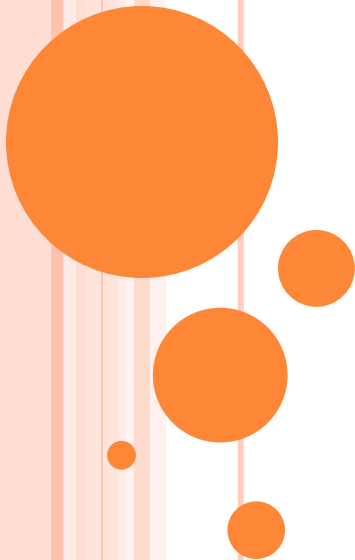


Wave properties of Particle

Ch.3 of Arthur Beiser

- Wave nature of particle,
- De Broglie waves, group waves,
- Phase velocity & group velocity,
- Davison-Germer experiment
- Uncertainty principle and its application



Light has a dual nature

Wave (electromagnetic) - Interference
- Diffraction

Particle (photons) - Photoelectric effect
- Compton effect

Wave - Particle Duality for light

What about Matter?

If light, which was traditionally understood as a wave also turns out to have a particle nature, might matter, which is traditionally understood as particles, also have a wave nature?

Yes!





Louis de Broglie's hypothesis

1905: Light behaves like a particle: $p = h / \lambda$

1924: Matter behaves like a wave



it turns out that everything's kind of mixed together at the fundamental microscopic level.

$$\lambda = \frac{h}{p}$$



de Broglie's wavelength

Both: Wave if $\lambda \gg \text{scale}$

Particle if $\lambda \ll \text{scale}$

Hypothesis in 1924, Nobel prize in 1929

the idea is: matter, because the momentum is so so so large compared to the photons, we'll have an extremely short wavelength.



Exp: What is the De Broglie wavelength of an electron that's moving at 2.2×10^6 m/s ?

Now, this is really really really fast. 2.2 million meters per second. But it's not relativistic. It's still slow compared to the speed of light so we can still do everything fairly classically.

$$p = mv = 9.1 \times 10^{-31} \times 2.2 \times 10^6 \text{ kg m/s} = 2 \times 10^{-24} \text{ N.s}$$

$$\lambda = h/p = 6.626 \times 10^{-34} / 2 \times 10^{-24} = 3.33 \times 10^{-10} \text{ m}$$

Now this is an important number: this speed: the kind of average speed of an electron in the ground state of hydrogen.

Let's estimate for De Broglie wavelength

For a non-relativistic free particle:

Momentum is $p = mv$, here v is the speed of the particle

For free particle total energy, E , is kinetic energy

$$E = K = \frac{p^2}{2m} = \frac{mv^2}{2}$$

$$\lambda_B = \frac{h}{p} = \frac{h}{mv} = \frac{h}{\sqrt{2Em}}$$



- **Bullet:** $m = 0.1 \text{ kg}; v = 1000 \text{ m/s} \Rightarrow \lambda_B \sim 6.63 \times 10^{-36} \text{ m}$

- **Electron at 4.9 V potential:**

$$m = 9.11 \times 10^{-31} \text{ kg};$$

$$E \sim 4.9 \text{ eV}$$

$$\Rightarrow \lambda_B \sim 5.5 \times 10^{-10} \text{ m} = 5.5 \text{ \AA}$$

- **Wavelength of electron with 50eV kinetic energy**

$$K = \frac{p^2}{2m_e} = \frac{h^2}{2m_e \lambda^2} \Rightarrow \lambda = \frac{h}{\sqrt{2m_e K}} = 1.7 \times 10^{-10} \text{ m}$$

- **Wavelength of Nitrogen molecule at room temperature**

$$K = \frac{3kT}{2}, \text{ Mass} = 28m_u$$

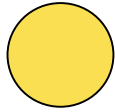
$$\lambda = \frac{h}{\sqrt{3MkT}} = 2.8 \times 10^{-11} \text{ m}$$

$$\lambda = \frac{h}{\sqrt{3MkT}} = 1.2 \times 10^{-6} \text{ m}$$

- **Wavelength of Rubidium(87) atom at 50nK**

Particle

Our traditional understanding of a particle...



“Localized” - definite position, momentum, confined in space

How do we associate a wave nature to a particle ?

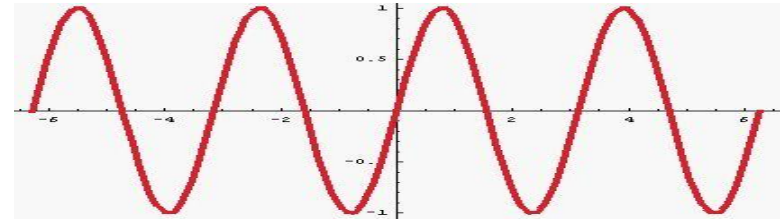
What could represent both wave and particle ?

