Quantum mechanics

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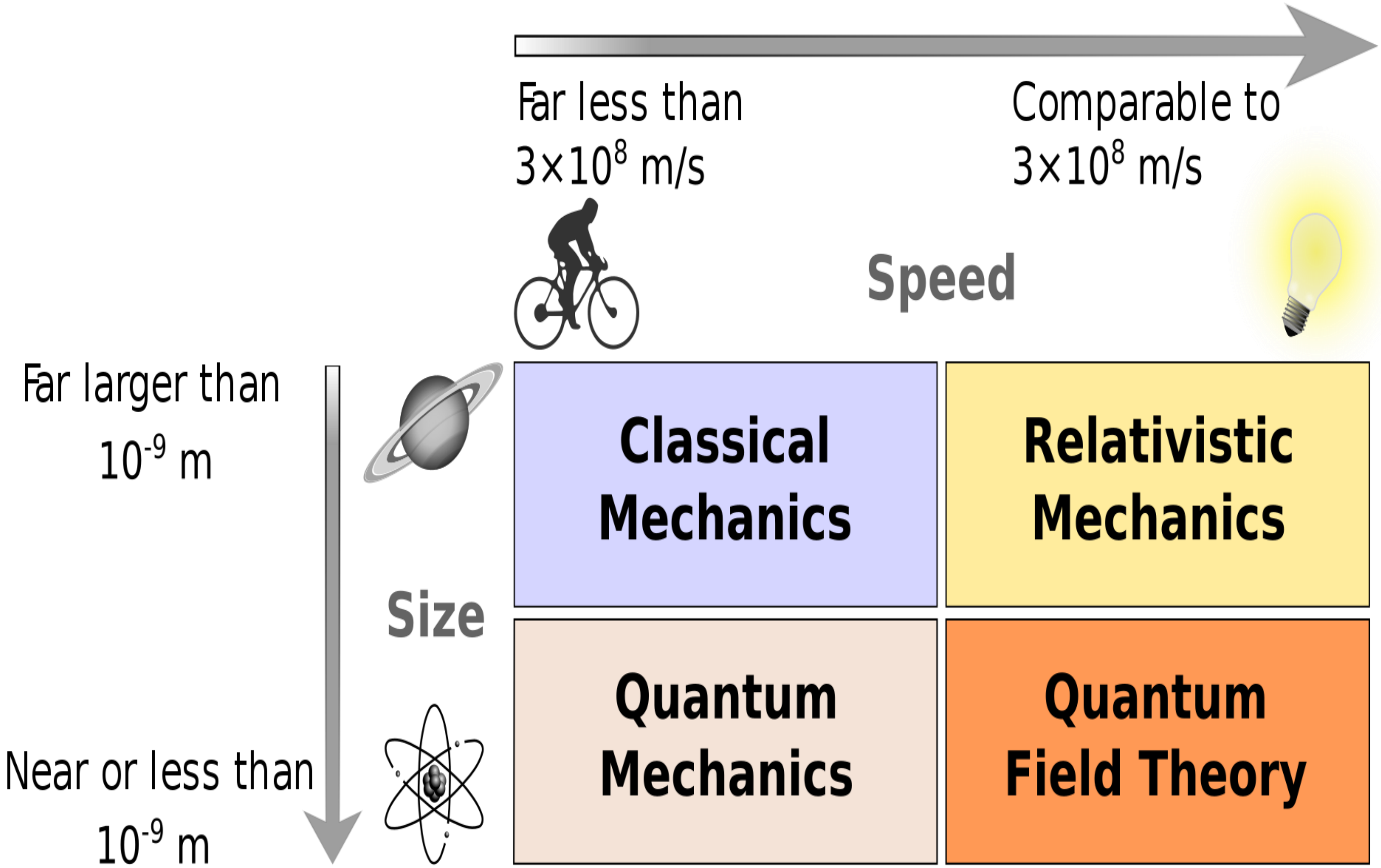
If quantum mechanics hasn't profoundly shocked you, you haven't understood it yet.

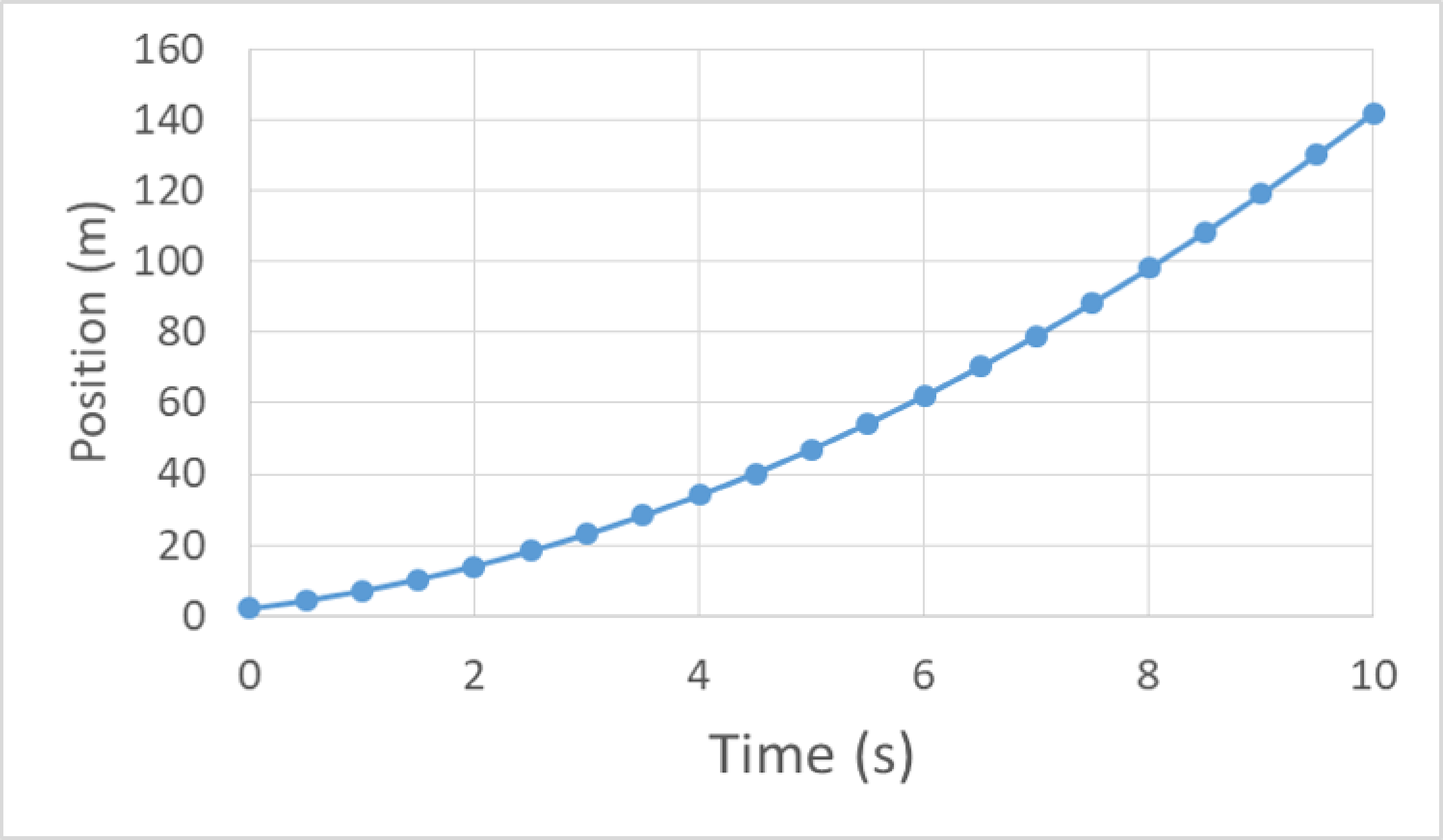
---- Niels Bohr

Niels Bohr, Danish Physicist, 1885-1962



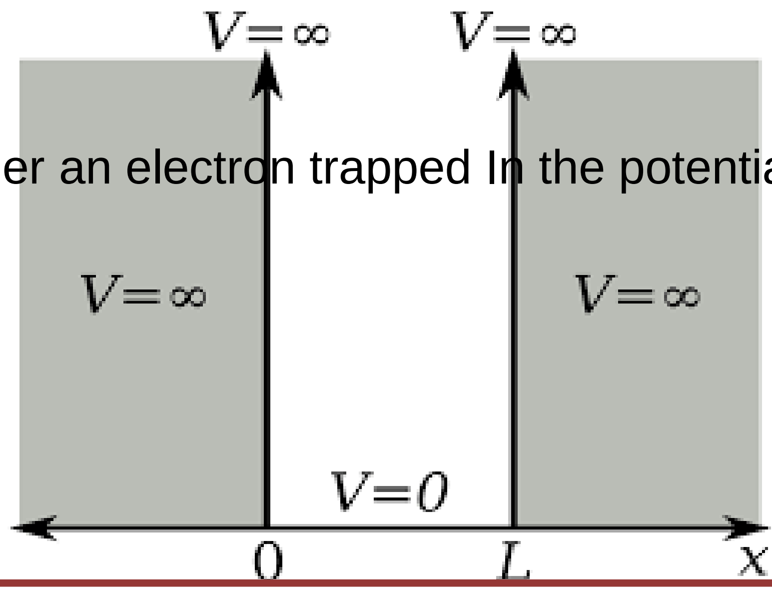
Far less than
3×10^8 m/s
Comparable to
3×10^8 m/s
Speed
Far larger than
10^{-9} m
Size
Near or less than
10^{-9} m
Classical Mechanics
Relativistic Mechanics
Quantum Mechanics
Quantum Field Theory

Classical mechanics or Newtonian mechanics



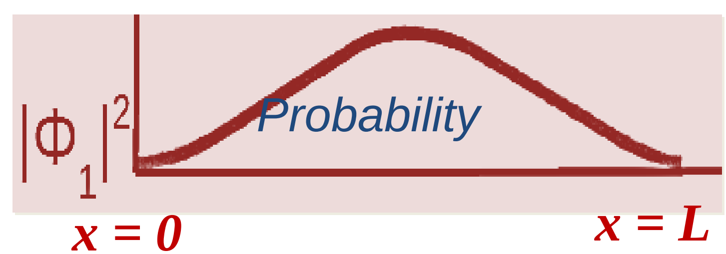
In classical physics, once the initial position and velocity of a particle and force acting on it is specified, we know it’s motion afterwards completely.

