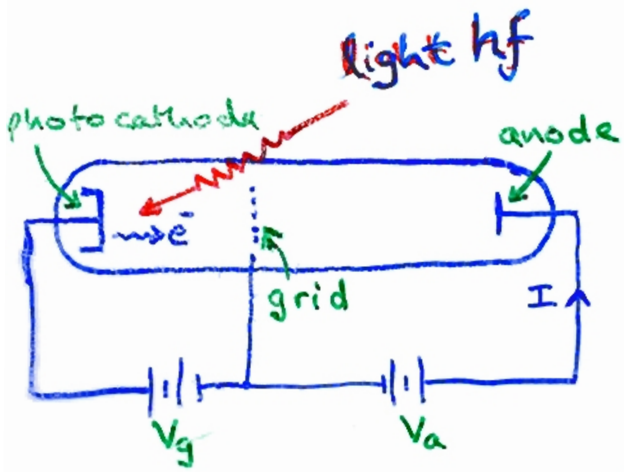
Quantum Mechanics

- **Accept that electrons can be particles or waves**
- **What happens when an electron is confined or bound**
- **Simple calculation of quantisation**
- **Tunnelling by wavelike electron**
- **Determination of band-gap from wave picture**
- **Concept of 'effective' mass**
- **Direct & Indirect band-gap**

Quantum Mechanical Effects

Early experiments on black body radiation could not be explained by classical theory. Max Planck showed that energy could only be absorbed or emitted by black body in discrete amounts (called quanta or photons).

Light as a particle: Photoelectric effect (*JA – pg. 2-7*)



Electrons emitted by photocathode only in hf> certain energy, depending on the grid voltage. Intensity does not matter! –unlike classical theory.

Energy = $\hbar\omega = hf$

ω = angular frequency

f = frequency

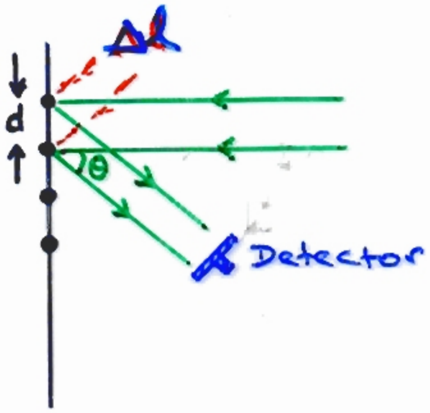
h = Planck's constant($\hbar = h/2\pi$)

$hf \geq e\phi_w$

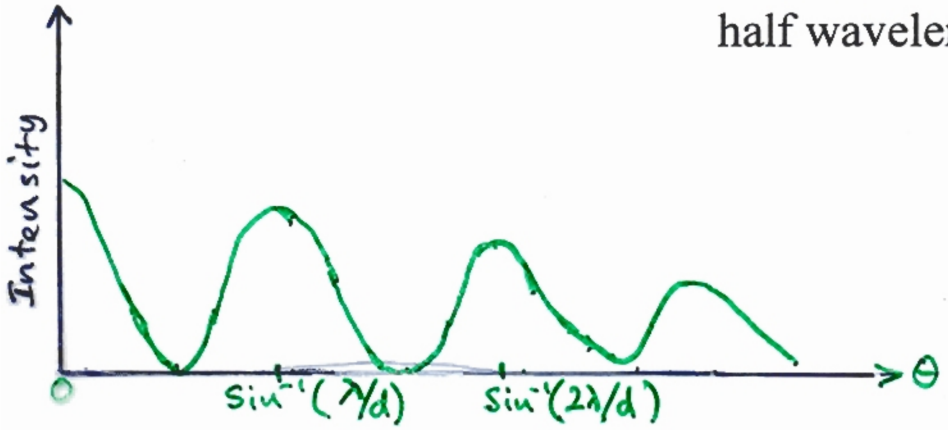
ϕ_w is the work function – minimum energy required to extract an electron from photocathode. Any extra energy results in increased kinetic energy (speed) of emitted electron. The kinetic energy of the electron can be measured by increasing the grid voltage until no current flows.

$$hf = e\phi_w + eV_{stop}$$

Light as a wave: Should demonstrate phenomena like diffraction



Constructive interference between waves when
$\Delta l = d.\sin(\theta) = n\lambda$
bright fringe when n = integer
Destructive interference when Δl = odd number of half wavelengths



Light therefore can exhibit particle-like or wave-like behaviour – dual nature of light.