Find a description of a particle which is consistent with our notion of **both** particles and waves.....

Fits the “wave” description
“Localized” in space

Wave

Our traditional understanding of a

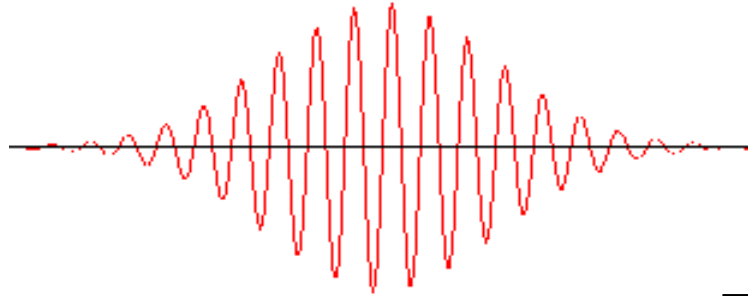


“de-localized” – spread out in space and time.



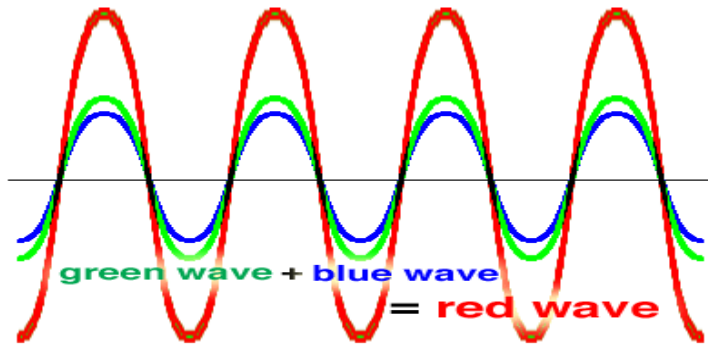
A "Wave Packet"

How do you construct a wave packet ?



What happens when you
add up waves?

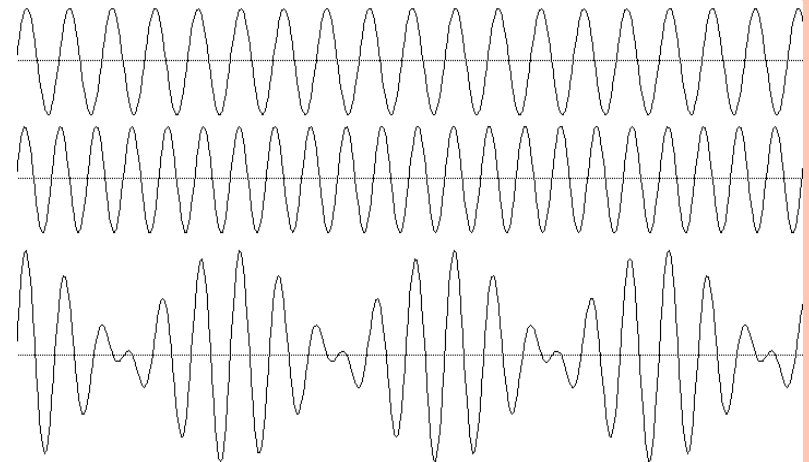
The Superposition principle



Waves of same frequency

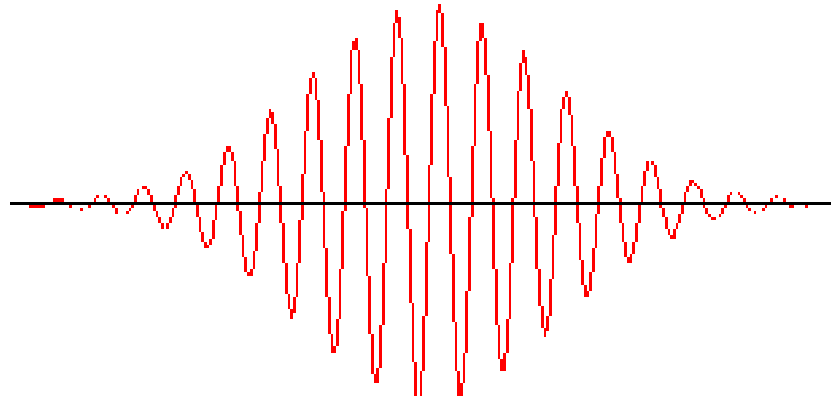
Adding up waves of different
frequencies.....

Waves of slight different frequency



Constructing a wave packet by adding up several waves

If several waves of different wavelengths (frequencies) and phases are superposed together, one would get a resultant which is a **localized wave packet**



A wave packet describes a particle

A **wave packet** is a group of waves with slightly different wavelengths interfering with one another in a way that the amplitude of the group (envelope) is non-zero only in the neighbourhood of the particle

A wave packet is **localized** – a good representation for a particle!



