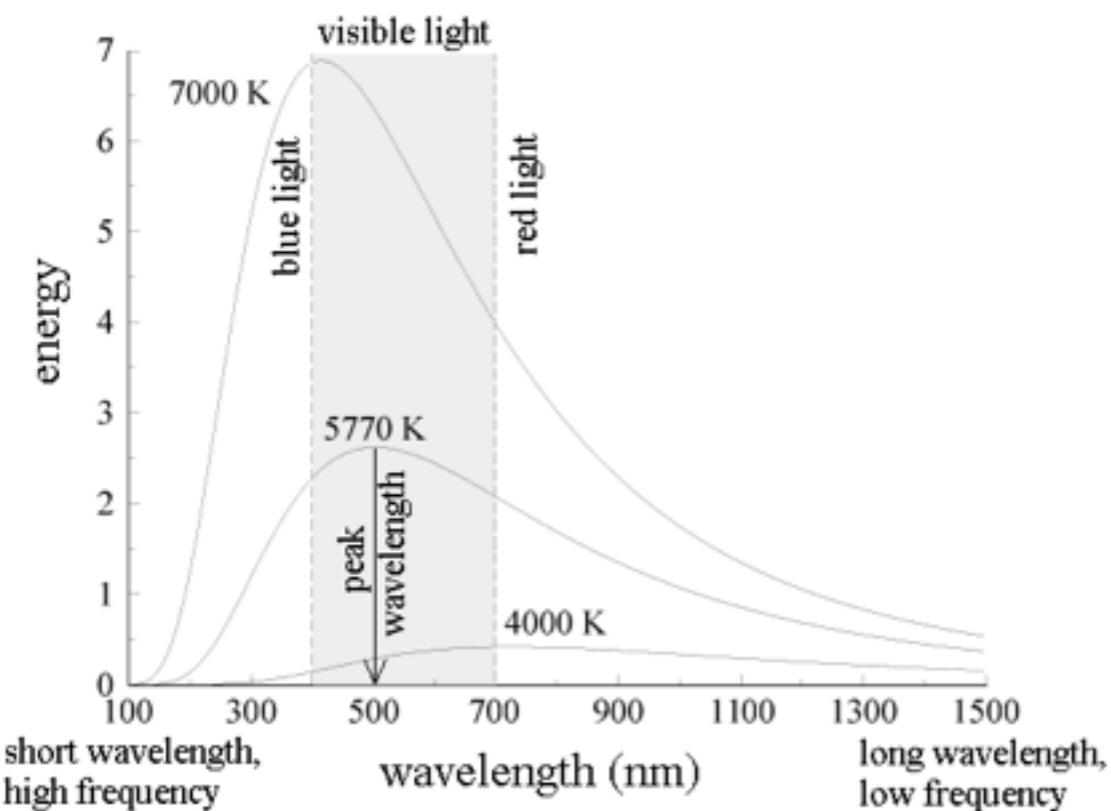


FAILURES OF CLASSICAL PHYSICS

1. Black Body radiation

Any object with a temperature above absolute zero emits light at all wavelengths. If the object is perfectly black (so it doesn't reflect any light), then the light that comes from it is called **blackbody radiation**.

The energy of blackbody radiation is not shared evenly by all wavelengths of light. The spectrum of blackbody radiation (below) shows that some wavelengths get more energy than others. Three spectra are shown, for three different temperatures. (One of the curves is for the surface temperature of the Sun, 5770 K.)



- a. The blackbody spectrum **depends only on the temperature of the object, and not on what it is made of**. An iron horseshoe, a ceramic vase, and a piece of charcoal --- all emit the same blackbody spectrum if their temperatures are the same.
- b. **As the temperature of an object increases, it emits more blackbody energy at all wavelengths.**
- c. **As the temperature of an object increases, the peak wavelength of the blackbody spectrum becomes shorter (bluer).** For example, **blue stars are hotter than red stars**.
- d. **The blackbody spectrum always becomes small at the left-hand side (the short wavelength, high frequency side).**

The explanation of classical physics:

Light is an electromagnetic wave that is produced when an electric charge vibrates. (Strictly speaking, "vibrates" means any change in how the charge moves --- speeding up, slowing down, or changing direction.) Now recall that heat is just the kinetic energy of random motion. In a hot object, electrons vibrate in random directions and produce light as a result. A hotter object means more energetic vibrations and so more light is emitted by a hotter object --- it glows brighter. So far, so good. **But classical physics could not explain the shape of the blackbody spectrum.**

The electrons in a hot object can vibrate with a range of frequencies, ranging from very few vibrations per second to a huge number of vibrations per second. In fact, there is no limit to how great the frequency can be. Classical physics said that each frequency of vibration should have the same energy. Since there is no limit to how great the frequency can be, there is no limit to the energy of the vibrating electrons at high frequencies. This means that, according to classical physics, there should be no limit to the energy of the light produced by the electrons vibrating at high frequencies.

WRONG!! Experimentally, the blackbody spectrum always becomes small at the left-hand side (short wavelength, high frequency).

Explained By Quantum Mechanics

At about 1900, Max Planck came up with the solution. He proposed that the classical idea that each frequency of vibration should have the same energy must be wrong. Instead, he said that energy is not shared equally by electrons that vibrate with different frequencies. Planck said that energy comes in clumps. He called a clump of energy a **quantum**.

The size of a clump of energy --- a quantum --- depends on the frequency of vibration. Here is Planck's rule for the a quantum of energy for a vibrating electron:

$$\text{energy of a quantum} = (\text{a calibration constant}) \times (\text{frequency of vibration})$$

or

$$E = hf = h\nu$$

where h , the calibration constant, is called Planck's constant. Its value is about 6.634×10^{-34} Js, very tiny!

So how does this explain the spectrum of blackbody radiation?

Planck said that **an electron vibrating with a frequency f could only have an energy of $1 hf$, $2 hf$, $3 hf$, $4 hf$, ... ; that is,**

$$\text{energy of vibrating electron} = (\text{any integer}) \times hf$$

But the electron has to have *at least* one quantum of energy if it is going to vibrate. If it doesn't have at least an energy of $1hf$, it will not vibrate at all and can't produce any light.

Planck said: at high frequencies the amount of energy in a quantum, hf , is so large that the high-frequency vibrations can never get going! This is why the blackbody spectrum always becomes small at the left-hand (high frequency) side.

2. The Photoelectric Effect

When light shines on the surface of a metallic substance, electrons in the metal absorb the energy of the light and they can escape from the metal's surface. This is called the **photoelectric effect**, and it is used to produce the electric current that runs many solar-powered devices.

Using the idea that **light is a wave with the energy distributed evenly throughout the wave**, classical physicists expected that when using very dim light, it would take some time for enough light energy to build up to eject an electron from a metallic surface.

WRONG!! Experiments show that if **light of a certain frequency can eject electrons from a metal**, it makes no difference how dim the light is. There is never a time delay.