Electron in a potential box



Consider an electron trapped In the potential box

A quantum particle is represented by wavefunction, the wavefunction has all the information about the particle



Quantum mechanics: a probabilistic description of the world?

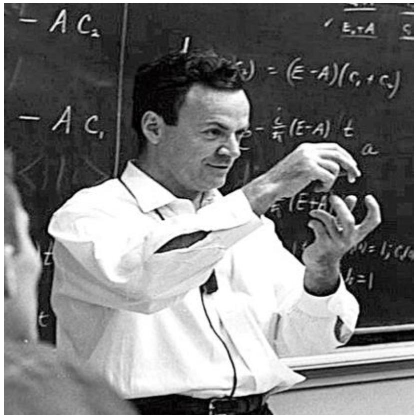
“God does not play dice with the universe.”

A. Einstein

Albert EINSTEIN
(1879-1955)

“I think I can safely say that nobody understands quantum mechanics.”

Richard Feynman

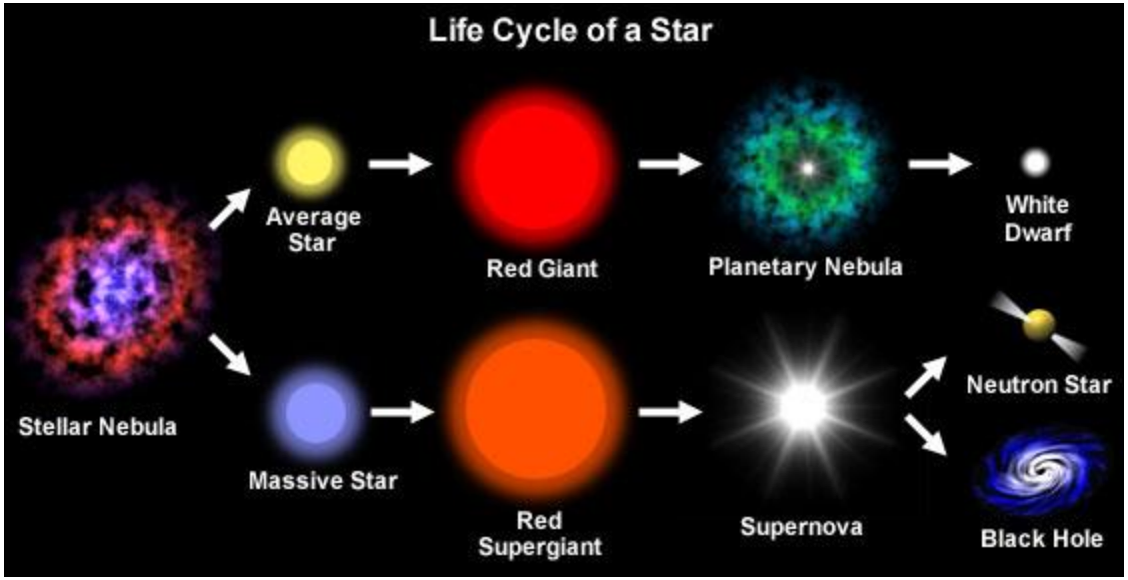


Richard Feynman
(1918-1988)

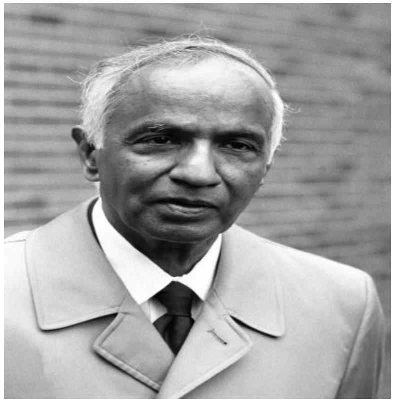
Stephen Hawkins
(1942-2018)

“Not only does God play dice but... he sometimes throws them where they cannot be seen.”

Stephen Hawking

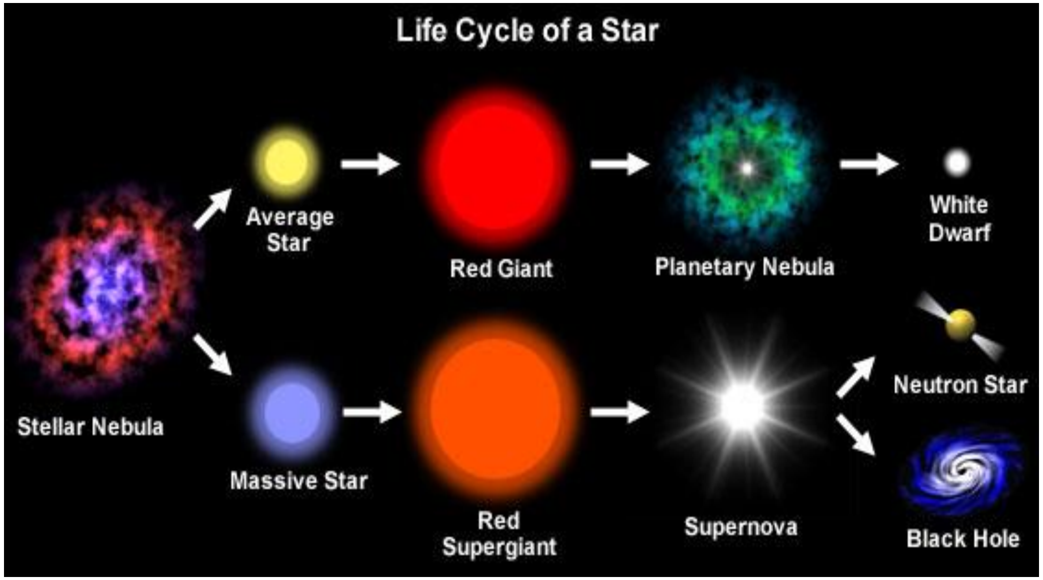


When all the hydrogen is converted into helium, the starts to die. Depending On mass of the star can turn into a white dwarf or black hole.



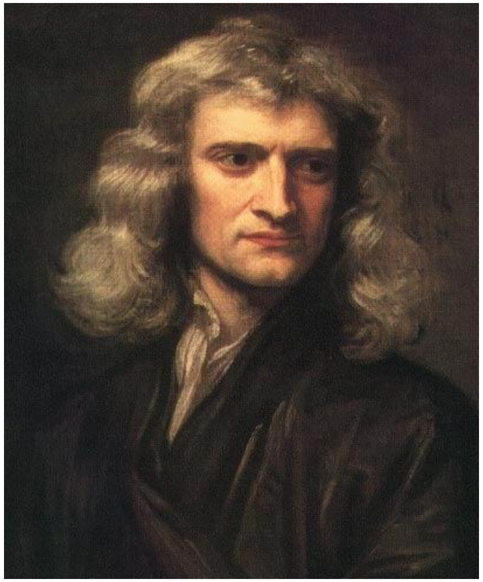
S. Chandrasekhar
1910-1995

S. Chandrasekhar used quantum mechanics with the special theory of relativity to explain the formation of white dwarf.



Light is a wave or a particle?

There had been continuous debate about the nature of light dating back to the 1600s, when competing theories of light were proposed by Huygens and Newton.



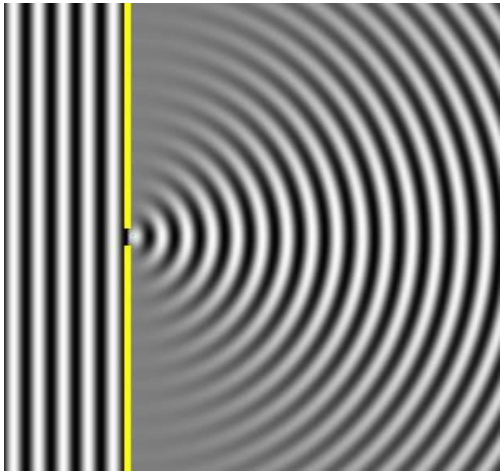
Christian Huygens
1629-1695
light is a wave

Sir Isaac Newton
1643-1727
light consists of particles (corpuscles)

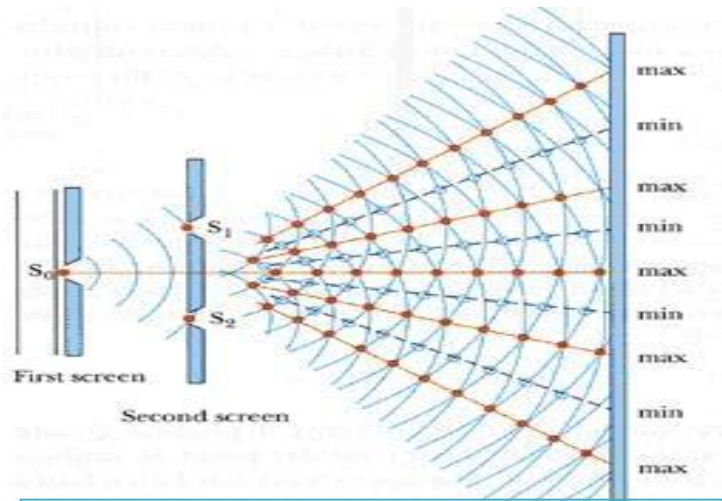
Light is a wave!!!

Light exhibits wave characteristics such as interference and diffraction, therefore it is wave .

Diffraction of waves: light bends around a corner when encounters an aperture or an obstacle.