- The spread of **wave packet** in wavelength depends on the required **degree of localization** in space – the central wavelength is given by

$$\lambda = \frac{h}{p}$$

- What is the **velocity** of the wave packet ?

Wave packet, phase velocity and group velocity

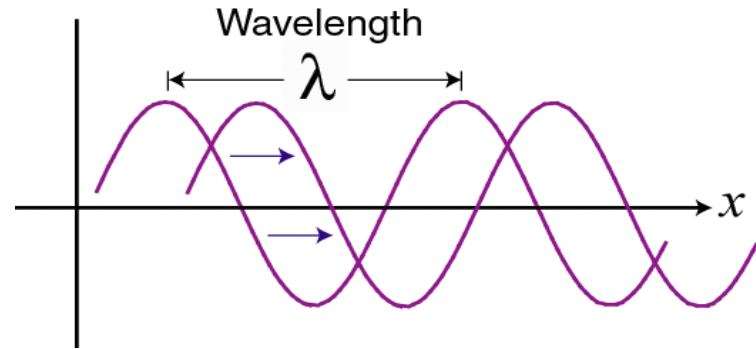
- The velocities of the individual waves which superpose to produce the wave packet representing the particle are different - the **wave packet as a whole** has a different velocity from the waves that comprise it
- **Phase velocity**: The rate at which the phase of the wave propagates in space
- **Group velocity**: The rate at which the envelope of the wave packet propagates



The Phase Velocity

How fast is the wave traveling?

Velocity is a reference distance divided by a reference time.



The phase velocity is the wavelength / period: $v = \lambda / \tau$

Since $f = 1/\tau$:

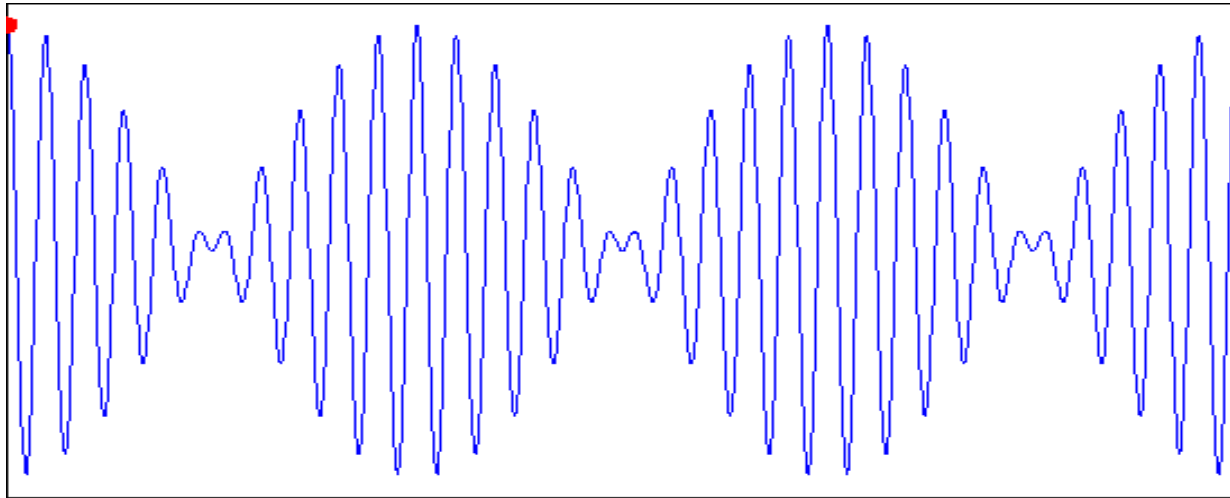
$$v = f \lambda$$

$$v = \omega / k$$

In terms of k , $k = 2\pi / \lambda$, and the angular frequency, $\omega = 2\pi / \tau$, this is:



The Group Velocity



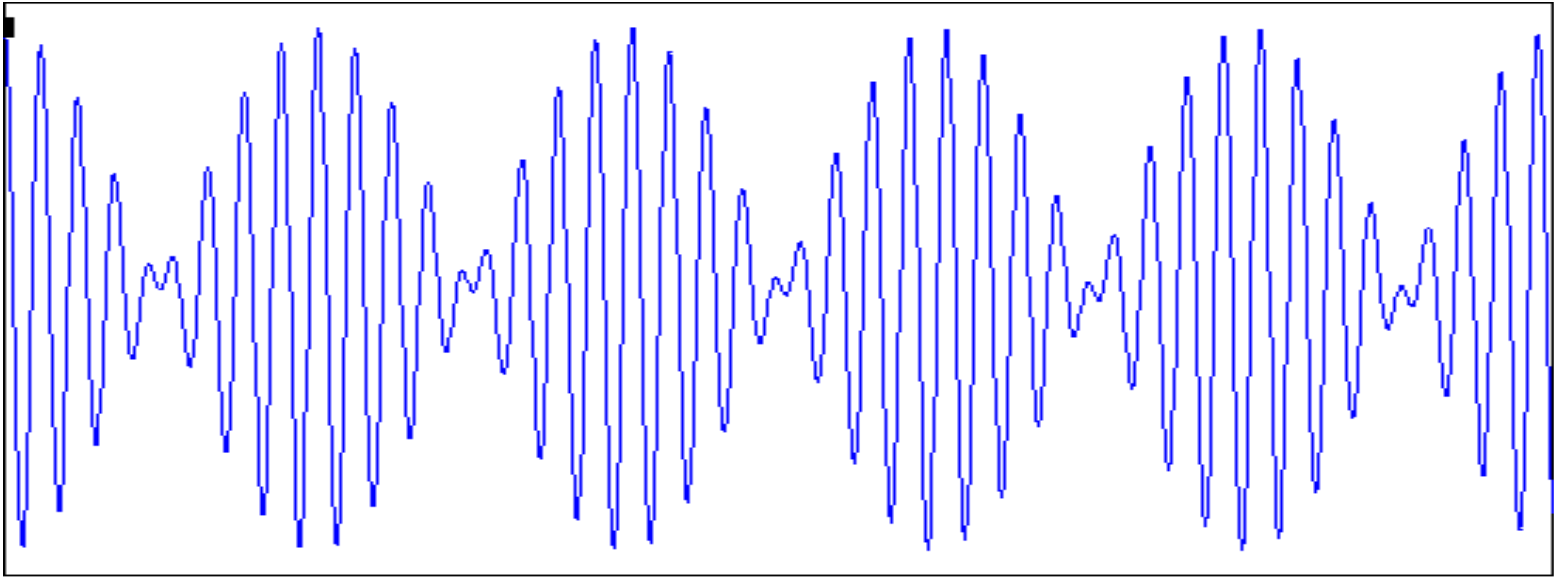
This is the velocity at which the overall shape of the wave's amplitudes, or the wave 'envelope', propagates. (= *signal velocity*)

Here, phase velocity = group velocity (the medium is *non-dispersive*):

The wave speed depends only on the physical properties of the medium. The wave speed is a constant and independent of frequency.



Dispersion: phase/group velocity depends on frequency

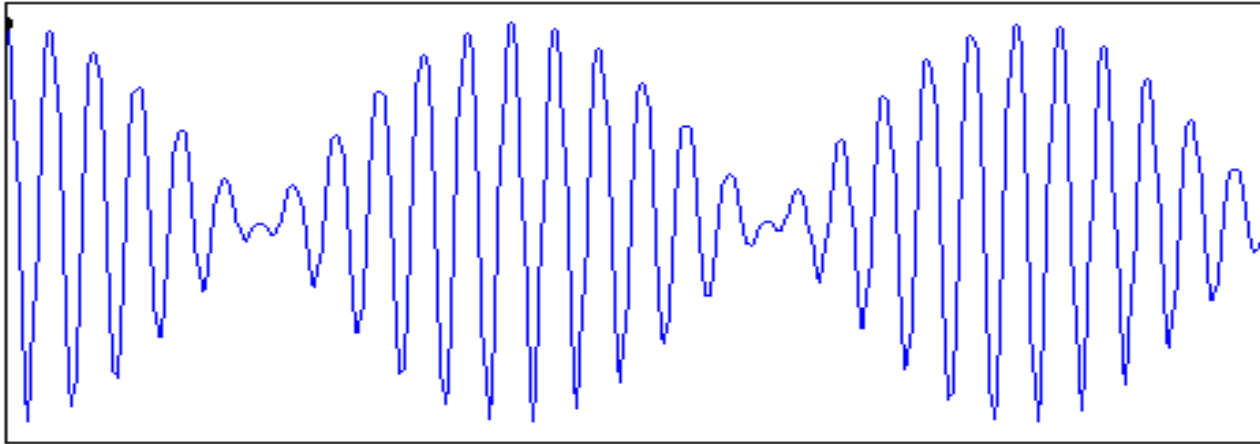


Black dot moves at phase velocity. **Red** dot moves at group velocity.

This is **normal** dispersion (refractive index decreases with increasing λ)



Dispersion: phase/group velocity depends on frequency



Black dot moves at group velocity. *Red* dot moves at phase velocity.