Wave Particle Duality

Photon energy, $E = hf$ Speed of light, $c = f\lambda$

If the photon energy E is transported at velocity 'c', its momentum $p = E/c$

Proof: dx F

←

External force F acts on photon over distance dx, such that there is a change in photon energy, dE

$dE = Fdx$

$F = dp/dt$ (Newton)

$dE = (dp/dt).dx = c.\ dp$ (since $dx/dt = c$)

Integrating, $p = E/c$

$$\boxed{p = \frac{E}{c} = \frac{E}{f\lambda} = \frac{hf}{f\lambda} = \frac{h}{\lambda}}$$

(de Broglie): **Photons (or any particles) with momentum p have an associated wavelength λ**

example 1: Apple (mass = 0.2kg) falls on ground with velocity 10m/s.
momentum $p = mv = 0.2 \times 10 = 2$kgm/s
associated $\lambda = h/p = 6.6 \times 10^{-34}/2 = 3.3 \times 10^{-34}$ m -this is a very, very short wavelength – impossible to measure, so treat as particle.

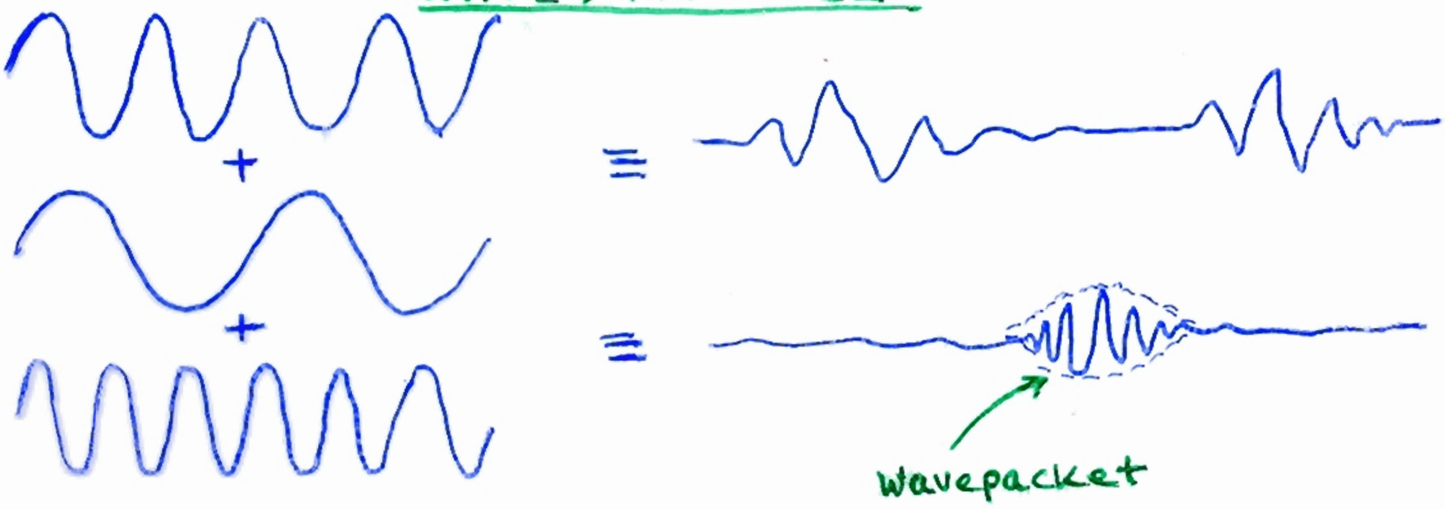
example 2: electron is accelerated through 100V.
Gain in K.E. = loss in P.E.

$$\tfrac{1}{2} mv^2 = eV$$

$$v = (2eV/m)^{1/2}$$

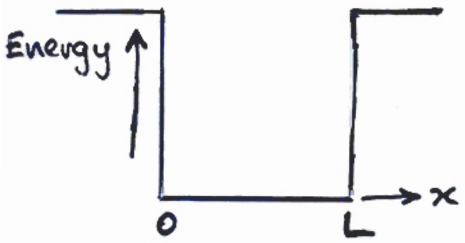
momentum $p = mv = (2eVm)^{1/2}$
associated $\lambda = h/p = h(2eVm)^{-1/2} = 1.225\ V^{-1/2}$ nm
For 100V, $\lambda = 0.12$nm -this is measurable and useful (electron microscopes).

WAVE / PARTICLE

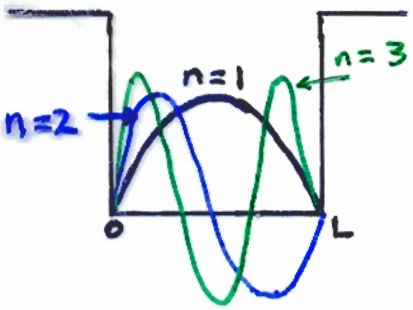


We can get region of constructive interference. Wavepacket has wave like properties, but also acts like a particle – it is localised in space.