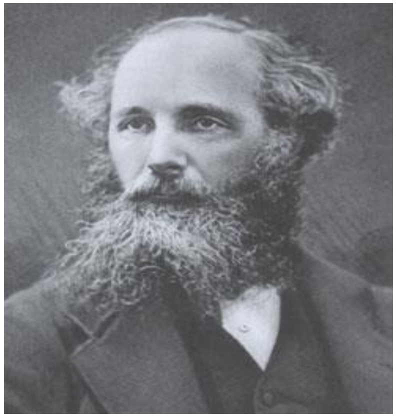
Thomas Young (1773 - 1829), a British scientist.



Young's double slit experiment

Light is a wave!!!

Light exhibits wave characteristics such as interference and diffraction, therefore it is wave .



James Clerk Maxwell (1831 – 1879), a Scottish scientist

Maxwell's Equations	Maxwell's Equations
Differential form	Integral form
$\nabla \cdot \vec{E} = \frac{\rho}{\varepsilon_0}$	$\oint \vec{E} \cdot d\vec{a} = \frac{Q_{enc}}{\varepsilon_0}$
$\nabla \times \vec{E} = \boxed{-\frac{\partial \vec{B}}{\partial t}}$	$\oint \vec{E} \cdot d\vec{l} = \boxed{-\int \frac{\partial \vec{B}}{\partial t} \cdot d\vec{a}}$
$\nabla \cdot \vec{B} = 0$	$\oint \vec{B} \cdot d\vec{a} = 0$
$\nabla \times \vec{B} = \mu_0 \vec{J} + \boxed{\mu_0 \varepsilon_0 \frac{\partial \vec{E}}{\partial t}}$	$\oint \vec{B} \cdot d\vec{l} = \mu_0 I_{enc} + \boxed{\mu_0 \varepsilon_0 \int \frac{\partial \vec{E}}{\partial t}}$

$$\frac{\partial^2 E}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 E}{\partial t^2} \quad \text{and} \quad \frac{\partial^2 B}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 B}{\partial t^2} \qquad (5)$$

for the electric Field　　　for the magnetic Field

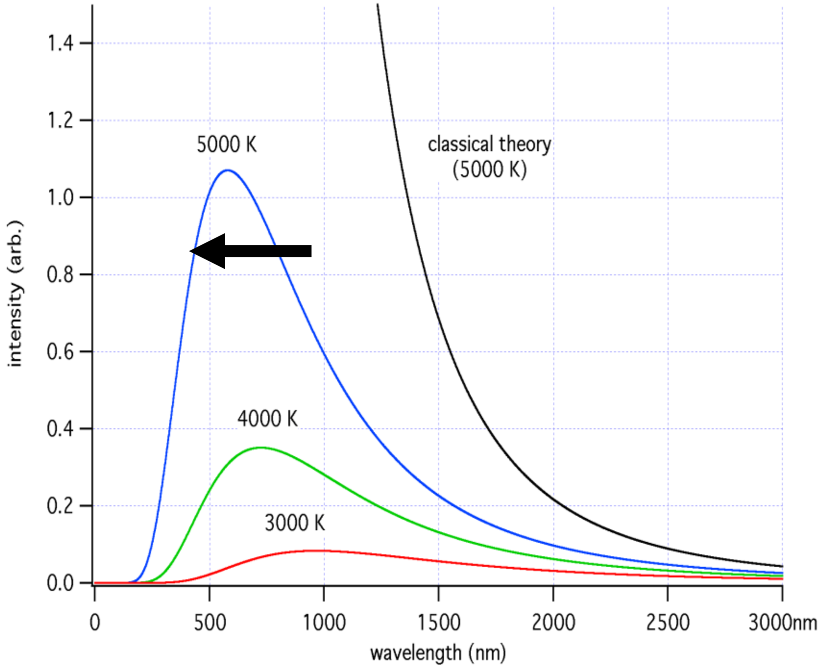
where $\frac{1}{c^2} = \varepsilon_o \mu_o$

Laws of electromagnetics, the electromagnetic wave equations.

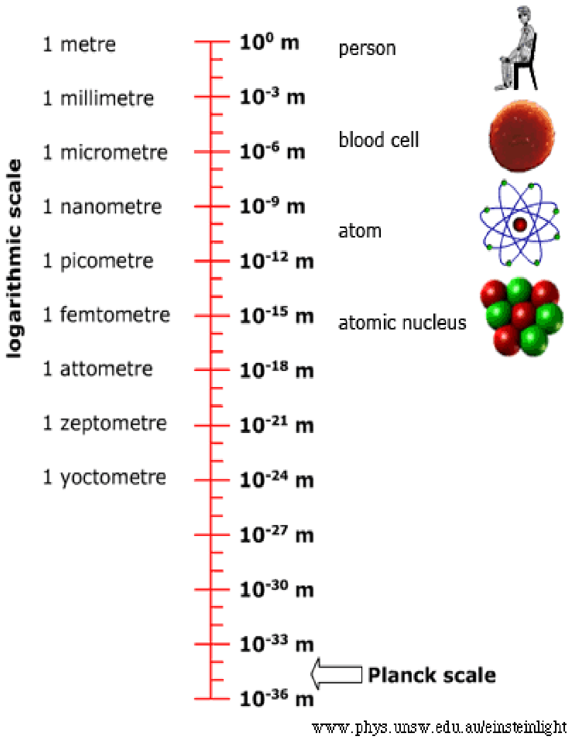
Light is a particle!!!

Black-body radiation

Electromagnetic wave should be quantized in order to explain the black body radiation (Quantization of Radiation, Max Plancks 1900)



Max Planck (1901)
Göttingen



RED
Small **n**

WHITE
Large **n**

Exchange of energy should be quantized

E* = *hv, *where n is an integer*

Plancks constant, $\boldsymbol{h} = 6.63 \times 10^{-34}$ *Js*

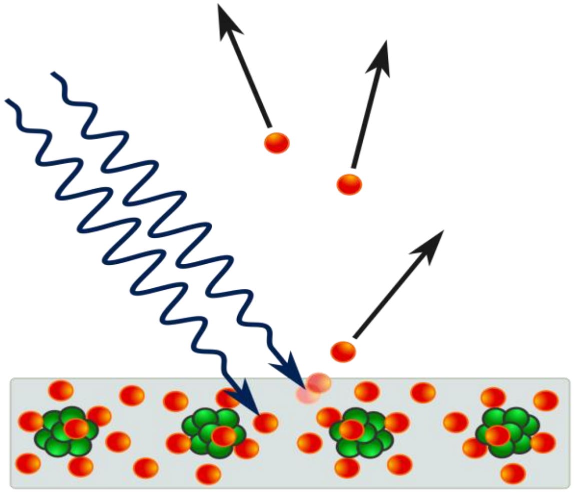
'

'

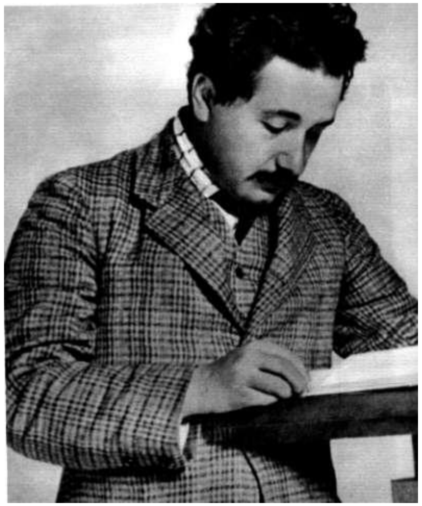
Light is a particle!!!

Photoelectric Effect (1887-1905)
discovered by Hertz in 1887 and explained in 1905 by Einstein

Heinrich HERTZ
(1857-1894)



$$K_{max} = h\nu - W$$



Albert EINSTEIN
(1879-1955)

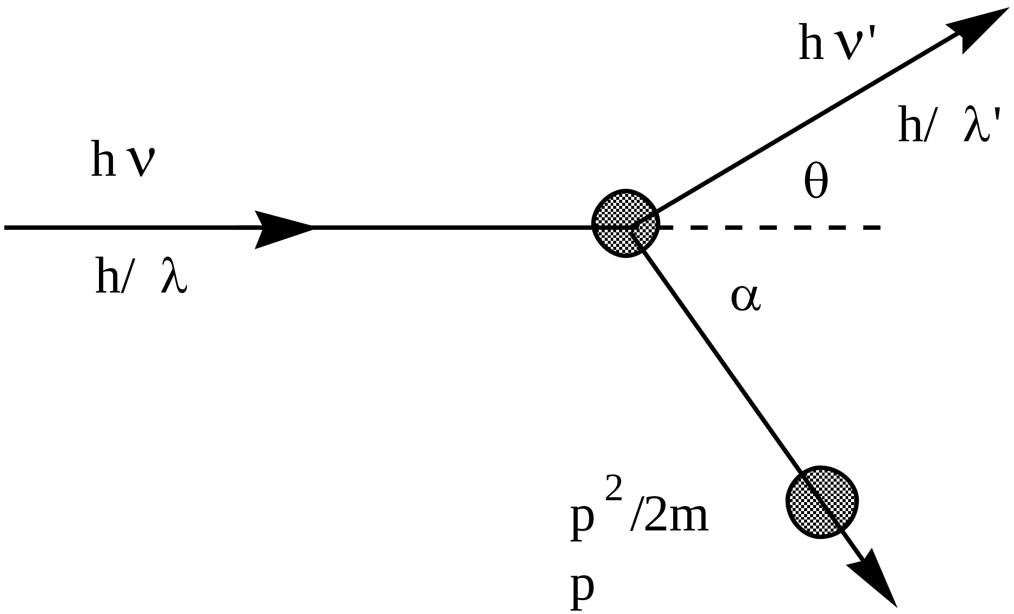
- Energy of the emitted electrons depend on the photon frequency.
- Number of emitted electrons depend on the photon intensity not on the frequency.

Striking out of an electron from metal surface involves only one electron and one photon.

Light is a particle!!!