This is *anomalous dispersion* (refractive index increases with increasing λ)



Phase velocity and group velocity

Phase velocity

$$v_p = \frac{\omega}{k} = \frac{E/\hbar}{p/\hbar} = \frac{E}{p}$$

$$v_p = \frac{E}{p} = \frac{\gamma mc^2}{\gamma mv} = \frac{c^2}{v} = \frac{c}{\beta}$$

$$v_p = \frac{c^2}{v}$$

Here C is the velocity of light and v is the velocity of the particle

$$v_g = v$$

$$v_g = v_p - \lambda \frac{dv_p}{d\lambda}$$

Group velocity

$$v_g = \frac{\partial \omega}{\partial k} = \frac{\partial(E/\hbar)}{\partial(p/\hbar)} = \frac{\partial E}{\partial p}$$

$$\begin{aligned} v_g &= \frac{\partial E}{\partial p} = \frac{\partial}{\partial p} \left(\frac{p^2}{2m} \right) \\ &= \frac{p}{m} \\ &= v \end{aligned}$$

$$\begin{aligned} v_g &= \frac{\partial E}{\partial p} = \frac{\partial}{\partial p} \left(\sqrt{p^2 c^2 + m^2 c^4} \right) \\ &= \frac{pc^2}{\sqrt{p^2 c^2 + m^2 c^4}} \\ &= \frac{p}{m \sqrt{(p/(mc))^2 + 1}} \\ &= \frac{p}{m\gamma} \\ &= \frac{mv\gamma}{m\gamma} \\ &= v. \end{aligned}$$

An electron has a de Broglie wavelength of $2.00 \text{ pm} = 2.00 \times 10^{-12} \text{ m}$. Find its kinetic energy and the phase and group velocities of its de Broglie waves.

(a) The first step is to calculate pc for the electron, which is

$$pc = \frac{hc}{\lambda} = \frac{(4.136 \times 10^{-15} \text{ eV} \cdot \text{s})(3.00 \times 10^8 \text{ m/s})}{2.00 \times 10^{-12} \text{ m}} = 6.20 \times 10^5 \text{ eV} \\ = 620 \text{ keV}$$

The rest energy of the electron is $E_0 = 511 \text{ keV}$, so

$$\text{KE} = E - E_0 = \sqrt{E_0^2 + (pc)^2} - E_0 = \sqrt{(511 \text{ keV})^2 + (620 \text{ keV})^2} - 511 \text{ keV} \\ = 803 \text{ keV} - 511 \text{ keV} = 292 \text{ keV}$$

(b) The electron velocity can be found from

$$E = \frac{E_0}{\sqrt{1 - v^2/c^2}}$$

to be

$$v = c \sqrt{1 - \frac{E_0^2}{E^2}} = c \sqrt{1 - \left(\frac{511 \text{ keV}}{803 \text{ keV}} \right)^2} = 0.771c$$

Hence the phase and group velocities are respectively

$$v_p = \frac{c^2}{v} = \frac{c^2}{0.771c} = 1.30c$$

$$v_g = v = 0.771c$$



De Broglie's Hypothesis:

predicts that one should see diffraction and interference of matter waves

For example we should observe

Electron diffraction

Atom or molecule diffraction

Wave nature of electron

Application : Electron Microscope

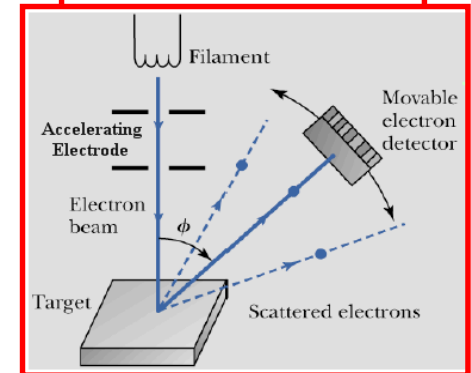
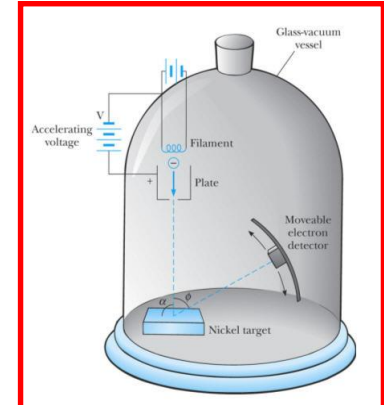
Davisson-Germer Experiment

provides experimental confirmation of the matter waves proposed by de Broglie

- If particles have a wave nature, then under appropriate conditions, they should exhibit diffraction
- Davisson and Germer measured the wavelength of electrons

