Quantum Physics PY1T20/PYU11P20

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Lecture 3: Particles as waves and the wavefunction

- Aims of this lecture
- Understand that particles, such as electrons or photons, can also show wave behaviour.
- Understand that this wave behaviour has a wavelength, the de Broglie wavelength.
- Understand that these wave-like behaviours lead to discrete energies.
- See how quantum mechanics describes a particle moving in one-dimension, with a particular momentum and a particular energy.

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Wave properties of particles

Recall, relativity shows photon has energy $E = pc$
and the photoelectric relates this to light-wave frequency $= hf$

So, since $c = f\lambda$, $p = h/\lambda$

de Broglie (1924) suggested that this relation is general:

any particle which has momentum p has an associated wavelength $\lambda = h/p = \frac{h}{mv}$

where m is relativistic mass. $m \approx m_0$ at non-relativistic speed.

Direct Experimental evidence (for things other than photons)??

N.B. $h = 6.6 \times 10^{-34} Js$ *so significance is for SMALL & LIGHT objects.*

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Davisson & Germer Experiment

"Diffraction of Electrons by a Crystal of Nickel"
The Physical Review 1927

"The investigation reported in this paper was begun as the result of an accident which occurred in this laboratory in April 1925….."

D & G had been working on electron scattering (1921) from polycrystalline nickel: during the accident the target became oxidised. After removing the oxide by heating, the scattering was dramatically altered :

The target was now more crystalline:
electrons were diffracted by the crystal, just like x-rays!

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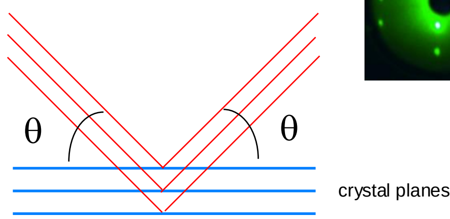
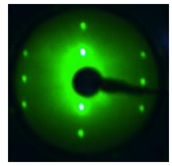
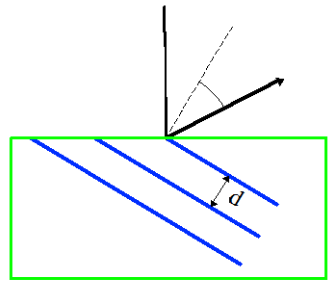
Davisson & Germer Experiment: Analysis

just like x-rays…







$$2d\sin\theta = n\lambda$$

θ : angle with planes
d : plane separation
(Bragg)

(planes drawn in blue)
electron energy $KE = 54$ eV
normal incidence
enhanced reflectivity at 50˚
to find θ bisect 50˚ (⇒25˚)
$\theta = 90˚ - 25˚ = 65˚$

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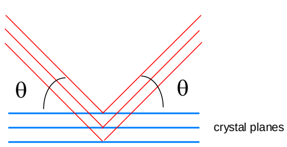
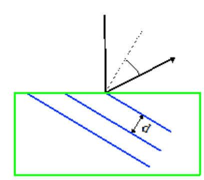
Davisson & Germer Experiment: Analysis



$$2d\sin\theta = n\lambda$$
$$\theta = 65^\circ$$

$$\lambda = h/p$$



Find p from kinetic energy, 54 eV (*<< 0.51 MeV (= m_oc^2) so non-relativistic)*

$KE = m_o v^2/2 = (m_o v)^2/2m_o$ so $p = m_o v = \sqrt{2m_0 KE}$

$$\lambda = \frac{h}{m_0 v} = \frac{h}{\sqrt{2m_0 KE}}$$

$$\lambda = \frac{6.63\times10^{-34}\,\text{Js}}{\sqrt{2\times(9.11\times10^{-31}\,\text{kg})(54\,\text{eV})(1.60\text{x}10^{-19}\,\text{J/eV})}} = \boxed{0.166\text{nm}}$$

(n=1)

$$\lambda = 2d\sin 65^\circ = 2(0.091\,\text{nm})(0.906) = \boxed{0.165\text{nm}}$$

