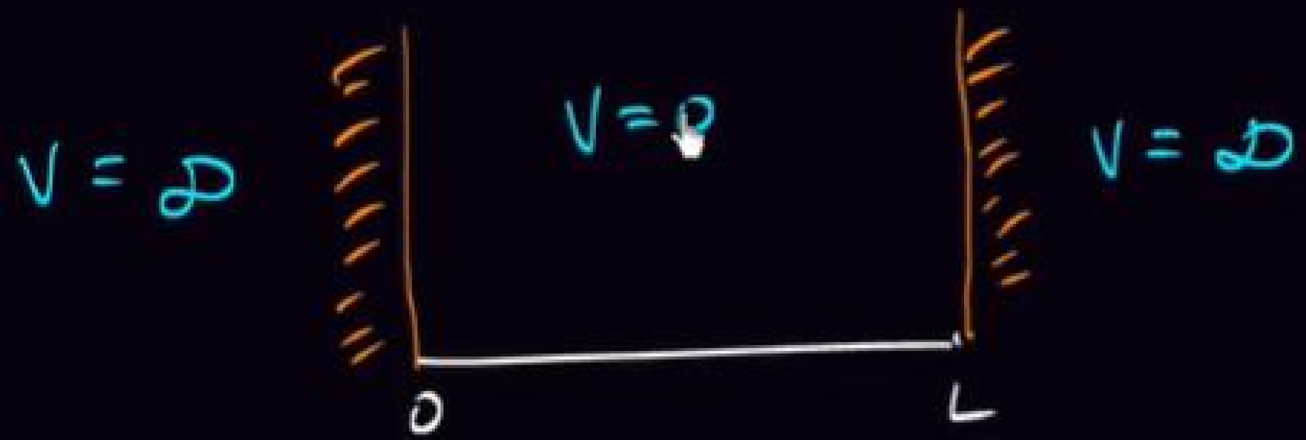


$$\psi(x) = A \sin\left(\frac{3\pi x}{L}\right) \quad n = 3$$

$\psi(x) = 0$ at $x = 0$ and $x = L$

Boundary

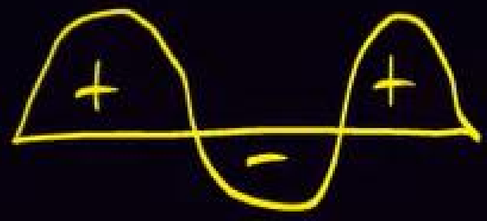
Particle in a box



$$\boxed{\frac{d^2}{dx^2}\psi(x) = -\left(\frac{2\pi}{\lambda}\right)^2\psi(x)}$$