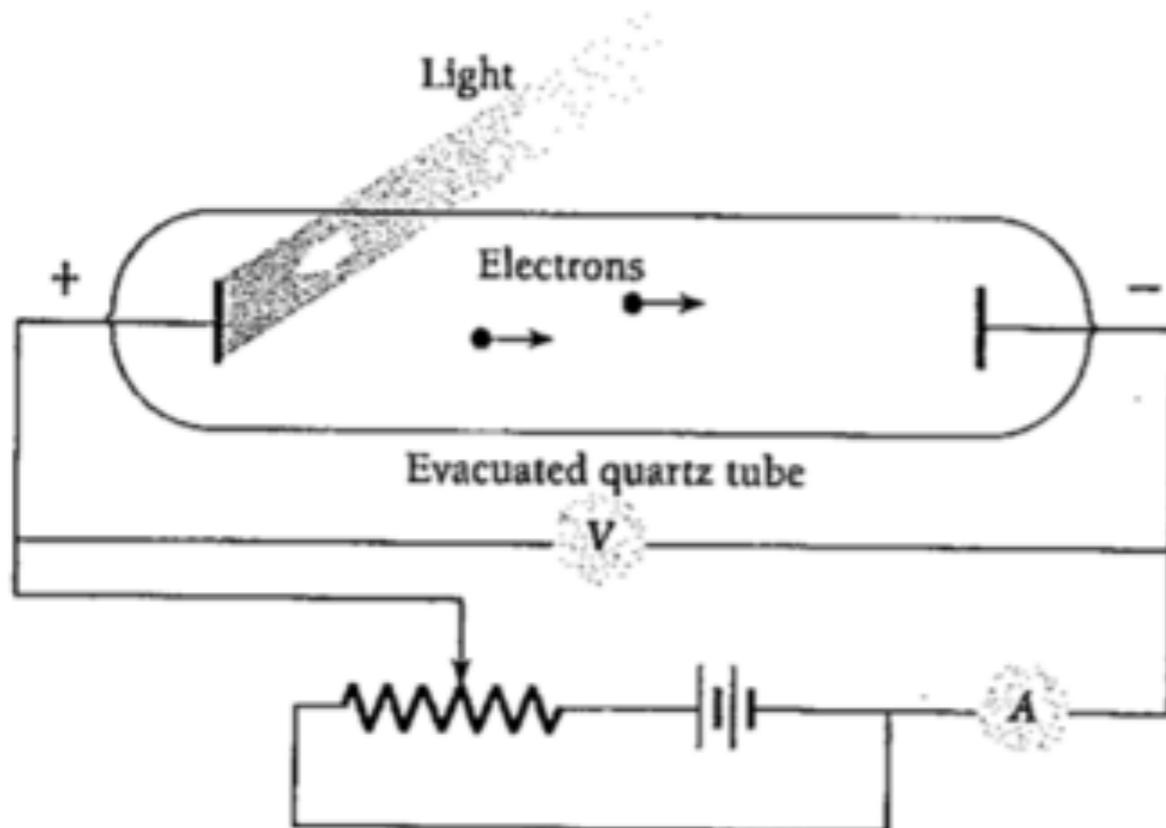


Figure 2.9 Experimental observation of the photoelectric effect.

- Electrons are ejected from a metal surface by absorption of a photon
- Electron ejection depends on frequency not on intensity
- The threshold frequency corresponds to $h\nu_0 = \phi$
 - ϕ is the work function (essentially equal to the ionization potential of the metal)
- The kinetic energy of the ejected particle is given by:
- $\frac{1}{2}mv^2 = h\nu - \phi$
- The photoelectric effect shows that the incident radiation is composed of photons that have energy proportional to the frequency of the radiation

Experimental Observations

1. The electrons were emitted immediately - **no time lag.**
2. Increasing the intensity of the light increased the number of photoelectrons, but not their maximum kinetic energy.
3. Red light will not cause the ejection of electrons, no matter what the intensity.
4. A weak violet light will eject only a few electrons, but their maximum kinetic energies are greater than those for intense light of longer wavelengths.

Explanation by Quantum Mechanics

In **1905, Albert Einstein** came up with the solution. If Max Planck's idea that energy comes in clumps (quanta) is correct, then **light must consist of a stream of clumps of energy**. Each clump of light energy is **called a photon**, said Einstein, and each photon **has an energy equal to hf** (Planck's constant times the frequency of the light).

Therefore the **energy of light is not evenly distributed along the wave, but is concentrated in the photons**. A dimmer light means **fewer photons**, but simply turning down the light (without changing its frequency) does not alter the energy of an individual photon. So for a specific frequency of light, if a single photon has enough energy to eject an electron from a metallic surface, then electrons will always be ejected immediately after the light is turned on and the photons hit the metal.

WAVES OR PARTICLES? BOTH!

When light passes through a **Young's double-slit**, an interference pattern consisting of bright bands and dark bands is seen on a screen. This is produced when the wave from one slit combines with the wave from the other slit. If two wave crests meet at the screen, the waves add and you get a bright band. If a wave crest from one slit meets a wave trough from the other slit, the waves cancel and you get a dark band. **This proves that light is a wave.**

On the other hand, the photoelectric effect proves that light consists of massless particles called photons.

Light acts like a wave if you want to know how it propagates, how it travels from one place to another. To describe how light travels from the double slits to the screen, you have to use the wave characteristics of light.

Light acts like particles (photons) if you want to know how light interacts with matter. To describe how light interacts with the electrons in a metal and how it ejects them from the metal's surface, you have to use the particle characteristics of light.

We say that **light exhibits a wave-particle duality**. It can behave like either waves or particles (but not both at the same time), depending on the situation.

Thinking about the photoelectric effect again, ***how can a photon (which has no mass) knock an electron***. Einstein used his ***theory of relativity*** to show that even massless photons have momentum.

Newton defined **momentum = (mass) x (velocity)** for a particle with mass, but **Einstein was able to show that the momentum of a massless photon depends on its wavelength:**

The smaller the wavelength, the greater the momentum of the photon.

De Broglie Hypothesis

In 1923, Prince Louis de Broglie of France had an idea.

Maybe the wave-particle duality applies to everything in nature. **He proposed that *everything* propagates like a wave, and that *everything* interacts like a particle.**

Question: What do you mean by the **wavelength of an electron**, or the **wavelength of a baseball**?

$$\lambda = h/p = h/mv$$

de Broglie rewrote Einstein's formula for the momentum of a photon and applied it to a particle with mass: **Planck's constant, *h*, is so tiny that we don't notice the wavelength of a thrown baseball, which is only about 10^{-35} meters!** But an electron's mass is also tiny, so it has a wavelength about 10,000 times shorter than the wavelength of visible light. This is useful, because microscopes that use electron waves instead of light waves can see several thousand times more detail!

The proof that electrons propagate like a wave came when electrons were passed through a double slit and counted as they hit a screen. If the electrons traveled like a stream of particles, they would have simply piled up at two locations behind the two slits. But they didn't. They showed a double-slit interference pattern, bright bands and dark bands just like the ones produced by light waves. Without a doubt, electrons exhibit the wave-particle duality of nature. In fact, every massive object exhibits the wave-particle duality of nature. It just isn't noticeable on the large scale of our everyday world.