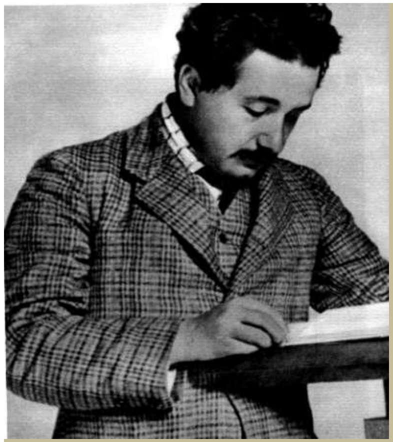
Compton effect 1923

Arthur Holly Compton
American, 1892-1962



Scattering of a photon by charged particle, usually an electron. If it results in a decrease in energy (increase in wavelength) of the photon it is called the **Compton effect**.

Einstein on wave particle duality and light



"It seems as though we must use sometimes one theory and sometimes the other, while at times we may use either. We are faced with a new kind of difficulty. We have two contradictory pictures of reality; separately neither of them fully explains the phenomena of light, but together they do."

Wave particle duality and matter wave

Louis de BROGLIE
French (1892-1987)

de Broglie hypothesis:

In a way similar to the light which can behave as wave as well as particle, electrons also have wave-like properties.

A photon of light of frequency v has the momentum

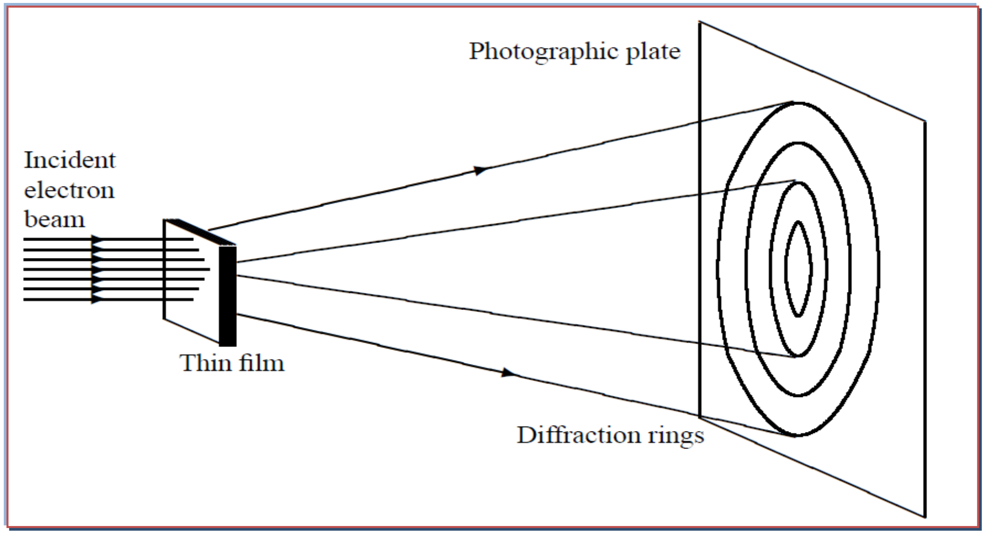
$$p=\frac{h\nu}{c}=\frac{h}{\lambda}\,;\, since\; c=\nu\lambda$$

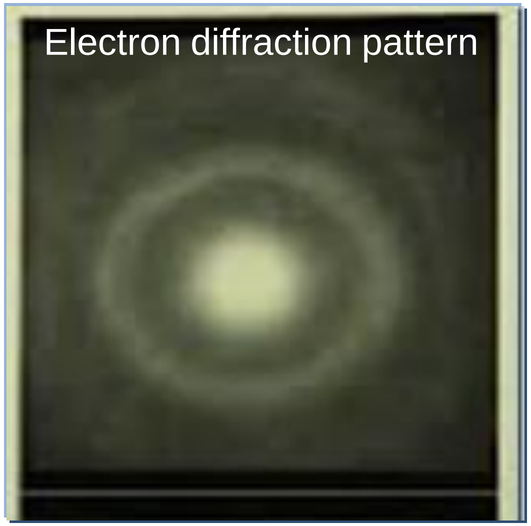
The wavelength of photon is specified by the momentum according to the relation

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

Thus, according to de Broglie the last relation connecting momentum and wavelength is not only valid for photons but also for matter wave (electrons, protons, etc).

Diffraction of electrons and Matter wave

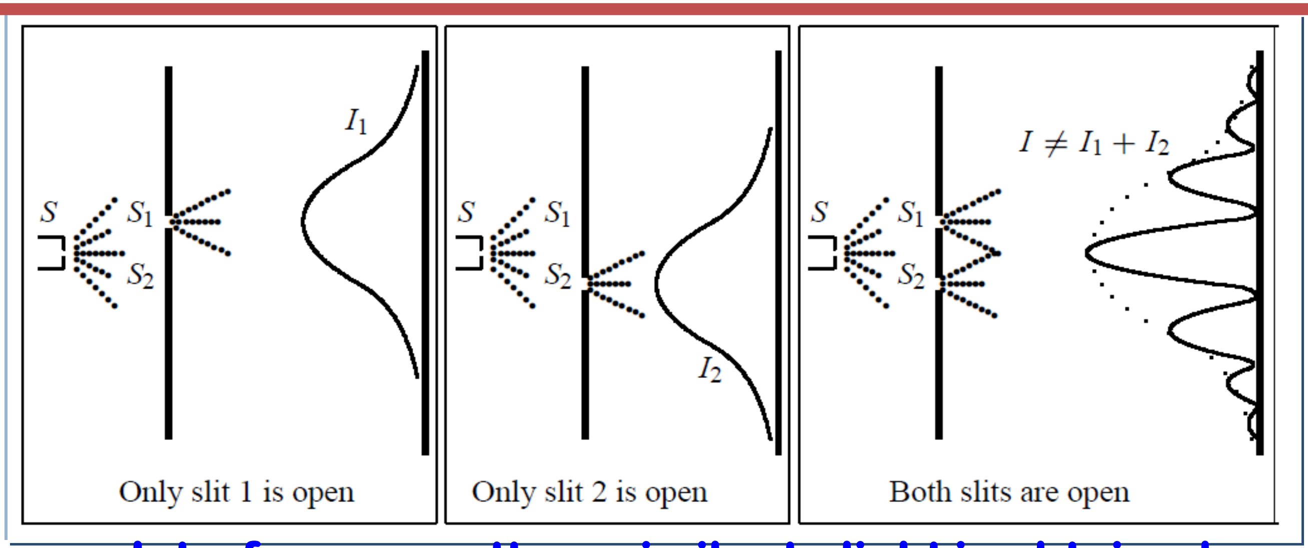




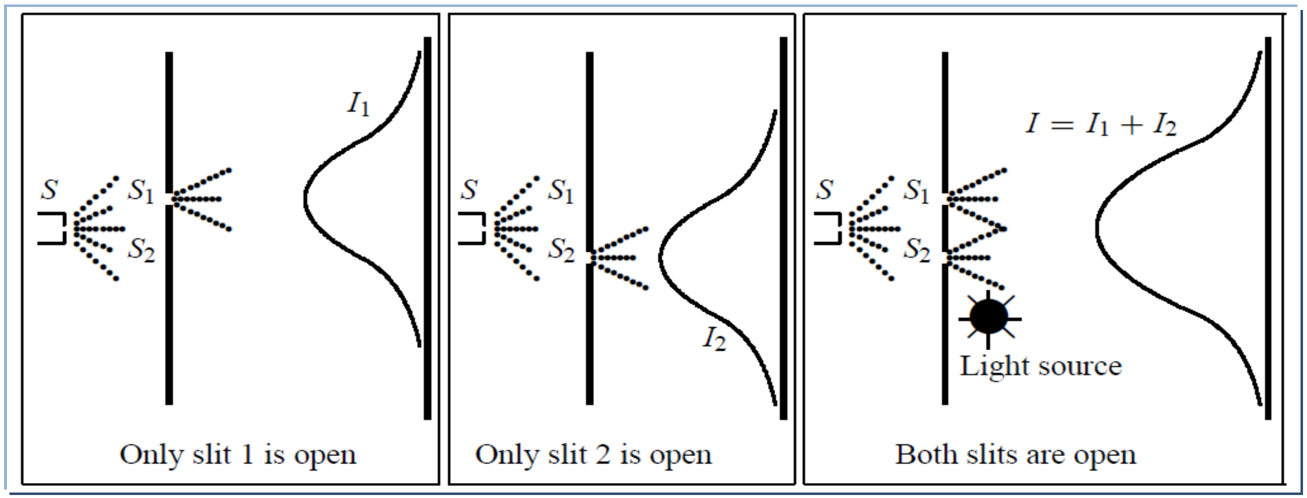
Electron diffraction obtained by George Paget Thomson, an English physicist (a Nobel Prize winner for physics)

G. P. Thomson's father J. J Thomson got the nobel prize for discovering electron which he believed to be a particle.

Double-slit experiment for electrons



Interference pattern similar to light is obtained



When tried to find through which slit the electron passes destroys the interference pattern.

Wave particle duality and complementary principle

The complementarity principle holds that objects have certain pairs of complementary properties which cannot all be observed or measured simultaneously.

Note: it has nothing to do with the resolution of the instruments used in the measurement process.

Niels Bohr, Danish Physicist, 1885-1962

Heisenberg uncertainty principle:position-momentum

It is impossible to determine both position and momentum of an object with infinite precision at any instant.”

$$\boxed{\Delta x \, \Delta p \geq \frac{h}{4\pi}}$$

Heisenberg,
German theoretical
Physicist, 1901-76

In other words, the product of uncertainties in position and momentum In a measurement cannot be less than a certain minimum value as indicated in above expression.

These uncertainties have nothing to do with the resolutions or other limitations of experimental set up. Rather it is indicative of probabilistic nature of particle dynamics.

Uncertainty principle: Energy-time

Similarly, the energy of a particle and the instant of its measurement cannot be determined with infinite precision.

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

Planck's constant *h* is so small that limitation imposed by uncertainty principle are significant only in the atomic scale.