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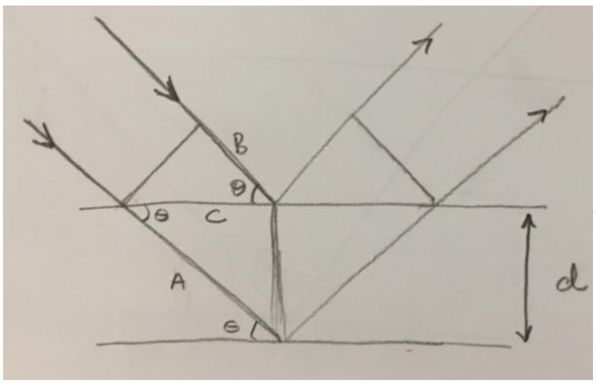
Bragg Condition Derivation

Physics of the Bragg condition is same as the double slit, but the geometry is a bit more involved.

Consider rays reflected from two successive planes of atoms separated by distance d.



Path difference between rays = $2(A-B)$

A is easy $A = \frac{d}{sin\theta}$

To get B note that $C = \frac{d}{\tan\theta}$ and then use this in :

$$B = C\cos\theta = \frac{d}{\tan\theta}\cos\theta = \frac{dcos\theta}{sin\theta}cos\theta = \frac{d\cos^2\theta}{\sin\theta}$$

Path difference = $2\left(\frac{d}{\sin\theta} - \frac{d\cos^2\theta}{sin\theta}\right) = 2d\sin\theta$

Constructive interference if (path difference)= $n\lambda$, n=1, 2, 3,...

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Conclude

- Particles like electrons can behave as waves too.
- Specifically ones with wavelength related to momentum by $p = h/\lambda$
- Diffraction becomes significant if λ is comparable to aperture sizes.
- Q. what if a particle or a wave is confined, e.g. in a ‘box’?

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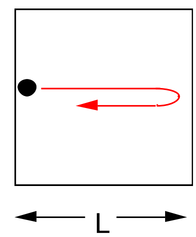
Particle in a Box

"confinement of quantum particle implies energy quantisation"

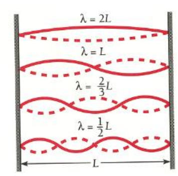
Particle in a box, making elastic collisions with rigid walls.
Cannot go outside box
Has a kinetic energy KE *(& zero potential energy change in box, i.e. V(x)=const.=0)*



Total energy *(non-relativistic)*

$$E = KE = \tfrac{1}{2} m_o v^2 = \frac{(m_o v)^2}{2 m_o} = \frac{(h/\lambda)^2}{2 m_o} = \frac{h^2}{2 m_o \lambda^2}$$

OK for particle, just bounces between walls.



What if it's a wave?
Means standing waves in box – nodes at walls
c.f. Guitar strings, Waves in cup, etc…

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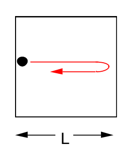
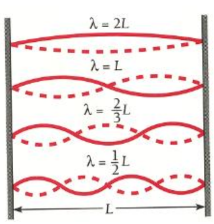
Particle in a Box *(cont.)*



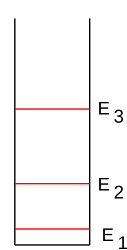


$\lambda_1 = 2L/1$
$\lambda_2 = 2L/2$
$\lambda_3 = 2L/3$
$\lambda_4 = 2L/4$

$$\boxed{\lambda_n = 2L/n}$$

Where n = 1, 2, 3, ….

$$E_n = \frac{p^2}{2m_0} = \frac{h^2}{2m_0\lambda_n^2} = \frac{h^2}{2m_0(2L/n)^2} = \frac{n^2h^2}{8m_0L^2}$$



E_n: "quantized" energy level.
n is the "quantum number"

$E \neq 0$ *(since n=0 implies infinite λ, cannot fit in box)*

So <u>lowest</u> energy level is E_1 *called* "the ground state"

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Conclude:

Confining a wave restricts possible wavelengths

⇒ only certain λ and hence Energies allowed!

Wider implication:

Confining a wave (particle) restricts possible states

e.g. Diffraction – possible directions affected by spacing d
Energy levels in atoms (later)
and much else….