De Broglie Wavelength

De Broglie first used Einstein's famous equation relating **matter and energy**:

$$E=mc^2 \quad (1)$$

E = energy, m = mass, c = speed of light

Using Planck's theory which states every quantum of a wave has a discrete amount of energy given by Planck's equation:

$$E=h\nu \quad (2)$$

E = energy, h = Plank's constant($6.62607 \times 10^{-34} \text{ Js}$), ν = frequency

Since de Broglie believes particles and wave have the same traits, the two energies would be the same:

$$mc^2=h\nu \quad (3)$$

Because real particles do not travel at the speed of light, De Broglie substituted v , velocity, for c , the speed of light.

$$mv^2 = h\nu \quad (4)$$

Through the equation λ , de Broglie substituted

v/λ for v and arrived at the final expression that relates wavelength and particle with speed.

$$mv^2 = h\nu/\lambda \quad (5)$$

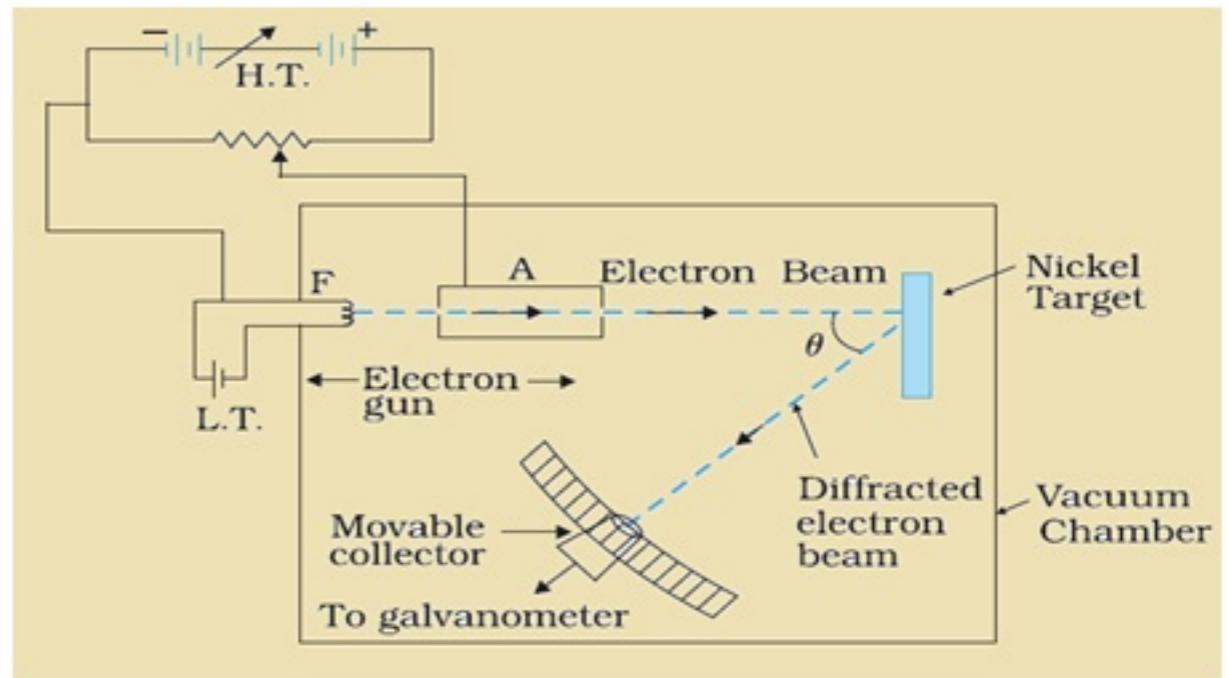
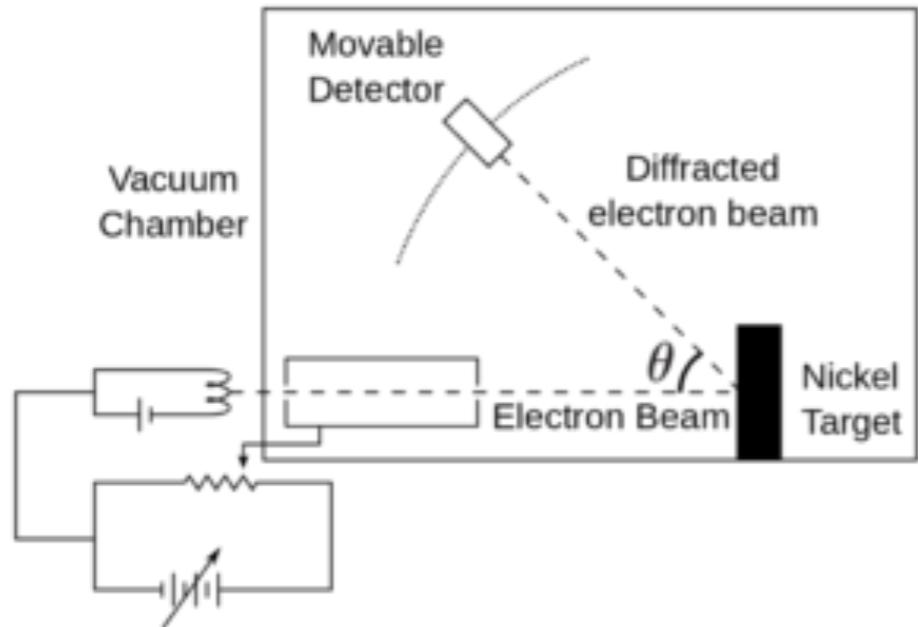
Hence:

$$\lambda = h\nu/mv^2 = h/mv \quad (6)$$

$$\lambda = h/p \quad (7)$$

The greater the particles momentum shorter is the wavelength.

Davisson and Germer Experiment

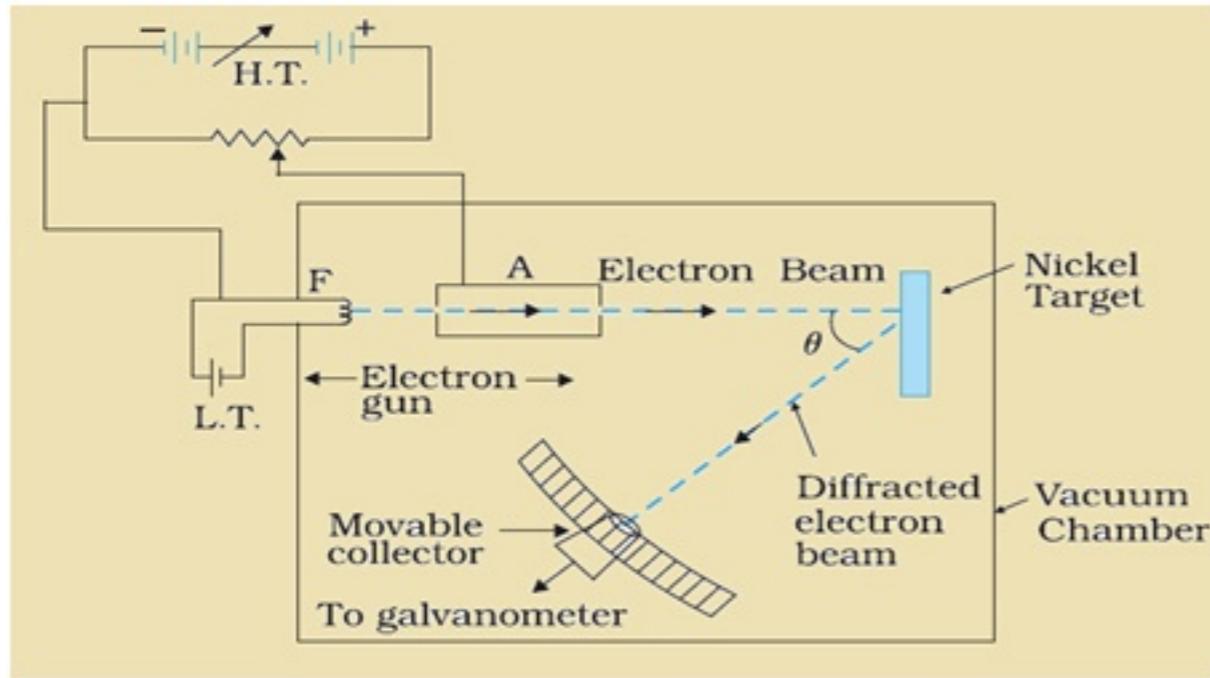


In the year 1927, two American physicists C.J Davisson and L.H Germer conducted an experiment **to explain the wave nature of electrons through electron diffraction like diffraction of light waves.**

This confirmed the earlier hypothesis by Louis de Broglie in 1924, which states that particles of matter like electron have wave-like properties. It was a historically important development in the establishment of quantum mechanics and Schrödinger equation.