These uncertainties have nothing to do with the resolutions or other limitations of experimental set up. Rather it is indicative of probabilistic nature of particle dynamics.

General Comments

Quantum mechanics provides the description of the behaviour of matter especially on atomic, subatomic, scale as well of light in all its details. Behavior of protons, neutrons, electrons etc. is very different from ordinary object that we experience in our life and therefore it is very difficult to understand these wave-like particles and get used to it.

In quantum mechanics, the concept trajectory does not exist. We can only talk about the probability of finding the particle at some given point. This is completely different from classical mechanics, where future of the particle is completely determined by its initial position, momentum and the forces acting upon it.

General Comments (cont..)

The classical or Newtonian mechanics is an approximation of quantum mechanics (in the limit $h \rightarrow 0$). For example, take $h \rightarrow 0$, you see de-Broglie wave-length $\lambda \rightarrow 0$ vanishes. this is precisely the classical limit.

The people who contributed mostly to the development of quantum mechanics

- Max Plank, (Quantization of radiation)
- Albert Einstein, (light consists of quantum of energy like a particle)
- Niels Bohr, (Bohr model of atom)
- Louis de Broglie, (Matter wave)
- Max Born, (Probabilistic interpretation of quantum mechanics)
- Paul Dirac, (Matter-antimatter)
- Werner Heisenberg, (Matrix formulation of quantum mechanics)
- Wolfgang Pauli,(two fermions cannot occupy the same state)
- Erwin Schrödinger, (wavefunction for the quantum particle)
- Richard Feynman (path integral formulation of quantum mechanics)

Note: the list is not exhaustive

Indeed, we don’t have immediate experience with quantum particles, but it is a fact that the quantum particles and their peculiar behavior play a central role in the appearance of matter whether on the earth or elsewhere in it’s current form. Therefore, quantum mechanics that describes the behavior of quantum particle is a very important tool in order to understand the universe.

Schrodinger Equation

We know how to describe wave or particle but what about something which exhibits both properties

Wave motion can be described by the solution of a second order differential equation involving derivative with respect to position as well as time.

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$$

Particle motion can be described by the solution of a second order differential equation involving time derivative.

$$\vec{F} = m\frac{d^2\vec{r}}{dt^2}$$

What kind of differential equation is needed to describe something which can exhibit wave or particle like properties in appropriate circumstances?

Schrodinger Equation

A quantum particle should be described by a complex wavefunction which is a solution of so called '**Schrodinger equation**".

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi}{\partial x^2}+\frac{\partial^2\Psi}{\partial y^2}+\frac{\partial^2\Psi}{\partial z^2}\right)+U\Psi$$

Here, *m* is mass of the particle and *U* is the potential energy of the particle. First order in time derivative and second order in position derivative.

This differential equation, whose solution are complex function, is fundamental to quantum mechanical description of a particle.

Erwin Schrödinger

If the particle motion is limited to 1-dimension (x,t) the above equation becomes

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi}{\partial x^2}\right)+U\Psi$$

In the following, we will try to understand this equation in more details

Before that let us ask a simple question. What is the Schrodinger equation for free particle?

Meaning and significance of the wave function

- The state of a quantum particle is described by a complex function which is often called a wavefunction. All the relevant information of particle motion can be obtained from it's wavefunction.

- The complex wavefunction contains the information about the phase of a particle, which is essential because the particle is behaving like a wave. Therefore, wave-like properties such as interference effect can be explained for the quantum particle.

- Although, the complex wave function $\Psi(x,y,z,t)$ itself is not an observable quantity (something which can be measured experimentally). But its modulus square $|\Psi(x,y,z,t)|^2$ gives the probability of finding the particle at point x, y, z, at time instant t.

- A larger value of $|\Psi(x,y,z,t)|^2$ means stronger probability of finding the object at a given point. A smaller value of $|\Psi(x,y,z,t)|^2$ means lesser probability of object's presence.

Normalization

The wave function must be normalizable. Since $|\Psi|^2$ is the *probability density* of finding object *described by* Ψ**,** integral of over all space must be finite and unity.

$$\boxed{\int_{-\infty}^{\infty} |\Psi|^2 dV = 1}$$

where dV = dxdydz, three dimensional integral

Non-normalizable wave function can not represent particle. A normalized wave function stays normalized for ever (particle conservation!!!).

Note: normalization simply states that the wavefunction should be chosen in such a wave that the overall probability of finding the particle in entire space should be one. The particle should be somewhere, it cannot simply disappear or a part of it shouldn't disappear(**It seems reasonable right!!!!!**).

Conditions for a well-behaved wave function

- The wavefunction Ψ of the particle must be continuous. So that there is no sudden jump in the probability. (Sudden jump in probability means as if there is some source or sink of a particle).

- It should also be single valued because probability can have one value at a particular place and time.

- The partial derivatives $\partial\Psi/\partial x$, $\partial\Psi/\partial y$ and $\partial\Psi/\partial z$ be finite and continuous. This requirement conforms to the fact that momentum of the particle is preserved.

- Ψ must be normalizable which means that Ψ must go to zero as $x\rightarrow\infty$.

How to extract information from a wave function

Expectation value : The wave function $\Psi(x,y,z,t)$ contains all information about the particle. Suppose if a particle is confined in x-direction, then

Expectation value <x> or the average location of the particle or simply the average position.

The probability P that the particle is found in interval dx at x. This probability is :

$$P = |\Psi|^2 \, dx$$

Where Ψ is the particle wave function at x. Making these substitutions in equation, the expectation value of the position of a single particle is given by

$$\langle x \rangle = \frac{\int_{-\infty}^{\infty} x |\Psi|^2 \, dx}{\int_{-\infty}^{\infty} |\Psi|^2 \, dx}$$

If Ψ is a normalized wave function then denominator is 1 (because the particle exists somewhere between x = +∞ and x = - ∞). In that case

Expectation value for position

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\Psi|^2 dx$$

Physically <x> is the average of a large number of independent hypothetical measurements performed in the state Ψ. Equivalently speaking, it can also be viewed as the average value of position for a large number of particles which are described by the same wavefunction.

For example, the expectation value of the radius of the electron in the ground state of the hydrogen atom is the average value you expect to obtain from making the measurement for a large number of hydrogen atoms.

Probability of finding the particle within a given interval (one dimensional case)

For a normalized wave function Ψ, the probability that the particle will be found between x_1 and x_2 (if motion is restricted in x direction) is given by

$$P_{x_1 x_2} = \int_{x_1}^{x_2} |\Psi|^2 \, dx$$

What about momentum or energy average?

How should we calculate?

For each observable, there is a corresponding operator

For position there is position operator, for momentum there is momentum operator, for energy there is energy operator

Consider a free particle wave function is given by

$$\Psi = A\, e^{-(i/\hbar)(Et - px)}$$

Differentiating above equation w.r.t. x and t gives

$$\frac{\partial \Psi}{\partial x} = \frac{i}{\hbar} p A\, e^{-(i/\hbar)(Et-px)} = \frac{i}{\hbar} p \Psi$$

$$\Rightarrow p\Psi = \frac{\hbar}{i}\frac{\partial}{\partial x}\Psi$$

$$\frac{\partial \Psi}{\partial t} = -\frac{i}{\hbar} E A\, e^{-(i/\hbar)(Et-px)} = -\frac{i}{\hbar} E \Psi$$

$$\Rightarrow E\Psi = i\hbar\frac{\partial}{\partial t}\Psi$$

If you substitute
$E = \hbar\omega$ and $p = \hbar k$
You will be able to show that free particle wave function changes to $\Psi = A\, e^{-i(\omega t - kx)}$, which looks familiar!!!!!

These operators may act on a wave function to yield the same wavefunction multiplied by a number, The number is called eigenvalue of the operator. The wave function is called eigen function.

Momentum and Energy Operators

$$p\Psi = \frac{\hbar}{i}\frac{\partial}{\partial x}\Psi \Rightarrow \hat{p} = -i\hbar\frac{\partial}{\partial x}$$

$$E\Psi = i\hbar\frac{\partial}{\partial t}\Psi \Rightarrow \hat{E} = i\hbar\frac{\partial}{\partial t}$$

Momentum operator
Energy operator

Just above we obtained the mathematical definition of momentum and energy operator. Note that even though they are derived for free particle, they are entirely general. Noting that energy operator is sum of kinetic energy and potential energy.

$$E = \frac{p^2}{2m} + U$$

multiplying both sides by Ψ

$$\Rightarrow E\Psi = \frac{p^2}{2m}\Psi + U\Psi$$

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi}{\partial x^2}\right) + U\Psi$$

Schrodinger equation in 1-d

where in the last line, we replaced momentum and energy by the momentum and energy operator, respectively.

Average value of momentum and energy

Expectation value of *p for normalized wave function* is given by

$$\langle p \rangle = \int_{-\infty}^{\infty} \Psi^* \hat{p} \Psi \, dx = \int_{-\infty}^{\infty} \Psi^* \left(-i\hbar \frac{\partial}{\partial x}\right) \Psi \, dx$$

$$= -i\hbar \int_{-\infty}^{\infty} \Psi^* \frac{\partial \Psi}{\partial x} dx$$

Expectation value of *E* is given by

$$\langle E \rangle = \int_{-\infty}^{\infty} \Psi^* \hat{E} \Psi \, dx = \int_{-\infty}^{\infty} \Psi^* \left(i\hbar \frac{\partial}{\partial t}\right) \Psi \, dx$$

$$= i\hbar \int_{-\infty}^{\infty} \Psi^* \frac{\partial \Psi}{\partial t} dx$$

Remember operators should be inserted between Ψ* and Ψ.
Expectation value of any observable G(x,p) can be calculated as

$$\boxed{\langle G(x,p) \rangle = \int_{-\infty}^{\infty} \Psi^* \hat{G} \Psi \, dx}$$

Time-independent Schrodinger equation

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi}{\partial x^2}\right)+U\Psi \qquad \textit{Where } U = U(x,t)$$

For a particle whose potential energy doesn't depend on time explicitly, forces acting on the particle and hence, potential energy U, vary with position of the particle only,i,.e, $U(x)$. In that case, Schrodinger equation can be simplified using variable separation method.