$$\psi(x) = A\sin\frac{2\pi x}{\lambda} + B\cos\frac{2\pi x}{\lambda}$$

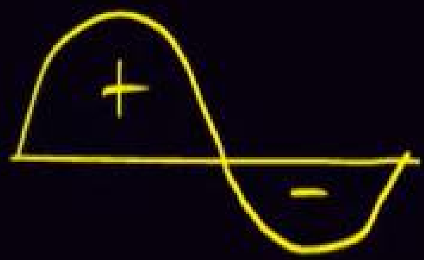
$$E_3 = \frac{9h^2}{8mL^2}$$



$$\psi_3 = A\sin\left(\frac{3\pi x}{L}\right)$$

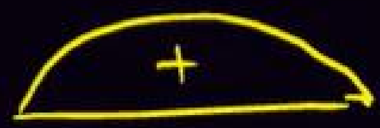
E

$$E_2 = \frac{4h^2}{8mL^2}$$



$$\psi_2 = A\sin\left(\frac{2\pi x}{L}\right)$$

$$E_1 = \frac{h^2}{8mL^2}$$



$$\psi_1 = A\sin\left(\frac{\pi x}{L}\right)$$

Interpreting the Wavefunction

Max Born

$\Psi^2 \longrightarrow$ probability density

Interpreting the Wavefunction

Max Born

$\Psi^2 \longrightarrow$ probability density

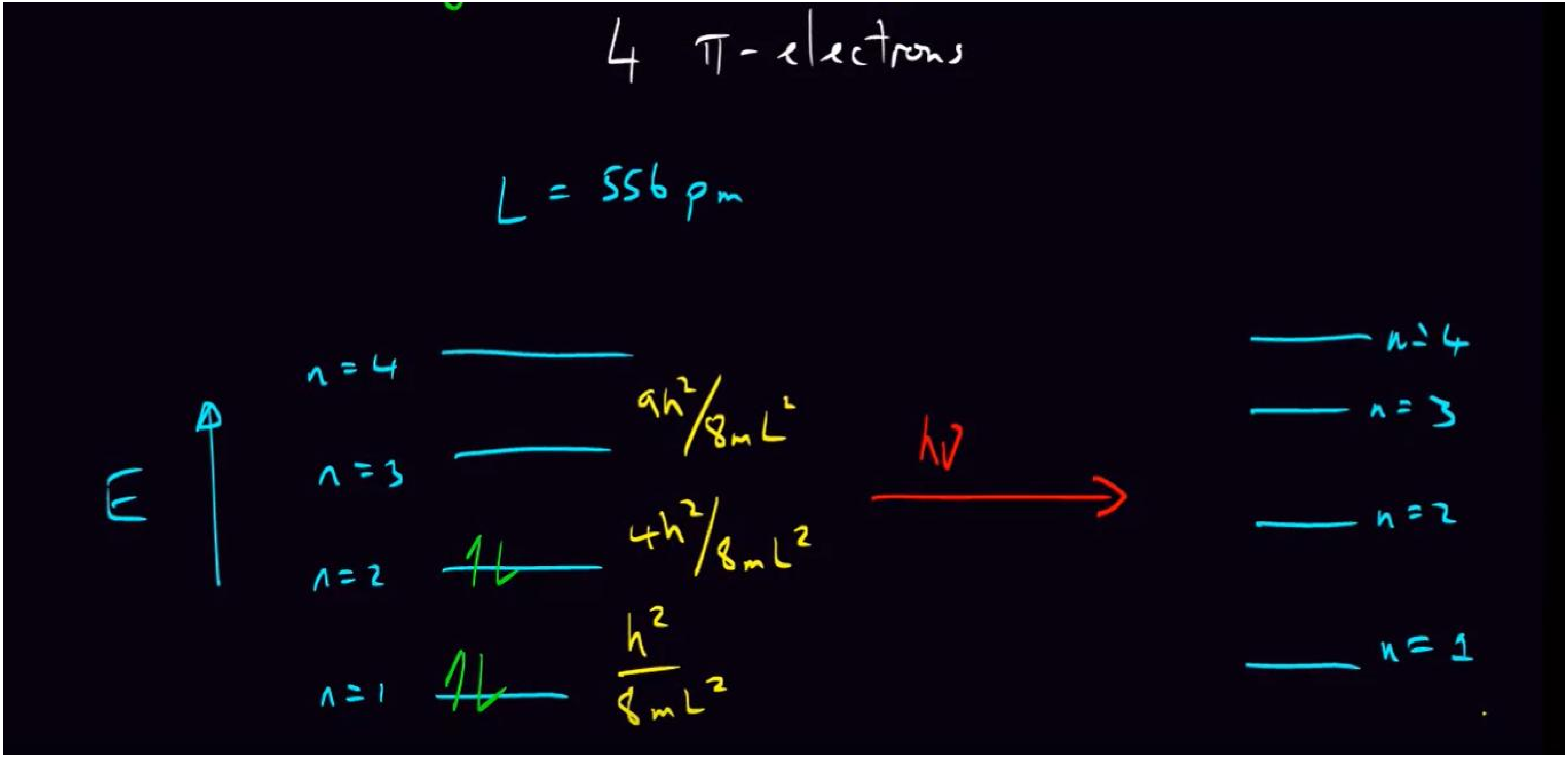
$\Psi^2 dx \longrightarrow$ probability

$x + dx$

$$\frac{A^2 L}{2} = 1$$

$$A = \sqrt{\frac{2}{L}} \quad \text{or} \quad \left(\frac{2}{L}\right)^{1/2}$$

Normalised wave function is $\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$


4 π - electrons
L = 556 pm
E
n = 4
n = 3
n = 2
n = 1
9h²/8mL²
4h²/8mL²
h²/8mL²
hν
n = 4
n = 3
n = 2
n = 1