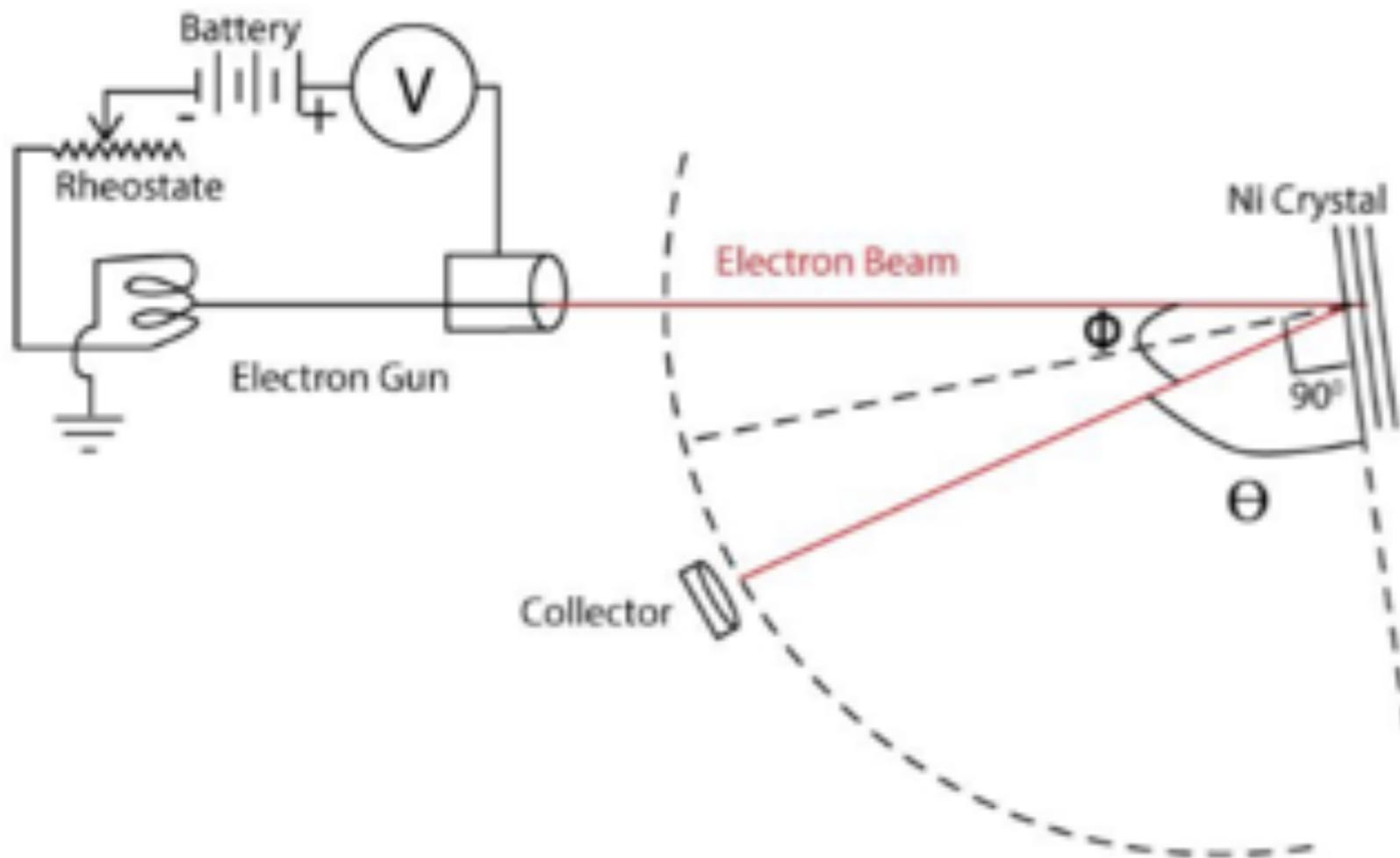
However, it is to be noted that the **Davisson Germer Experiment was not intended to confirm De Broglie's hypothesis but rather they were studying the surface of a nickel (Ni)**. This was somewhat an accidental discovery.

The experimental setup for the Davisson and Germer experiment is enclosed within a vacuum chamber. Thus the deflection and scattering of electrons by the medium are prevented.



The main parts of the experimental setup are as follows:

- **Electron gun:** An electron gun is a **Tungsten filament** that emits electrons via **thermionic emission** i.e. it emits electrons when heated to a particular temperature.
- **Electrostatic particle accelerator:** Two opposite charged plates (positive and negative plate) are used to accelerate the electrons at a known potential.
- **Evacuated Chamber:** For free movement of an electron without air resistance
- **Collimator:** The accelerator is enclosed within a cylinder that has a narrow passage for the electrons along its axis. Its function is **to render a narrow and straight (collimated) beam of electrons ready for acceleration.**
- **Target:** The target is a **Nickel crystal**. The electron beam is **fired normally** on the Nickel crystal. The crystal is placed such that **it can be rotated about a fixed axis**.
- **Galvanometer:** Used to **measure the small values of current**.
- **Detector:** A detector is used **to capture the scattered electrons from the Ni crystal**. The detector can be moved in a semicircular arc as shown in the diagram above.

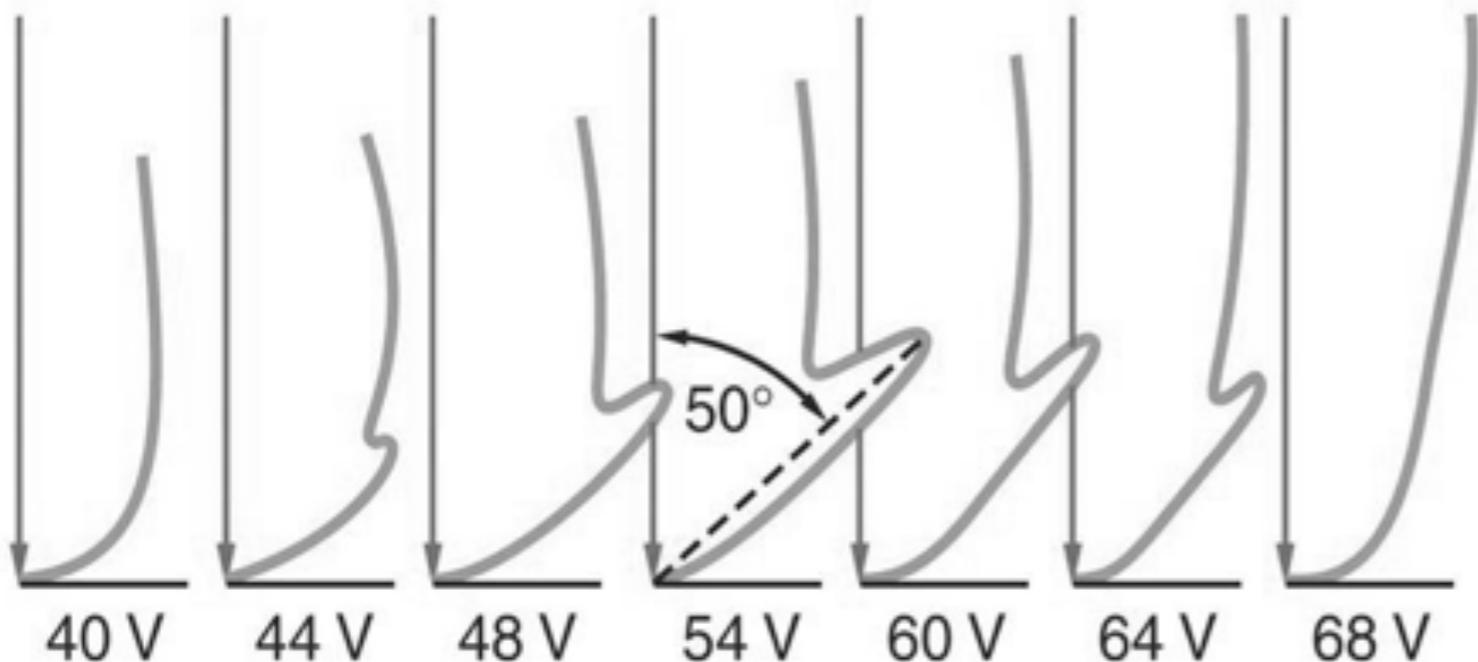


Observations of the Davisson and Germer Experiment

The detector used here can only detect the presence of an electron in the form of a particle. As a result, the detector receives the electrons in the form of an electronic current. The intensity (strength) of this electronic current received by the detector and the scattering angle is studied. We call this current as the **electron intensity**.