The wave function can be written as $\Psi(x,t)=\phi(x)\, f(t)$

$$\frac{\partial\Psi(x,t)}{\partial x}=\frac{d\varphi(x)}{dx}f(t)$$

$$\frac{\partial^2\Psi(x,t)}{\partial x^2}=\frac{d^2\varphi(x)}{dx^2}f(t)$$

$$\frac{\partial\Psi(x,t)}{\partial t}=\varphi(x)\frac{df(t)}{dt}$$

Time-independent Schrodinger equation

Using above equations in Schrodinger equations

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi}{\partial x^2}\right)+U\Psi$$

$$i\hbar\varphi(x)\frac{df(t)}{dt}=-\frac{\hbar^2}{2m}f(t)\frac{d^2\varphi(x)}{dx^2}+U\varphi(x)f(t)$$

Finally we divide by $\phi(x)\,f(t)$ on both sides to obtain

$$i\hbar\frac{1}{f(t)}\frac{df(t)}{dt}=-\frac{\hbar^2}{2m}\frac{1}{\varphi(x)}\frac{d^2\varphi(x)}{dx^2}+U$$

L.H.S. is function of time t only and the R.H.S. is function of diplacement x only, which possible only when both sides are equal to some constant.

Time-independent Schrodinger equation

Let the constant is E. Then

$$i\hbar \frac{1}{f}\frac{df}{dt} = E$$

$$\Rightarrow \frac{df}{dt} = -\frac{iE}{\hbar} f$$

$$f(t) = C\,\mathrm{e}^{\frac{-iEt}{\hbar}}$$

(I am getting rid of writing f as function of t and Φ as function of x).

And $$-\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2} + U\varphi = E\varphi$$

You can easily see that E is energy of the particle (why?)

Therefore, general solution for equation is given by

$$\Psi(x,t) = \varphi(x)\,\mathrm{e}^{\frac{-iEt}{\hbar}}$$

where constant C is absorbed in Φ(x).

This is time-independent (steady state) Schrodinger equation. It is called steady state because the probability doesn't depend on time

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2}+U\varphi=E\varphi$$

can be generalized to three dimension as follows

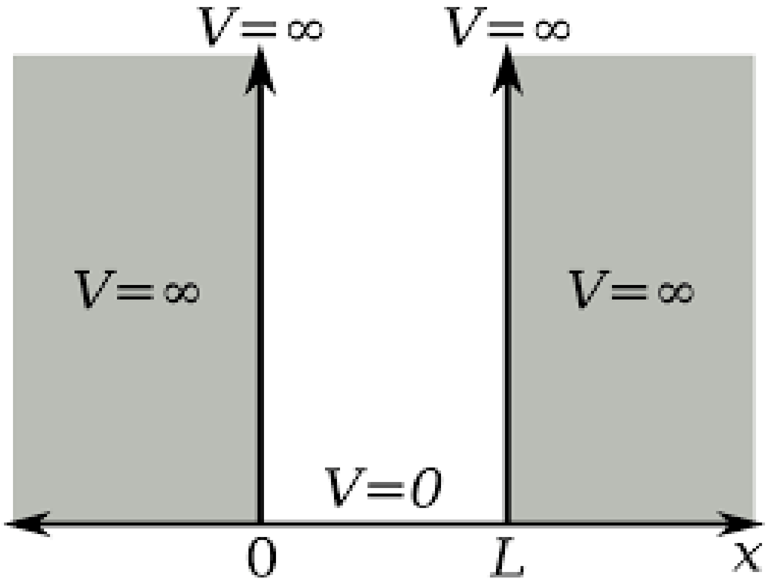
$$-\frac{\hbar^2}{2m}\left(\frac{d^2\varphi}{dx^2}+\frac{d^2\varphi}{dy^2}+\frac{d^2\varphi}{dz^2}\right)+U\varphi=E\varphi$$

Particle in a box or infinite well

❖ Consider a particle of mass *m* trapped in a box of length L, the particle motion is restricted to $x = 0$ to $x = L$. It is a one dimensional box.

❖ The potential corresponding to the box, is taken to be zero inside the box and infinite for $x < 0$ and $x > L$.

❖ Since particle can not have infinite energy, it can not be found outside box, and so the wave function Φ and hence the probability $|\Phi|^2$ is zero for $x \leq 0$ and $x \geq L$.



Solving the Schrodinger equation for particle in a box

The Schrodinger equation is given by (potential does not depend on time)

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2}+U\varphi=E\varphi$$

For particle inside the box, above equation becomes

$$\frac{d^2\varphi}{dx^2}+\frac{2mE}{\hbar^2}\varphi=0$$

The general solution of this equation (S.H.O.) is given by

$$\varphi=A\sin\frac{\sqrt{2mE}}{\hbar}x+B\cos\frac{\sqrt{2mE}}{\hbar}x$$

The wave function must vanish for x=0 and x=L (i.e. Φ=0 for x=0 and x=L). A and B are constants to be calculated.

Note: Boundary condition is the reflection of the fact that particle cannot enter into the region of infinite potential or it cannot penetrate the infinite potential wall. Because it will need infinite energy which it does not have. If it has infinite energy then it will simply escape the potential well.

Solving the Schrodinger equation for particle in a box

$$\varphi = A\sin\frac{\sqrt{2mE}}{\hbar}x + B\cos\frac{\sqrt{2mE}}{\hbar}x$$

At x=0, first term vanishes because sin(0) = 0. But cos(0) =1, therefore second term does not vanish. But, we require that φ to vanish at $x = 0$ as the probability of the particle should vanish at both x = 0 and x = L. Therefore, ***B*** should vanish. The new wavefunction is

$$\varphi = A\sin\frac{\sqrt{2mE}}{\hbar}x$$

But this φ will vanish at x = L only when

$$\frac{\sqrt{2mE}}{\hbar}L = n\pi \qquad n = 1,2,3\ldots\ldots$$

Why don't we include n = 0 and E = 0 ?

Energy of the particle in infinite potential well

Thus,
$$\frac{\sqrt{2mE}}{\hbar} L = n\pi \qquad n = 1,2,3.....$$

$$\sqrt{(2mE_n)} = \frac{n\pi\hbar}{L} \Rightarrow 2mE_n = \frac{n^2\pi^2\hbar^2}{L^2}$$

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

Unlike classical particle, the quantum particle can only take discretized or quantized energy as you can see it through the dependence of energy on integer n. These energies are often called energy levels.

Salient features of particle in a box problem

- Trapped particle can not have an arbitrary energy. Boundary conditions or its confinement restricts its wave function and hence particle is allowed to have only certain specific energies and no others (No counterpart in classical). Exact energies depend on mass of particle and nature of the trapping potential.

- Because Planck's constant is so small – quantization of energy clearly noticeable only when *m* and *L* are also small.

- A trapped particle can not have zero energy. The de Broglie wavelength ($\lambda = h/mv$) is infinite when v=0. There is no way a trapped particle can have an infinite wavelength, so particle must have at least some kinetic energy. Exclusion of E=0 has no counterpart in classical physics.

- Energy levels are not equally spaced. E_n is proportional to integer n^2

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \qquad n=1,2,3 \ldots\ldots$$

Wavefunction in the nth eigenstate

- The wavefunction of particle in a box whose energy is E_n is given by

$$\varphi_n = A \sin \frac{\sqrt{2mE_n}}{\hbar} x$$

- Substituting, $E_n = \dfrac{n^2 \pi^2 \hbar^2}{2mL^2}$

- We obtain

$$\varphi_n = A \sin \frac{\sqrt{2m \dfrac{n^2\pi^2\hbar^2}{2mL^2}}}{\hbar} x = A \sin \frac{\dfrac{n\pi\hbar}{L}}{\hbar} x = A \sin \frac{n\pi x}{L}$$

- Thus, the wavefunction is given by

$$\varphi_n = A \sin \frac{n\pi x}{L}$$ n=1,2,3 ……

Φ_n is a well-behaved wave function because for each value of n, Φ_n is finite, single valued function of x and Φ_n and $\partial\Phi_n/\partial x$ are continuous.

Normalization of the wave function

$$\int_{-\infty}^{\infty} |\varphi_n|^2 dx = \int_0^L |\varphi_n|^2 dx = A^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx$$

$$= \frac{A^2}{2} \int_0^L \left(1 - \cos\left(\frac{2n\pi x}{L}\right)\right) dx$$

$$= \frac{A^2}{2} \left[\int_0^L dx - \int_0^L \cos\left(\frac{2n\pi x}{L}\right) dx\right]$$

$$= \frac{A^2}{2} \left[\int_0^L dx - \int_0^L \cos\left(\frac{2n\pi x}{L}\right) dx\right]$$

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

$$= \frac{A^2}{2} \left[L - \frac{L}{2n\pi} \sin\left(\frac{2n\pi L}{L}\right) - 0 - \frac{L}{2n\pi} \sin\left(\frac{2n\pi 0}{L}\right)\right]$$

$$= A^2\left(\frac{L}{2}\right)$$

In other words $\Rightarrow \int_{-\infty}^{\infty} |\varphi_n|^2 dx = A^2\left(\frac{L}{2}\right)$

But if Φ_n is to be normalized that means A should be assigned a value such that total probability will be equal to 1.

$$\Rightarrow \int_{-\infty}^{\infty} |\varphi_n|^2 dx = A^2\left(\frac{L}{2}\right) = 1$$

$$\Rightarrow A = \sqrt{\frac{2}{L}}$$

Therefore, the normalized wave function Φ_n is given by

$$\varphi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \qquad n = 1,2,3\ldots$$

First few wavefunctions

Ground state wavefunction $\varphi_1 = \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L}$

First excited wavefunction $\varphi_2 = \sqrt{\frac{2}{L}} \sin \frac{2\pi x}{L}$