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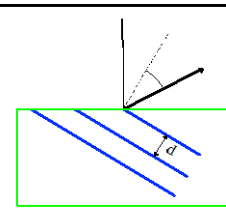
Waves of what?
Classical vs Quantum Theory

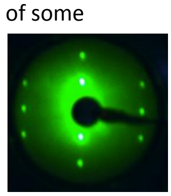


In classical mechanics we ascribe position and momentum to a particle – and view these as real, unambiguous quantities.

And we can use Newton's equations-of-motion to figure out how these quantities change with time.

Waves in classical physics are just a form of motion of some physical quantity,

Light: electric and magnetic fields
Water: height
Sound: acoustic pressure/displacement



which we also regard as real and unambiguous quantities.

In quantum mechanics the complete information about the system (e.g. a particle moving in a potential) is contained in the 'wavefunction'.

We can use a wave equation to figure out how the wavefunction changes with time.

It tells us everything there is to know about every measurable property, e.g. if we measure the position of a particle (e.g. by the electron or photon hitting a screen at some place).

BUT, the wave function tells us only the probabilities of different outcomes (e.g. where the electron is more or less likely to hit the screen).

'waves of possibility'

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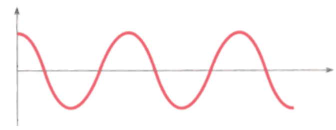
General fomula for waves

1-D wave: Simple harmonic function of time t and distance x

At $x = 0$: $y = A\cos 2\pi ft = A\cos\omega t$ (amplitude A, frequency f)



At general x? - *travelling wave "speed"* v
wave travels a distance x in time $t = x/v$

Amplitude at any x, at any time t,
is amplitude at $x = 0$ but at the earlier time $t - x/v$

$$y = A\cos 2\pi f\left(t - x/v\right) = A\cos 2\pi\left(ft - fx/v\right) = A\cos 2\pi\left(ft - x/\lambda\right)$$

Also written $\boxed{y = A\cos\left(\omega t - kx\right)}$ $\omega = 2\pi f$ Velocity $v = f\lambda$ $k = 2\pi/\lambda$

Or $y = Re[Ae^{i(kx-\omega t)}]$

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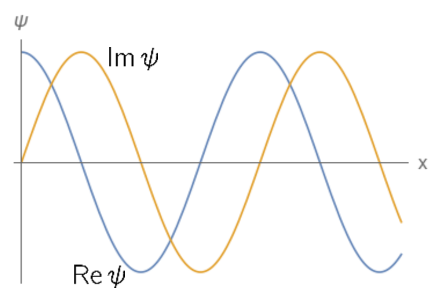
Guessing the wavefunction

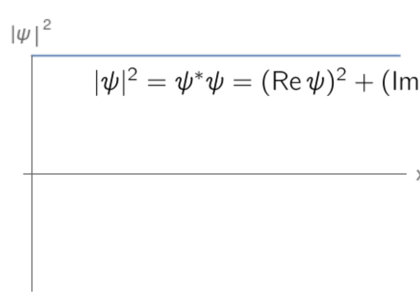


- Suppose we have a particle moving freely (no forces), with a momentum p and an energy E.
- de-Broglie /Davisson-Germer experiment: diffraction like a wave of wavelength $\lambda = h/p$
- Planck/Photoelectric experiments: we associate the energy E with angular frequency $E = h\omega/(2\pi)$
- So for 1D we might guess that the wavefunction is a travelling harmonic wave with this wavelength and frequency :

$$y = Re[Ae^{i(kx-\omega t)}]$$

- In fact the wavefunction takes complex values (remember: not observable so OK)
- and, for a particle of momentum p, energy E, moving in 1D is :

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



$$|\psi|^2 = \psi^*\psi = (\mathrm{Re}\,\psi)^2 + (\mathrm{Im}\,\psi)^2$$

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Lecture 3: Particles as waves and the wavefunction

- We have:
- Looked at how particles, such as electrons or photons, can also show wave behaviour.
- Seen that this wave behaviour has a wavelength, the de Broglie wavelength.
- Seen how these wave-like behaviours lead to discrete energies.
- Seen the wavefunction for a particle moving in one-dimension, with a particular momentum and a particular energy.

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