The intensity of the scattered electrons is not continuous. It shows a maximum and a minimum value corresponding to the maxima and the minima of a diffraction pattern produced by X-rays.

The intensity of scattered electrons is studied from various angles of scattering and potential difference. For a particular voltage (**54V**, say) the maximum scattering happens at a fixed angle only (**50**) as shown below:



Plots between I – the intensity of scattering (X-axis) and the angle of scattering θ for given values of Potential difference.

Conclusions:

1. The scattered electrons have the same pattern as observed with waves.
2. High intensity of electron was at 54V at an angle of 50 degree.
3. The wavelength was discovered to be 0.167nm via Bragg's Law.

The Thought Behind the Experimental Setup

The basic **thought** behind the Davisson and Germer experiment was that **the waves reflected from two different atomic layers of a Ni crystal will have a fixed phase difference**. After reflection, these waves will interfere either constructively or destructively. Hence **producing a diffraction pattern**. In the Davisson and Germer experiment **electrons were used in place of waves**. These electrons formed a diffraction pattern. The dual nature of matter was thus verified. We can relate the de Broglie equation and the Bragg's law as shown below: From the de Broglie equation, we have:

$$\lambda = h/p = h/mv = h/\sqrt{2mE} = h/\sqrt{2meV} \quad \dots (1)$$

$$(E = mv^2/2 \text{ and } E = eV)$$

where, m is the mass of an electron, e is the charge on an electron and h is the Plank's constant. Therefore for a given V, an electron will have a wavelength given by equation (1). The following equation gives Bragg's Law:

$$n\lambda = 2d \sin(90^\circ - \theta/2) \quad \dots (2)$$

Since the value of d was already known from the X-ray diffraction experiments. Hence for various values of θ , we can find the wavelength of the waves producing a diffraction pattern from equation 2.

Results of the Davisson and Germer Experiment

From the Davisson and Germer experiment, we get a value **for the scattering angle θ** and a corresponding value of **the potential difference V at which the scattering of electrons is maximum**. Thus these two values from the data collected by Davisson and Germer, when used in equation (1) and (2) give the same values for λ . Therefore, this establishes the de Broglie's wave-particle duality and verifies his equation as shown below:

From (1), we have:

$$\lambda = h/\sqrt{2meV}$$

For $V = 54$ V, we have.

$$\lambda = 12.27/\sqrt{54} = 0.167 \text{ nm} \quad \dots (3)$$

Now the value of ' d ' from X-ray scattering is 0.092 nm. Therefore for $V = 54$ V, the angle of scattering is 50, using this in equation (2), we have:

$$n\lambda = 2 (0.092 \text{ nm})\sin(90 - 50/2)$$

For $n = 1$, we have:

$$\lambda = 0.165 \text{ nm} \quad \dots (4)$$

Therefore the **experimental results are in a close agreement with the theoretical values got from the de Broglie equation**. The equations (3) and (4) verify the de Broglie equation. Thus, Davisson Germer experiment confirms the wave nature of electrons and De Broglie relation.

Schrodinger's time independent wave equation

Suppose an electron is moving with a velocity v in a wave motion.

According to classical theory, if there is a wave motion, there must be vibrations, frequency, amplitude and phase. We have to consider a wave equation.

Let $\psi = \psi_0 \sin(\omega t - kx)$ ————— ①

It is a simple harmonic wave eqn, where,

ψ \Rightarrow wave function.

ω \Rightarrow angular velocity

t \Rightarrow time period

k \Rightarrow wave vector

x \Rightarrow displacement.

+ Let us differentiate eqn ①, partially, w.r.t x .

$$\frac{\partial \psi}{\partial x} = \psi_0 \cos(\omega t - kx) \cdot (-k)$$

Again differentiate $\omega \propto t \cdot x$, partially,

$$\Rightarrow \frac{\partial^2 \psi}{\partial x^2} = -\psi_0 \sin(\omega t - kx) (-k) (-k)$$

$$\Rightarrow \frac{\partial^2 \psi}{\partial x^2} = -k^2 \underbrace{\psi_0 \sin(\omega t - kx)}_{\text{ll}}$$

From eqⁿ ①, $\psi = \psi_0 \sin(\omega t - kx)$

$$\Rightarrow \frac{\partial^2 \psi}{\partial x^2} = -k^2 \psi$$

$$\Rightarrow \left\{ \frac{\partial^2 \psi}{\partial x^2} + k^2 \psi = 0 \right\} \rightarrow ②$$

Now, we have to eliminate classical terms into quantum terms. First, we need to eliminate K term.

* we know $\Rightarrow k = \frac{2\pi}{\lambda}$ which is a wave vector,

Put the value of 'k' in eqⁿ ② -

$$\Rightarrow \frac{\partial^2 \psi}{\partial x^2} + \frac{4\pi^2}{\lambda^2} \psi = 0 \quad \text{--- } ③$$

* Now, Acc. to de-Broglie's hypothesis,

$$\lambda = \frac{h}{mv} \quad \left. \right\} \rightarrow \text{Put in eqⁿ } ③$$

$$\Rightarrow \frac{\partial^2 \psi}{\partial x^2} + \frac{4\pi^2 m^2 v^2}{h^2} \psi = 0 \quad \text{--- } ④$$

* we have to replace, $m^2 v^2$ -

- . o -

As we know, total energy = K.E. + P.E.

$$\Rightarrow E = K + V$$

K \Rightarrow K.E.

V \Rightarrow P.E.

E \Rightarrow Total energy

$$\Rightarrow E = \frac{1}{2}mv^2 + V$$

$$\Rightarrow 2(E - V) = mv^2$$

Multiply both sides by 'm',

$$\Rightarrow 2m(E - V) = m^2v^2$$

Put things in eqn (1)

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{4\pi^2}{h^2} (2m(E - V)) \psi = 0$$

$$\boxed{\frac{\partial^2 \psi}{\partial x^2} + \frac{8\pi^2 m (E - V)}{h^2} \psi = 0}$$

①

Now, Acc. to Bohr $\Rightarrow \frac{h}{\lambda} = \frac{h}{2\pi}$ (30)

or $\frac{\hbar^2}{4\pi^2} = \frac{h^2}{\lambda^2} \Rightarrow$ Put in eqⁿ (A).

or
$$\left[\frac{\partial^2 \Psi}{\partial x^2} + \frac{2m [E - V]}{\hbar^2} \Psi = 0 \right] \rightarrow (B)$$

Eqⁿ (A) or (B), ^{represents} a Schrodinger's time independent wave eqⁿ in one dimensional.