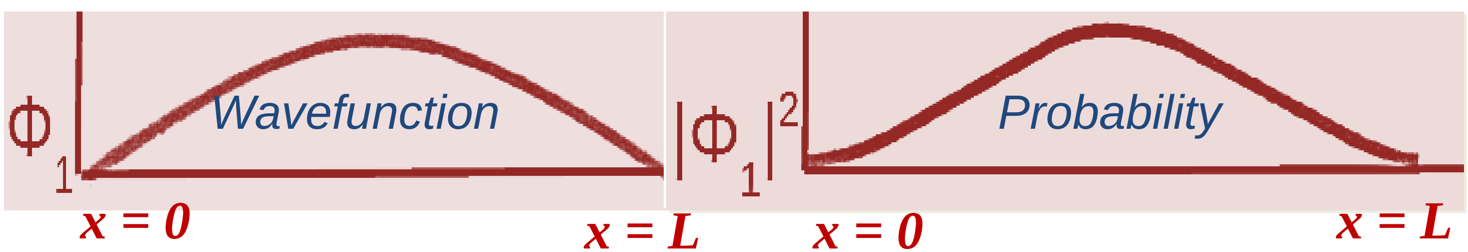
Second excited wavefunction $\varphi_3 = \sqrt{\frac{2}{L}} \sin \frac{3\pi x}{L}$

Ground State

The ground state wave function of the particle is

$$\varphi_1 = \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L}$$

It is not hard to see that $\Phi_1(0) = 0$, $\Phi_1(L/2) = \text{Max}$, $\Phi_1(L) = 0$.
Thus, the wavefunction and corresponding probability function can be plotted as

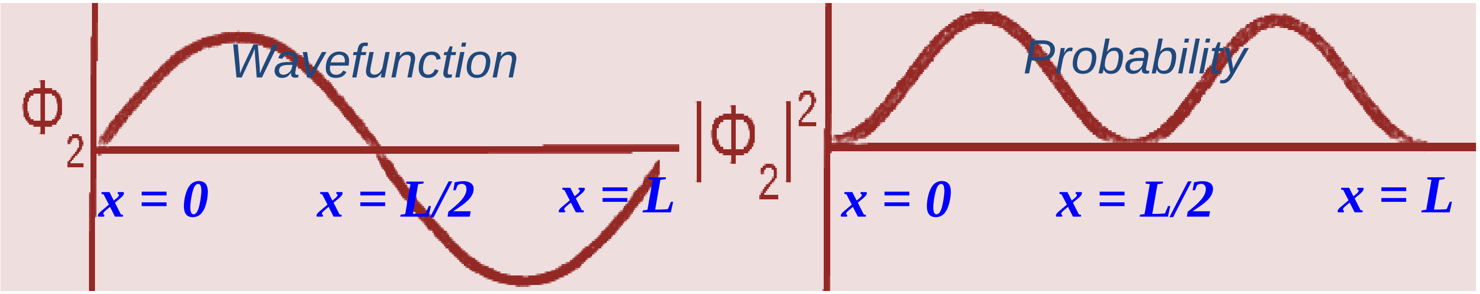


Particle has the maximum probability to be in the middle of box in the lowest energy state.

First excited state

$$\varphi_2 = \sqrt{\frac{2}{L}} \sin \frac{2\pi x}{L}$$

Note that $\Phi_2(0) = 0$, $\Phi_2(L/4) = \mathrm{Max}$, $\Phi_2(L/2) = 0$, $\Phi_2(3L/4) = \mathrm{Min}$, $\Phi_2(L) = 0$. Thus, the wavefunction and corresponding probability function can be plotted as

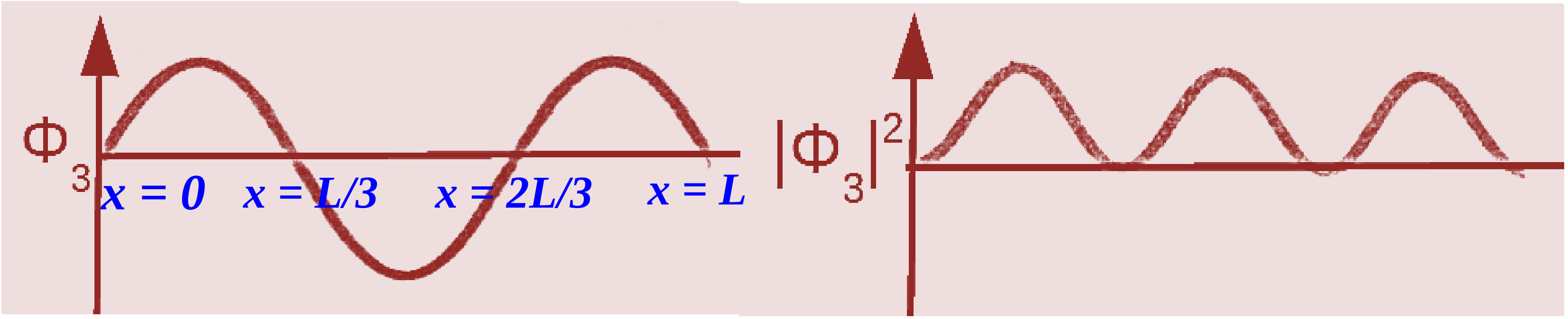


Particle has the minimum (vanishing) not only on the Boundaries but also in the middle of potential well.

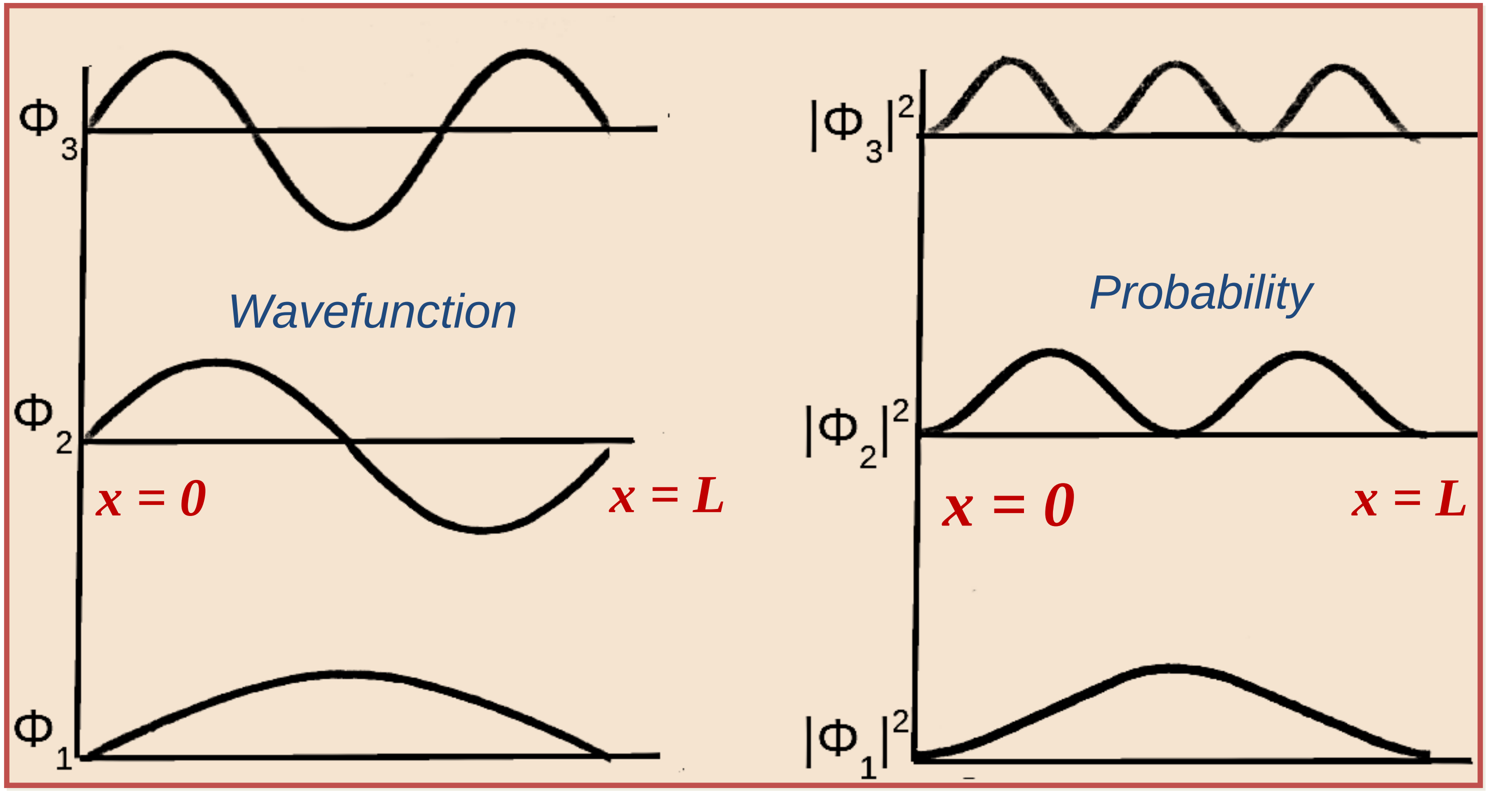
Second excited state

$$\varphi_3 = \sqrt{\frac{2}{L}} \sin \frac{3\pi x}{L}$$

How should the plot of wavefunction and corresponding probability look like?