Bound Particles – electron in a well



Assume that electron is bound by the well, i.e. it exists only within the well. Classical theory states that electron can have *any* energy within well.



As a wave however, only certain wavelengths (λ) are possible – those that fit between 0 and L. *

$n\lambda/2 = L$ satisfies this requirement.

i.e. a whole number of ½ wavelengths must fit in the well.

$\lambda = 2L/n$, $E = p^2/2m = h^2/2m\lambda^2$

$E = \frac{1}{2}mv^2$
$= \frac{1\, m^2v^2}{2m}$

Substitute for λ,

$$E_n = \frac{n^2h^2}{8mL^2} \qquad n = 1,2,3....$$

i.e. electrons surprisingly can only take up values given by E_n above - called **quantisation**. In most everyday cases, L is large (mm or larger).

Example: electron confined between two atoms in a crystal, L = 1nm

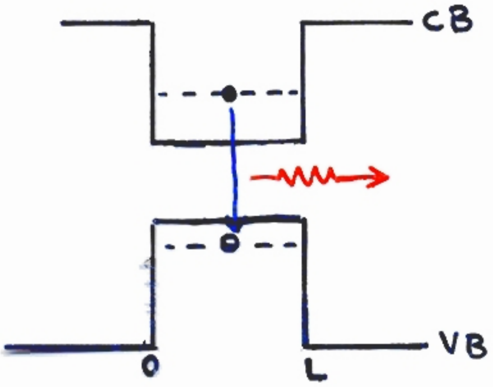
* This is a highly simplified treatment. A more rigorous treatment involves the solution of the Schrödinger's time independent equation.

$$E_n = \frac{n^2h^2}{8mL^2}$$

Let n=1,

$$E = \frac{\left(6.6\text{x}10^{-34}\right)^2}{8\text{x}9.1\text{x}10^{-31}\text{x}\left(10^{-9}\right)^2} = 6.02\text{x}10^{-20}\,\text{J} = 0.38\text{eV}$$

this is substantial on an atomic scale.



Use in QW laser
Same quantisation effect for holes – just different effective mass

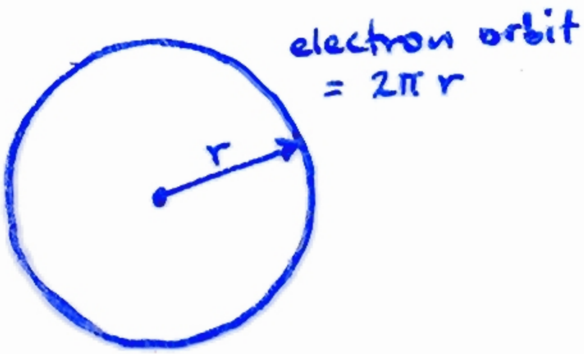
$m_e^* \approx 0.06\, m_o$

$m_h^* \approx 0.5\, m_o$

m_o = electron rest mass

If L = 1mm, energy levels are 10^{12} smaller – effectively continuous.

Bohr model for hydrogen atom



For the electron orbit to be stable, the electron wave must fit into 2πr, i.e. the electron must come back on

Calculation of electron energy levels

Equate centrifugal force $\frac{mv^2}{r}$

$= $ coulomb force $q^2/4\pi\varepsilon_0 r^2$

$p = h/\lambda$ (de Broglie)

$= \frac{hn}{2\pi r}$ $\quad$ ($2\pi r = n\lambda$ for stable orbit)

$$\frac{mv^2}{r} = \frac{p^2}{mr} = \frac{q^2}{4\pi\varepsilon_0 r^2} \quad \text{—— } ①$$

$$\frac{p^2}{mr} = \frac{h^2 n^2}{4\pi^2 r^3 m} = \frac{q^2}{4\pi\varepsilon_0 r^2} \quad \text{(substitute for } p\text{)}$$

$$\therefore \; r = \frac{\varepsilon_0 h^2 n^2}{\pi q^2 m}$$

$$\text{Energy } E_n = \frac{1}{2}mv^2 = \frac{q^2}{8\pi\varepsilon_0 r} \quad \text{(from ①)}$$

substitute for r

$$E_n = \frac{q^2}{8\pi\varepsilon_0 \cancel{r}} \cdot \frac{\pi q^2 m}{\varepsilon_0 h^2 n^2} = \frac{q^4 m}{8\varepsilon_0^2 h^2 n^2}$$

$$= -\frac{13.6}{n^2} \text{ eV}$$

(Derivation not required for examinations) itself "in-phase" otherwise get destructive interference. i.e. $n\lambda = 2\pi r$