Also,
$$\left[\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} + \frac{2m [E - V]}{\hbar^2} \Psi = 0 \right] \rightarrow (C)$$

\hookrightarrow Schrodinger's wave eqⁿ (time independent) in 3 Dimensional

Eqⁿ (C) can be re-written as —

$$\left[\nabla^2 \Psi + \frac{2m [E - V]}{\hbar^2} \Psi = 0 \right]$$

Particle in a one Dimensional Box

A particle in a box in which a particle of mass m is moving in between the walls of one dimensional box having length 'a' at $x=0$ and $x=a$.

$$\text{So, } V(x) = 0$$

inside the walls

(P.E. = 0)

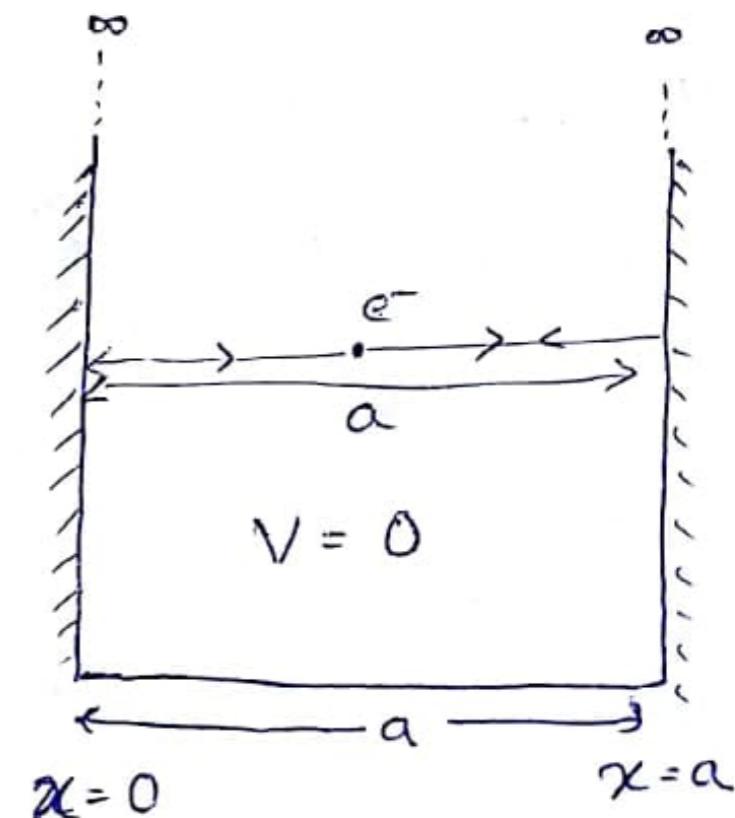
$$V(x) = \infty$$

outside the walls

(P.E. = ∞)

Now, consider a time independent Schrodinger's wave eqn \Rightarrow

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{8\pi^2 m}{h^2} (E - V) \psi = 0$$



Applying boundary conditions as —

$$\text{At } x=0, \quad V = 0$$

$$\text{So, } \frac{\partial^2 \psi}{\partial x^2} + \frac{8\pi^2 m}{h^2} E \psi = 0$$

Let $K^2 = \frac{8\pi^2 m E}{h^2}$ } → is a constant independent of 'x'.

$$\text{So, } \frac{\partial^2 \psi}{\partial x^2} + K^2 \psi = 0$$

We know the solution of wave eq'n as -

$$\psi(x) = A \sin Kx + B \cos Kx$$

Apply boundary condition as, $x = 0, \psi(x) = 0$

$$0 = A \sin 0 + B \cos 0 \Rightarrow B = 0 \quad \text{--- (1)}$$

At $x = a, \psi(a) = A \sin Ka + B \cos Ka$

From eq" ① $\rightarrow B = 0$

So, $\psi(a) = A \sin ka$

So, $A \sin ka = 0$

$$\sin ka = 0$$

So, $\sin ka = \sin n\pi$

or $Ka = n\pi$

or

$$K = \frac{n\pi}{a}$$

Also, at $x = a$,
 $\psi(a) = 0$.

$$\sin n\pi = 0$$

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

where $n = 1, 2, 3, \dots$

So, $K^2 = \frac{n^2 \pi^2}{a^2}$

Already we know that, $K^2 = \frac{8\pi^2 m E}{h^2}$

So, $\frac{8\pi^2 m E}{h^2} = \frac{n^2 \pi^2}{a^2}$

$$E = \frac{n^2 \pi^2 h^2}{8 m a^2}$$

$$\boxed{E = \frac{n^2 h^2}{8 m a^2}}$$



Quantized energy of
a particle in a one
dimensional box.

$$n = 1, 2, 3, \dots$$

So, we can say that "Energy depends upon the
quantum number 'n', which can have any integral
value", the energy levels of the particle in
a box are QUANTIZED"

The wave function of a particle in a box whose energies are E_n with $B=0$ are:

$$\Psi_n(x) = A \sin kx = A \sin \frac{n\pi}{a} x \quad \text{--- } ①$$

These are the eigenfunctions corresponding to the energy eigen values E_n .

For each quantum number n , Ψ_n is a finite, single valued function of x and Ψ_n & $\frac{\partial \Psi_n}{\partial x}$ are continuous (except at the ends of the box).

The integral of $|\Psi_n|^2$ over all space is finite.

So integrating $|\Psi_n|^2$ w.r.t x .

$$\int_{-\infty}^{\infty} |\Psi_n|^2 dx = \int_0^a |\Psi_n|^2 dx = A^2 \int_0^a \sin^2 \left(\frac{n\pi x}{a} \right) dx$$
$$= \frac{A^2}{2} \left[\int_0^a dx - \int_0^a \cos \left(\frac{2n\pi x}{a} \right) dx \right] \quad \left[\because \sin^2 \theta = \frac{1 - \cos 2\theta}{2} \right]$$

$$= \frac{A^2}{2} \left[a - \left(\frac{a}{2n\pi} \right) \sin \frac{2n\pi a}{a} \right]_0^a$$

$$\int_{-\infty}^{\infty} |\Psi_n|^2 dx = A^2 \left(\frac{a}{2}\right) \quad \rightarrow ②$$

To normalize Ψ we must assign a value to A such that $|\Psi_n|^2 dx$ is equal to the probability P_{dx} of finding the particle between x & $x+dx$, so