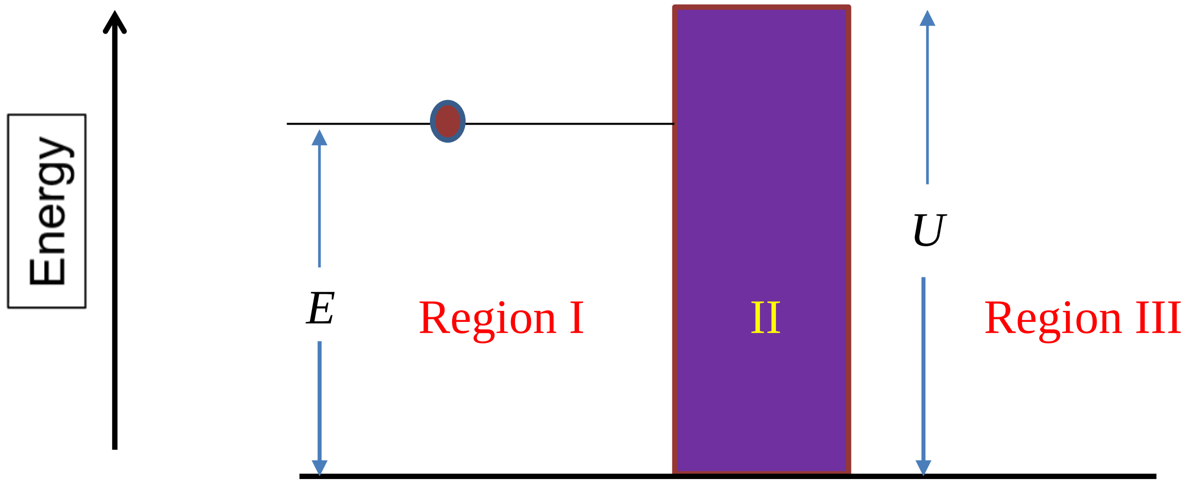
Wave functions and corresponding probabilities for first three excited state



Question: what is the probability of finding a classical particle with a given energy inside an infinite box?

Answer: Same probability everywhere in the box!!!! (why?)

Tunneling

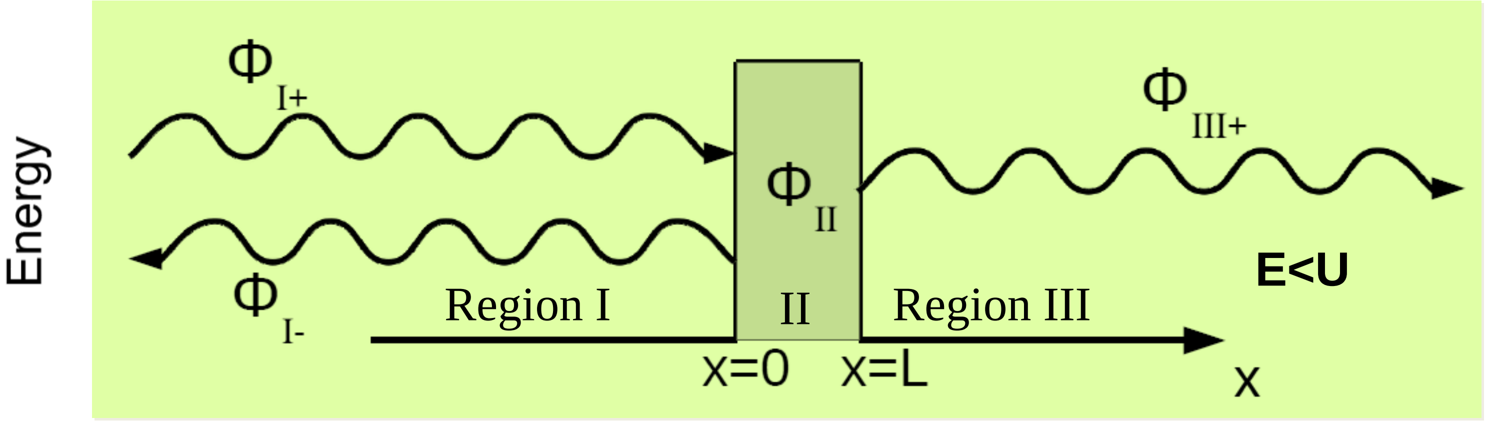


Can a classical particle with kinetic energy E<U enter region II or III?

No, of course

What about quantum particle? if yes, then does not it violate the energy conservation principle?

On both sides of barrier U=0, no forces act on the particle there. Barrier height is “U” and width is “L”.



Φ_{I+} is incoming part of the wavefunction for the particle (moving to the right in region I). Φ_{I-} represents reflected part of the wavefunction moving to the left. Φ_{II} is wavefunction inside the barrier. Φ_{III} represents transmitted part of the wavefunction moving to the right.

The **transmission probability** for a particle to pass through the barrier is equal to fraction of incident beam that gets through the barrier. Transmission probability is given by

$$T = e^{-2k_2 L}$$

Factor multiplying the exponential is not included.The relation is valid when E<<U.

where $$k_2 = \frac{\sqrt{2m(U-E)}}{\hbar}$$

where m is mass of the particle, E is the kinetic energy and U is the height of potential barrier, L is width of the barrier.

Important points

❖ Classical Mechanically, when energy of the particle is less than barrier height U, particle is reflected back.

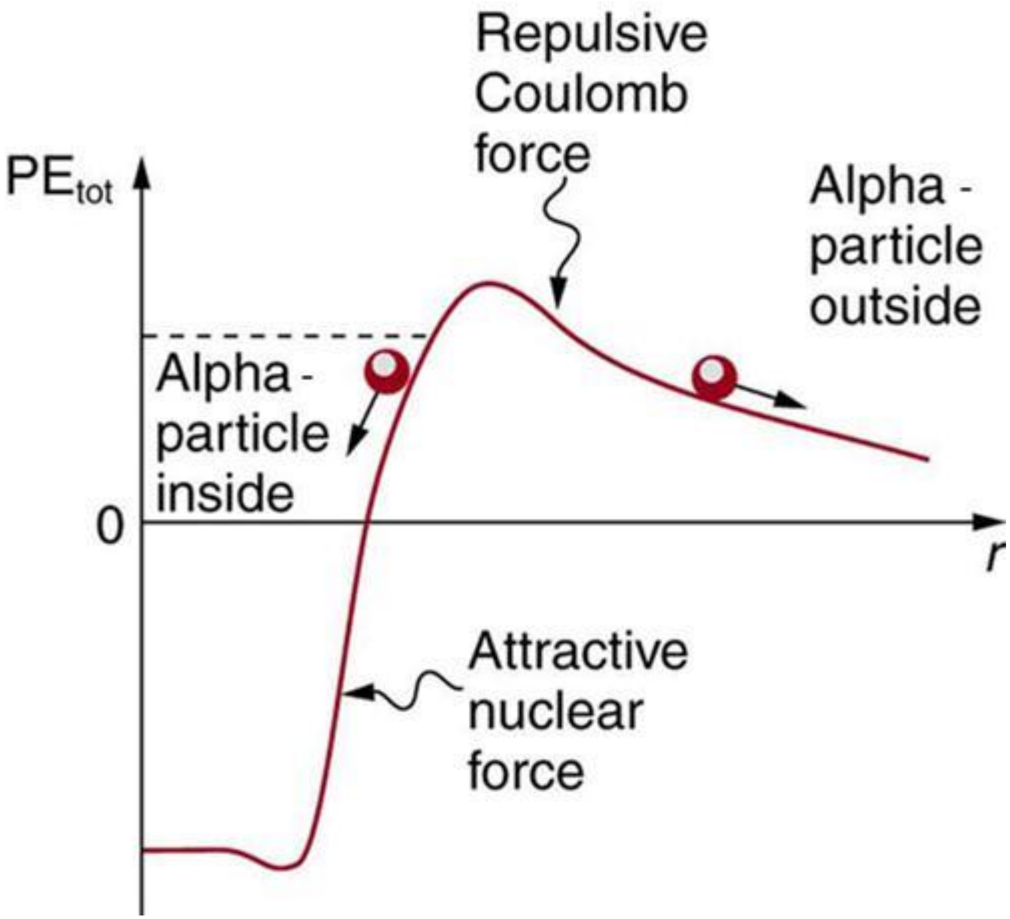
❖ According to quantum mechanics, the wavefunction of the particle does not vanish inside the potential barrier as well as on the other side even though $E<U$. In other words, the particle is partially reflected and partially transmitted.

❖ If the barrier is infinitely thick then the transmission probability will be zero. But if it is of finite thickness there is finite probability-however small- for particle to tunnel through region II and emerge in region III.

❖ The higher the barrier and wider it is, less will be the chance that the particle can get through the barrier.

Applications: radioactive decay, nuclear fusion, tunnel junction, tunnel diode, scanning tunneling microsope

Alpha particle decay



A few questions

Does the electron in the photoelectric effect tunnel when it escapes the metal surface?

The answer is strictly no. Because the electrons are trapped inside the metal just like a particle in finite potential well. I am saying "finite" because the electrons can indeed escape with certain minimum energy provided via photons.

This leads to next question. If the potential barrier is finite at the metal boundary, then electron can tunnel through this barrier into the space. But this does not happen why?

The potential inside the metal is negative and outside it is zero.
In other words, the potential barrier length L is very large, therefore tunneling probability becomes zero (check the expression of tunneling probability). So electrons cannot escape the metal through tunneling.

Quantum mechanics and computation (quantum computation)

- The basic unit of information in quantum computation is a quantum bit or qubit, which is a two-level quantum mechanical system

$$|\psi\rangle = \alpha_1 |0\rangle + \alpha_2 |1\rangle$$

where α_1 and α_2 are complex numbers and $|\alpha_1|^2 + |\alpha_2|^2 = 1$.

- It is coherently superposed state and it simultaneously in both of the states |1> and |0>.

- Eamples: (i) photon polarization (horizontal, vertical) (ii) electronic spin (up, down)

Note that a classical bit can correspond to either 0 or 1 not both at the same time

- Unlike classical bits, qubits can be entangled, which means there is certain degree of correlation between them. This can enhance the computation power (parallel computation, which requires quantum algorithm).

- More secure because any attempt of unauthorized decryption would lead to the disturbance in the system, which can be detected easily. This is unlike the information stored in classical computer which can be decrypted with powerful computational device.

Challenges with quantum computation:

- The computer should be isolated otherwise it's interaction with environment can lead to quantum decoherence or loss of information. It also means that it should be maintained at low temperature.

- The measurement intended to find in which state the qubit also introduces decoherence.