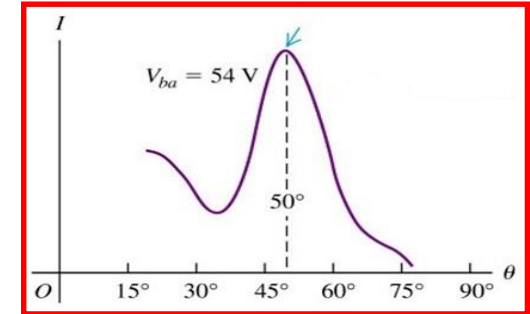
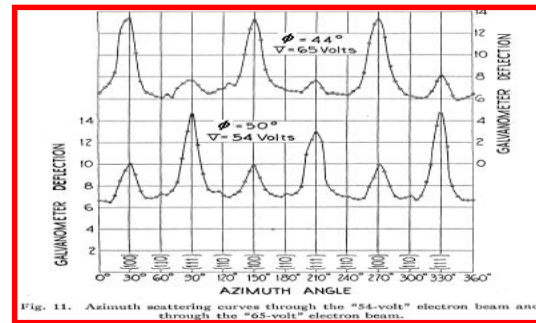
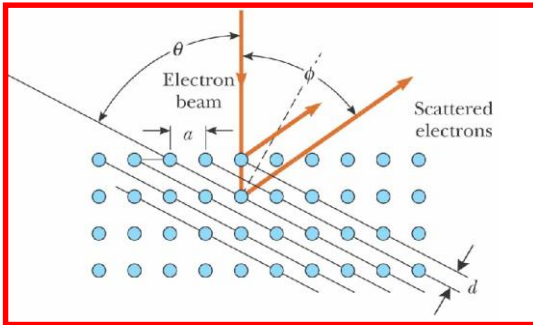
Electrons were directed onto nickel crystals

Accelerating voltage is used to control electron energy:
 $E = |e|V$



Continue...

If electrons are “just” particles, we expect a smooth monotonic dependence of scattered intensity on angle and voltage because only elastic collisions are involved. Diffraction pattern similar to X-rays would be observed if electrons behave as waves.



- ➡ Intensity was stronger for certain angles for **specific** accelerating voltages (i.e. for specific electron energies)
- ➡ Electrons were reflected in almost the same way that X-rays of comparable wavelength
- ➡ Current vs accelerating voltage has a maximum, i.e. the highest number of electrons is scattered in a specific direction
- ➡ This can't be explained by particle-like nature of electrons \Rightarrow electrons scattered on crystals behave as waves

For $\varphi \sim 50^\circ$ the maximum is at $\sim 54\text{V}$

For X-ray Diffraction on Nickel

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

$$d_{\langle 111 \rangle} = 0.91 \text{ \AA}; \lambda_{\text{X-ray}} = 1.65 \text{ \AA}$$

$$\Downarrow$$

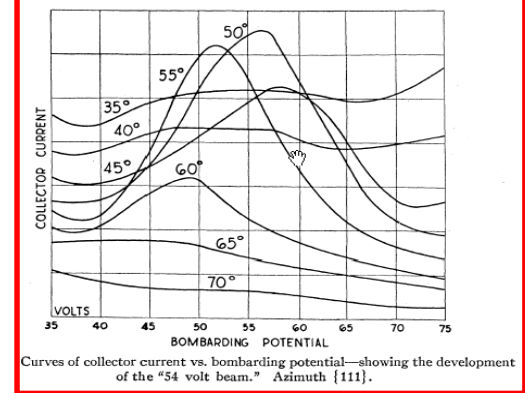
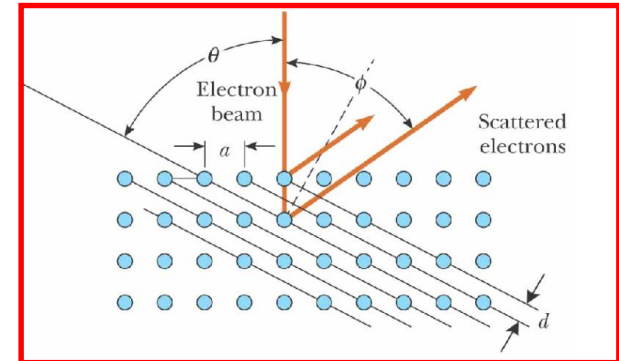
$$\theta = 65^\circ \Rightarrow \phi = 50^\circ$$

Ex: Assuming the wave nature of electrons **we can use de Broglie's approach** to calculate wavelengths of a matter wave corresponding to electrons in this experiment

$$V = 54 \text{ V} \Rightarrow E = 54 \text{ eV} = 8.64 \times 10^{-18} \text{ J}$$

$$E = \frac{p^2}{2m}, \quad p = \sqrt{2mE}, \quad \lambda_B = \frac{h}{\sqrt{2mE}}$$

$$\lambda_B = \frac{6.63 \times 10^{-34} \text{ J} \cdot \text{sec}}{\sqrt{2 \times 9.1 \times 10^{-31} \text{ kg} \times 8.6 \times 10^{-18} \text{ J}}} = 1.67 \text{ \AA}$$



excellent agreement with wavelengths of X-rays diffracted from Nickel!