$$\int_{-\infty}^{\infty} |\Psi_n|^2 dx = 1 \quad \rightarrow ③$$

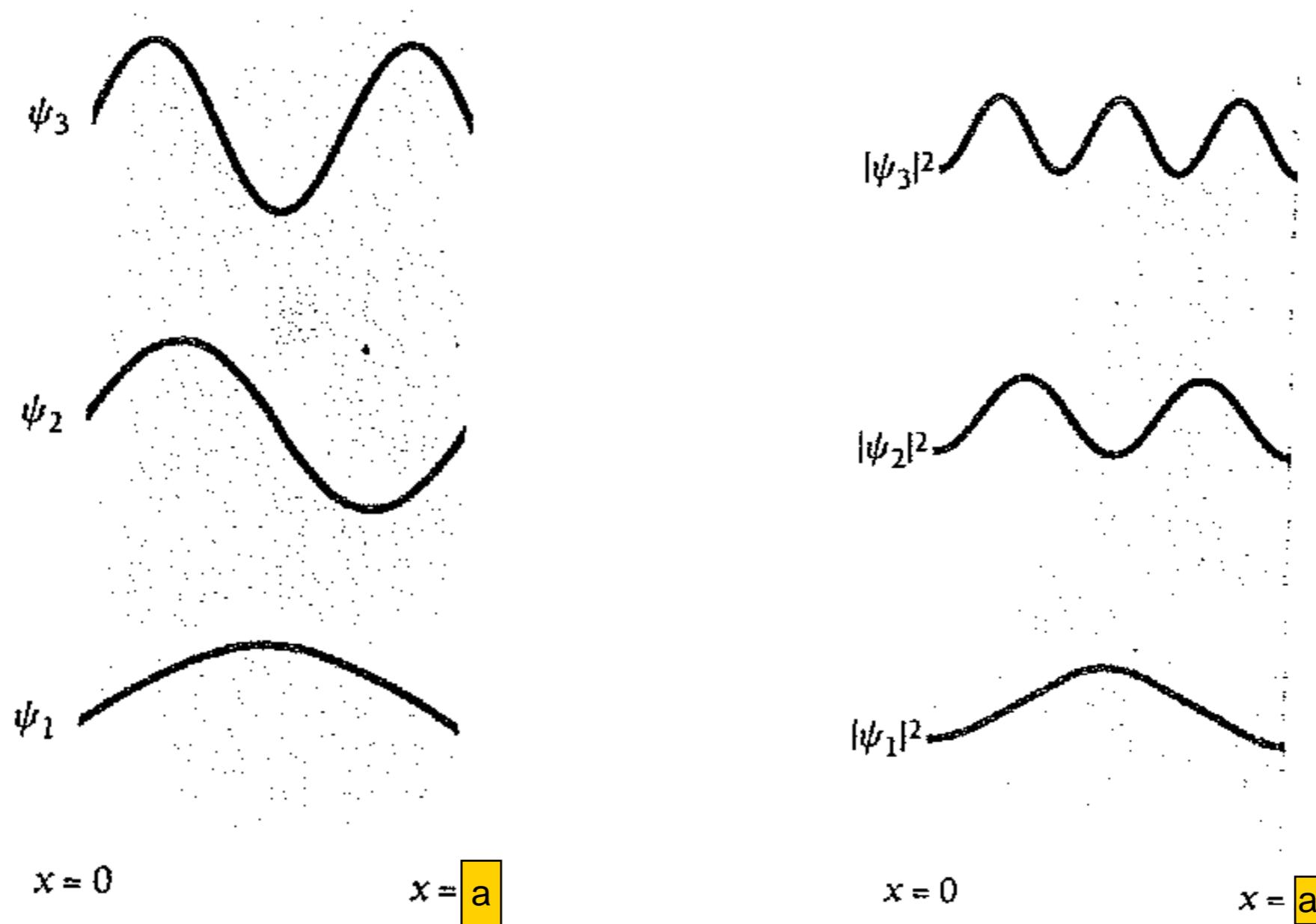
\therefore using ② & ③, we get

$$A^2 \left(\frac{a}{2}\right) = 1 \Rightarrow A = \sqrt{\frac{2}{a}}$$

\therefore The Normalized wave functions of the particle are

$$\boxed{\Psi_n = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}} \quad (n=1, 3, \dots)$$

The wave functions may be negative as well as positive, but the probability is never negative.

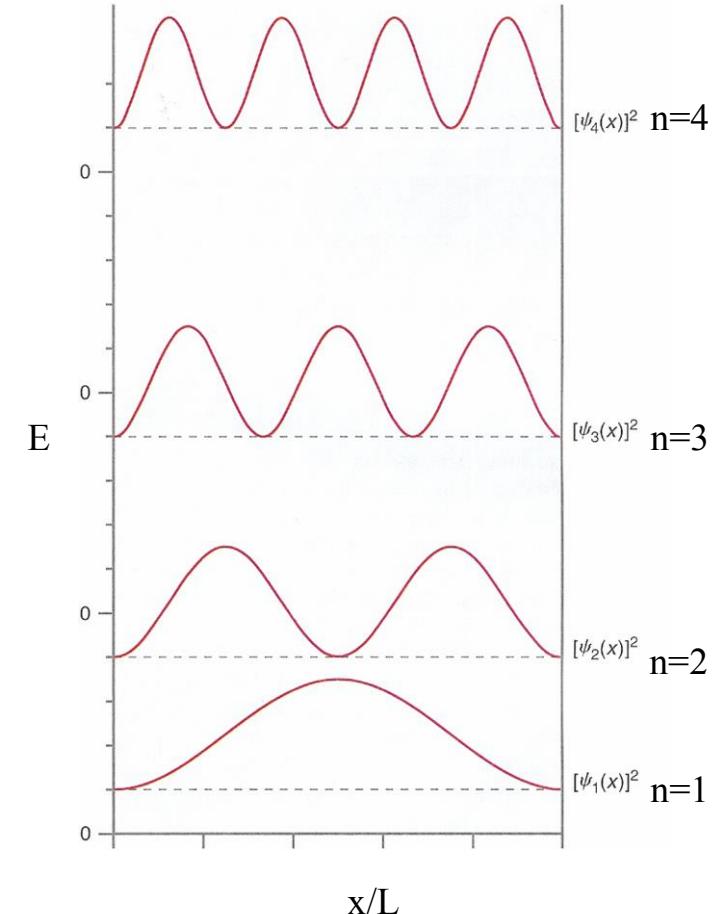
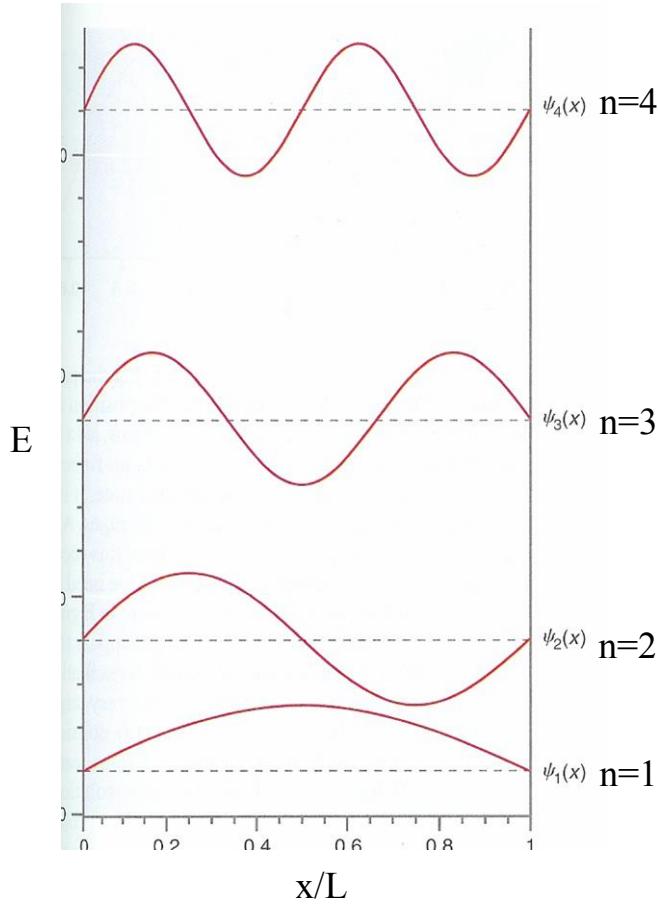


Wave functions and probability densities of a particle confined to a box with rigid walls

Graphical representation of Wavefunction, Energy and Probability

Size of the box is L here, in previous discussion we have represented it by 'a')

$$\psi_{II} = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \quad \xrightarrow{\text{Applying the Born Interpretation}} \quad |\psi_{II}|^2 = \frac{2}{L} \left(\sin \frac{n\pi x}{L} \right)^2$$



Quantum Harmonic Oscillator: Schrodinger Equation

The [Schrodinger equation](#) for a [harmonic oscillator](#) may be obtained by using the classical [spring potential](#)

$$V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2x^2 \quad \omega = \sqrt{\frac{k}{m}} = \text{angular frequency}$$
$$\omega = 2\pi \cdot \text{frequency}$$