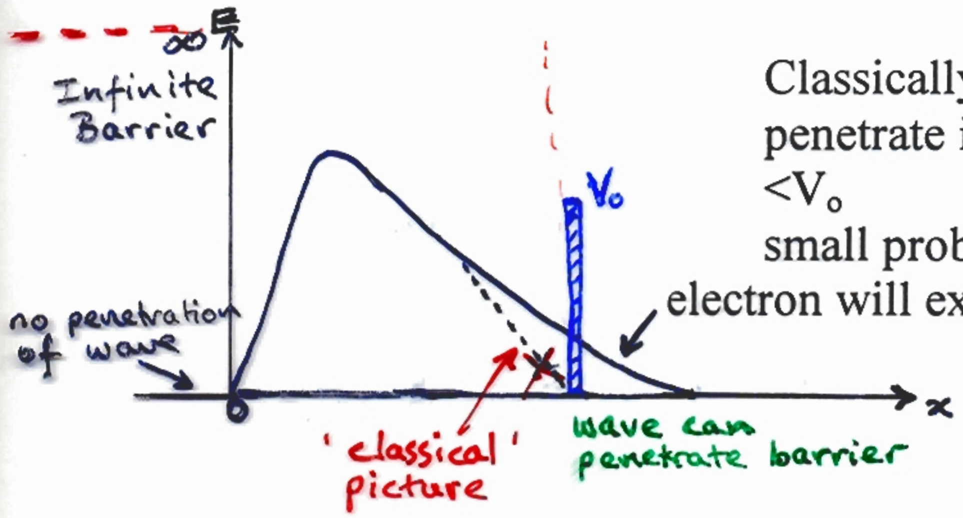
Centrifugal force = mv^2/r = coulomb force = $e^2/4\pi\varepsilon_o r^2$

Calculate the electron energy as a sum of PE & KE, substituting for v and r, to get (*see JA-pg. 8-10 for details*);

$$E_n = -\frac{e^4 m}{8h^2\varepsilon_o^2 n^2} = -\frac{13.6}{n^2}\,\text{eV} \qquad \text{as quoted earlier}$$

Tunnelling

The wave picture of an electron gives an explanation of tunnelling – important for modern devices.
Only infinitely high and infinitely thick barriers (as assumed in 'particle in well' example) can stop an electron wave. Otherwise the electron can have a probability of tunnelling through a thin, finite height barrier.
e.g. consider a particle in a well but with one side having a finite, thin barrier.

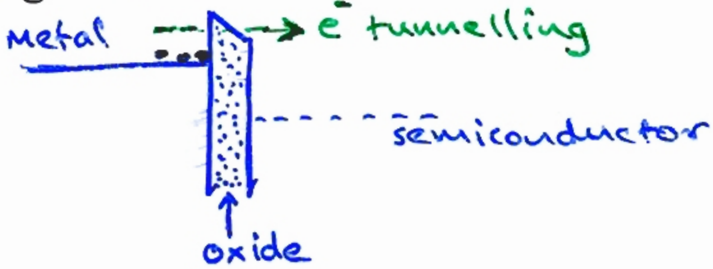


Classically, electron will not penetrate if electron energy $< V_o$

small probability that electron will exist here

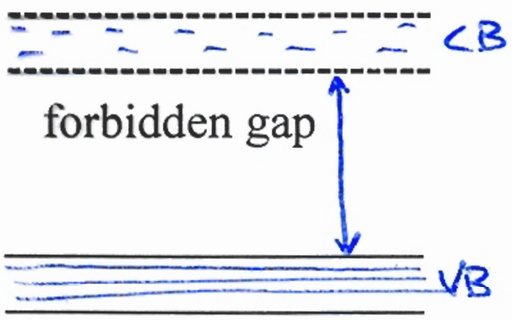
Amplitude of the wave describing the electron relates to the probability of finding the electron at that point.

Practical examples of tunnelling:
Zener diode – see later
MOSFET – oxide between the gate and channel is very thin for modern devices as miniaturisation proceeds, resulting in tunnel leakage current.



Wave Picture of Forbidden Bandgaps in Semiconductors

Before we saw that electrons were 'not allowed' in the forbidden gap between the V.B. and C.B.



How does this arise?

Consider an electron in a vacuum
$E = ½mv^2 = p^2/2m$ (since momentum $p = mv$)