Particle in a BOX

The wave nature of a moving particle when it is restricted to a certain region of space instead of free

The simplest case: particle that bounces back and forth between the walls of a box. Walls of the box are infinitely hard

Particle trapped in a box: standing wave in a string stretched between the box's walls.

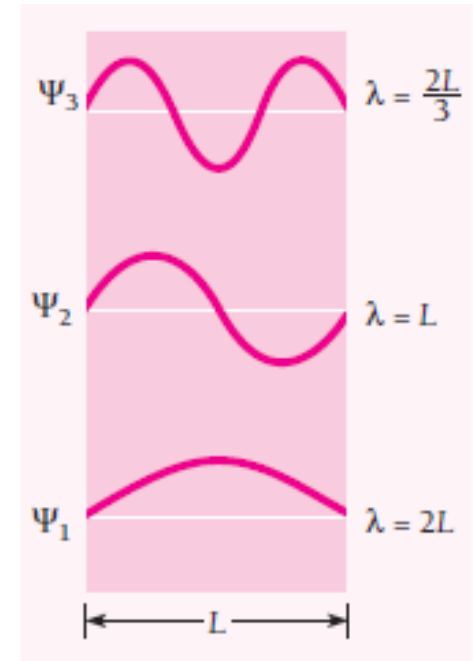
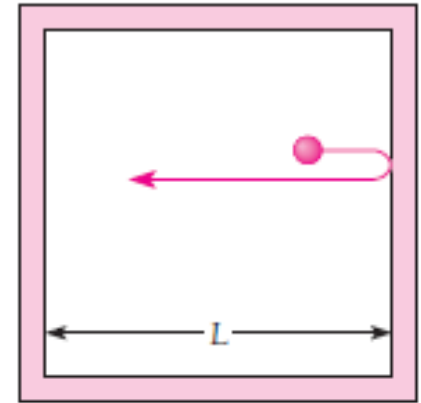
Wave function ψ must be 0 at the walls.

de Broglie wavelengths of the particle are determined by the width L

The longest wavelength is $\lambda = 2L$, the next by $\lambda = L$, then $\lambda = 2L/3$ etc.

The general formula for the permitted wavelengths is

$$\lambda_n = 2L / n, n = 1, 2, 3, \dots$$



Because $mv = h/\lambda$, the restrictions on de Broglie wavelength imposed by the width of the box are equivalent to limits on the momentum of the particle and, in turn, to limits on its kinetic energy.

The kinetic energy of a particle of momentum m is
$$\text{KE} = \frac{1}{2}mv^2 = \frac{(mv)^2}{2m} = \frac{h^2}{2m\lambda^2}$$

Energy level for particle in a Box:


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

Conclusions:

1: A trapped particle cannot have an arbitrary energy. Depends on the mass of the particle and on the details of how it is trapped.

2: A trapped particle cannot have zero energy. Since the de Broglie wavelength of the particle is $\lambda = h/mv$, a speed of $v = 0$ means an infinite wavelength. Such a particle must have at least some kinetic energy. $E = 0$ is not allowed for a trapped particle.

3: Because Planck's constant is so small — only 6.63×10^{-34} J.s — quantization of energy is conspicuous only when m and L are also small. This is why we are not aware of energy quantization in our own experience.



Example

An electron is in a box 0.10 nm across, which is the order of magnitude of atomic dimensions. Find its permitted energies.

Here $m = 9.1 \times 10^{-31}$ kg and $L = 0.10$ nm $= 1.0 \times 10^{-10}$ m, so that the permitted electron energies are

$$\begin{aligned} E_n &= \frac{(n^2)(6.63 \times 10^{-34} \text{ J} \cdot \text{s})^2}{(8)(9.1 \times 10^{-31} \text{ kg})(1.0 \times 10^{-10} \text{ m})^2} = 6.0 \times 10^{-18} n^2 \text{ J} \\ &= 38n^2 \text{ eV} \end{aligned}$$

A 10-g marble is in a box 10 cm across. Find its permitted energies

With $m = 10$ g $= 1.0 \times 10^{-2}$ kg and $L = 10$ cm $= 1.0 \times 10^{-1}$ m,

$$\begin{aligned} E_n &= \frac{(n^2)(6.63 \times 10^{-34} \text{ J} \cdot \text{s})^2}{(8)(1.0 \times 10^{-2} \text{ kg})(1.0 \times 10^{-1} \text{ m})^2} \\ &= 5.5 \times 10^{-64} n^2 \text{ J} \end{aligned}$$



Uncertainty principle

Heisenberg 1932 Nobel



- **Uncertainty Principle** is an important consequence of the wave-particle duality of matter and radiation and is **inherent** to the quantum description of nature
- Simply stated, it is **impossible** to know both the exact position and the exact momentum of an object simultaneously

A fact of Nature!