The Schrodinger equation with this form of potential is

$$\frac{-\hbar^2}{2m} \frac{d^2\Psi(x)}{dx^2} + \frac{1}{2}m\omega^2x^2\Psi(x) = E\Psi(x)$$

Since the derivative of the wavefunction must give back the square of x plus a constant times the original function, the following form is suggested:

$$\Psi(x) = Ce^{-\alpha x^2/2}$$

Substituting this function into the Schrodinger equation by evaluating the second derivative gives

$$\frac{d\Psi}{dx} = -C \frac{\alpha}{2} e^{-\alpha x^2/2} 2x$$

$$\frac{d^2\Psi}{dx^2} = -C\alpha e^{-\alpha x^2/2} + C\alpha^2 x^2 e^{-\alpha x^2/2}$$

$$\frac{-\hbar^2}{2m}[-\alpha + \alpha^2 x^2]\Psi + \frac{1}{2}m\omega^2 x^2\Psi = E\Psi$$

For this to be a solution to the Schrodinger equation for all values of x , the coefficients of each power of x must be equal. That gives us a method for fitting the boundary conditions in the differential equation. Setting the coefficients of the square of x equal to each other:

$$\frac{-\hbar^2\alpha^2}{2m} + \frac{1}{2}m\omega^2 = 0 \quad \alpha = \frac{m\omega}{\hbar}$$

Then setting the constant terms equal gives the energy

$$\frac{-\hbar^2}{2m} \frac{m\omega}{\hbar} = E_0 = \frac{\hbar\omega}{2}$$

This is the smallest energy allowed by the uncertainty principle. [Show](#)

The energy of the quantum harmonic oscillator must be at least

$$E = \frac{(\Delta p)^2}{2m} + \frac{1}{2}m\omega^2(\Delta x)^2 \quad \begin{aligned}\Delta x &= \text{position uncertainty} \\ \Delta p &= \text{momentum uncertainty}\end{aligned}$$

Taking the lower limit from the uncertainty principle

$$\Delta x \Delta p = \frac{\hbar}{2}$$

Then the energy expressed in terms of the position uncertainty can be written

$$E = \frac{\hbar^2}{8m(\Delta x)^2} + \frac{1}{2}m\omega^2(\Delta x)^2$$

Minimizing this energy by taking the [derivative](#) with respect to the position uncertainty and setting it equal to zero gives

$$-\frac{\hbar^2}{4m(\Delta x)^3} + m\omega^2\Delta x = 0$$

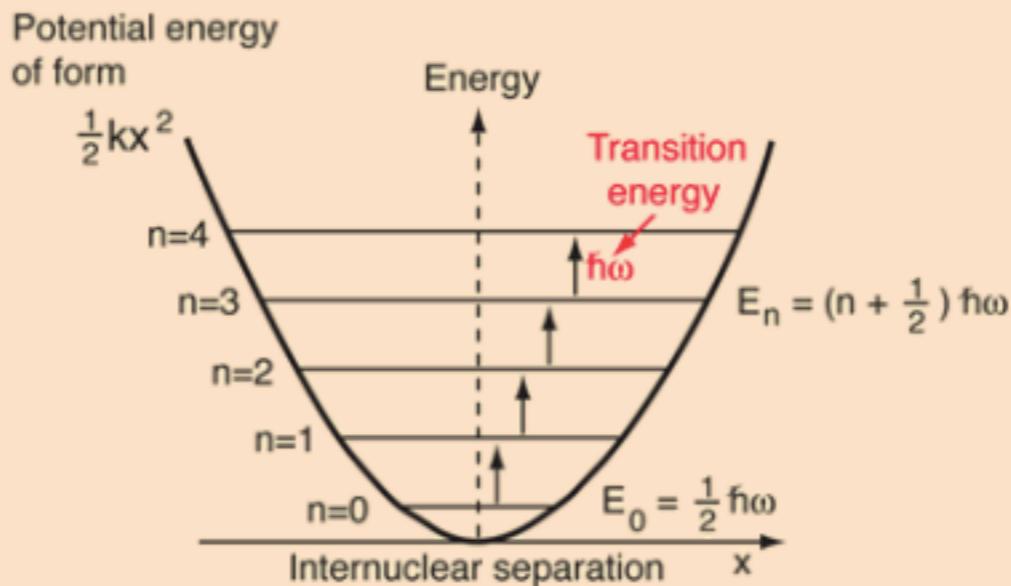
Solving for the position uncertainty gives

$$\Delta x = \sqrt{\frac{\hbar}{2m\omega}}$$

Substituting gives the minimum value of energy allowed.

$$E_0 = \frac{\hbar^2}{8m(\Delta x)^2} + \frac{1}{2}m\omega^2(\Delta x)^2 = \frac{\hbar\omega}{4} + \frac{\hbar\omega}{4} = \frac{\hbar\omega}{2}$$

The general solution to the Schrodinger equation leads to a sequence of evenly spaced energy levels characterized by a quantum number n.



The wavefunctions for the quantum harmonic oscillator contain the Gaussian form which allows them to satisfy the necessary boundary conditions at infinity. In the wavefunction associated with a given value of the quantum number n, the Gaussian is multiplied by a polynomial of order n called a Hermite polynomial. The expressions are simplified by making the substitution

$$y = \sqrt{\alpha} x \quad \text{where} \quad \alpha = \frac{m\omega}{\hbar}$$

The general formula for the normalized wavefunctions is

$$\Psi_n(y) = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(y) e^{-y^2/2}$$

$H_n(y)$ = Hermite polynomial

Comparison of classical and quantum probabilities

First four harmonic oscillator normalized wavefunctions

$$\Psi_0 = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-y^2/2}$$

$$\Psi_1 = \left(\frac{\alpha}{\pi}\right)^{1/4} \sqrt{2}y e^{-y^2/2}$$

$$\Psi_2 = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{2}}(2y^2 - 1)e^{-y^2/2}$$

$$\Psi_3 = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{3}}(2y^3 - 3y)e^{-y^2/2}$$

$$\alpha = \frac{m\omega}{\hbar} \quad y = \sqrt{\alpha}x$$

The solution of the Schrodinger equation for the first four energy states gives the normalized wavefunctions at left. These functions are plotted at left in the above illustration. The probability of finding the oscillator at any given value of x is the square of the wavefunction, and those squares are shown at right above. Note that the wavefunctions for higher n have more "humps" within the potential well. This corresponds to a shorter wavelength and therefore by the [deBroglie relationship](#) they may be seen to have a higher momentum and therefore higher energy.

The most probable value of position for the lower states is very different from the classical harmonic oscillator where it spends more time near the end of its motion. But as the quantum number increases, the probability distribution becomes more like that of the classical oscillator - this tendency to approach the classical behavior for high quantum numbers is called the [correspondence principle](#).

n	$H_n(y)$	E_n
0	1	$\frac{1}{2}\hbar\omega$
1	$2y$	$\frac{3}{2}\hbar\omega$
2	$4y^2 - 2$	$\frac{5}{2}\hbar\omega$
3	$8y^3 - 12y$	$\frac{7}{2}\hbar\omega$
4	$16y^4 - 48y^2 + 12$	$\frac{9}{2}\hbar\omega$
5	$32y^5 - 160y^3 + 120y$	$\frac{11}{2}\hbar\omega$

When the Schrodinger equation for the harmonic oscillator is solved by a series method, the solutions contain this set of polynomials, named the Hermite polynomials.

The [Schrodinger equation](#) for a [harmonic oscillator](#) may be solved to give the wavefunctions illustrated below.