Uncertainty in Position :

$$\Delta x$$

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

Uncertainty in Momentum:

$$\Delta p_x$$

energy-time uncertainty relation

$$\Delta E \Delta t \geq \frac{h}{4\pi}$$



Consequences: The more accurately we know the energy of a body, the less accurately we know how long it possessed that energy

The energy can be known with perfect precision ($\Delta E = 0$), only if the measurement is made over an infinite period of time ($\Delta t = \infty$)

- applies to all “conjugate variables”

These uncertainties are due not to inadequate apparatus but to the imprecise character in nature of the quantities involved.

Any instrumental or statistical uncertainties that arise during a measurement only increase the product $\Delta x \Delta p$.

Since we cannot know exactly both where a particle is right now and what its momentum is, we cannot say anything definite about where it will be in the future or how fast it will be moving then.



Consequences of the Uncertainty Principle

- The path of a particle (trajectory) is **not well-defined** in quantum mechanics.
- Electrons cannot exist inside a nucleus.
- Atomic oscillators possess a certain amount of energy known as the **zero-point energy**, even at absolute zero.

Do Electrons Exist Within the Nucleus?

Estimate the kinetic energy of an electron confined within a nucleus of size 10^{-14} m by using the uncertainty principle.

Solution: Taking x to be the *half-width of the confinement* length in the equation , we have

$$\Delta p_x \geq \frac{h}{2\Delta x}$$

$$\Delta p_x \geq \frac{6.58 \times 10^{-16} \text{ eV.s}}{10^{-14} \text{ m}} \times \frac{3 \times 10^8 \text{ m/s}}{c}$$

or

$$\Delta p_x \geq 2 \times 10^7 \text{ eV} / c$$

This means that measurements of the component of momentum of electrons trapped inside a nucleus would range from less than 20 MeV/c *to greater than 20 MeV/c and that some electrons would have momentum* at least as large as 20 MeV/c . *Because this appears to be a large momentum*, to be safe we calculate the electron's energy relativistically.

$$\begin{aligned}
 E^2 &= p^2 c^2 + (m_e c^2)^2 \\
 &= (20 \text{ MeV}/c)^2 c^2 + (0.511 \text{ MeV})^2 \\
 &= 400 (\text{MeV})^2
 \end{aligned}$$

or

$$E \geq 20 \text{ MeV}$$

Finally, the kinetic energy of an intranuclear electron is $K = E - m_e c^2 \geq 19.5 \text{ MeV}$

Since electrons emitted in radioactive decay of the nucleus (beta decay) have energies much less than 19.5 MeV (about 1 MeV or less) and it is known that no other mechanism could carry off an intranuclear electron's energy during the decay process, we conclude that electrons observed in beta decay do not come from within the nucleus but are actually created at the instant of decay.

Why isn't the uncertainty principle apparent to us in our ordinary experience...?

$$\Delta x \Delta p_x \geq \frac{h}{2\pi}$$

Planck's constant, again!!

$$h = 6.6 \times 10^{-34} \text{ J.s}$$

Planck's constant is **so small** that the uncertainties implied by the principle are also **too small to be observed**. They are only significant in the domain of microscopic systems



Example: A measurement establishes the position of a proton with an accuracy of $\pm 1.00 \times 10^{-11}$ m. Find the uncertainty in the proton's position 1 s later. Assume $v \ll c$.

Let us call the uncertainty in the proton's position Δx_0 at the time $t = 0$. The uncertainty in its momentum at this time is therefore, from Eq. (3.22),

$$\Delta p \geq \frac{\hbar}{2\Delta x_0}$$

Since $v \ll c$, the momentum uncertainty is $\Delta p = \Delta(mv) = m \Delta v$ and the uncertainty in the proton's velocity is

$$\Delta v = \frac{\Delta p}{m} \geq \frac{\hbar}{2m \Delta x_0}$$

The distance x the proton covers in the time t cannot be known more accurately than

$$\Delta x = t \Delta v \geq \frac{\hbar t}{2m \Delta x_0}$$

Hence Δx is inversely proportional to Δx_0 : the *more* we know about the proton's position at $t = 0$, the *less* we know about its later position at $t > 0$. The value of Δx at $t = 1.00$ s is

$$\begin{aligned} \Delta x &\geq \frac{(1.054 \times 10^{-34} \text{ J} \cdot \text{s})(1.00 \text{ s})}{(2)(1.672 \times 10^{-27} \text{ kg})(1.00 \times 10^{-11} \text{ m})} \\ &\geq 3.15 \times 10^3 \text{ m} \end{aligned}$$



