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Wave Mechanics

Engineering Physics
G V Khandekar
HOD FE SKNSITS

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Objectives

- ✔To understand the wave nature of matter waves.
- ✔To understand the relation between wave and matter.
- ✔To understand Schroedinger's wave equation and apply it for simple quantum mechanical problems.

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Syllabus

Wave particle duality of radiation and matter, de Broglie's concept of matter waves, Expressing de Broglie wavelength in terms of kinetic energy and potential , concept and derivation of group velocity and phase velocity;

Heisenberg's uncertainty principle,

Illustration of it by electron diffraction at a single slit.

Why an electron can not exist inside the nucleus.

Syllabus

Concept of wave function and probability interpretation,
Physical significance of the wave function,
Schrodinger's time independent and time dependent wave equations,
Applications of Schrodinger's time independent wave equations to problems of

(i) Particle in a rigid box (infinite potential well), Comparison of predictions of classical mechanics with quantum mechanics

(ii)Particle in a non-rigid box (finite Potential Well)-Qualitative (results only)

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Syllabus

Tunneling Effect

Tunnel diode

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Introduction

This unit is small, introductory part of Quantum mechanics.

Limitations of Classical Mechanics

1. High speed(comparable to the speed of light) phenomenon

2. Mechanics in microscopic bodies(Atoms, electrons, protons etc.)

can not be explained by classical mechanics

Failure of Classical Mechanics and Need of Quantum Mechanics

- Photoelectric effect
- Radioactivity
- Compton effect

These phenomenon can not be explained by classical (Newtonian) mechanics.
Quantum mechanics can explain these phenomenon satisfactorily.

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Nature of Light

Is the nature of light that of a wave or a particle?

Light has a dual(double) nature

1. Wave nature (electromagnetic) – can be proved by Interference and Diffraction phenomenon

2. Particle nature (photons) – can be proved by Photoelectric effect and Compton effect

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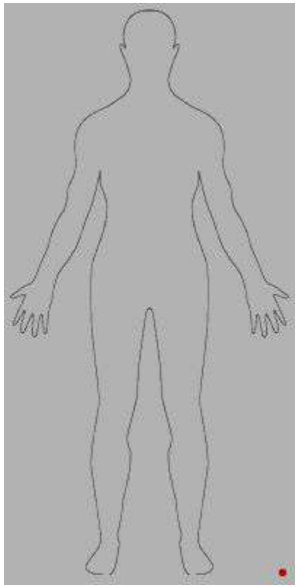
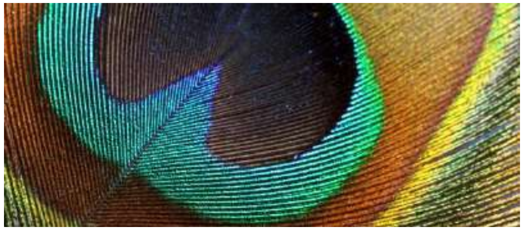
Hence light initially considered as wave also possesses particle i.e. matter nature.

What about Matter?

Nature loves symmetry





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De Broglie's Concept of Matter Waves

In his thesis in 1923, Prince Louis de Broglie suggested that mass particles should have wave properties similar to electromagnetic radiation.

The wavelength of a matter wave is called **the de Broglie wavelength**

Louis V. de Broglie (1892-1987)

de Broglie's hypothesis

A particle with momentum p has a *matter wave* associated with it, whose wavelength is given by

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

Wave Particle

De-Broglie wavelength of particle by Analogy with Radiation (Dec-09)

We know for a photon, $E = h\nu$ Also $E = mc^2$

$$\therefore mc^2 = h\nu = h\frac{c}{\lambda}$$

$$\nu = \frac{c}{\lambda}$$

$$\therefore \lambda = \frac{h}{mc}$$

This is for a photon.

Similarly for a particle with velocity v , we can write

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

De-Broglie Wavelength in terms of Kinetic Energy (May-05,08)

K. E. of the particle is given by, $E = \frac{1}{2}mv^2$

$$\therefore E = \frac{m^2v^2}{2m} = \frac{p^2}{2m} \qquad \therefore p^2 = 2mE$$

$$\therefore p = \sqrt{2mE}$$

By de Broglie's hypothesis,

$$\lambda = \frac{h}{p} \qquad \therefore \lambda = \frac{h}{\sqrt{2mE}}$$

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De-Broglie wavelength of an Electron

(Dec-05,06,09)

When electron is accelerated by a potential V it will get K. E.

$$E = \frac{1}{2}mv^2 = eV$$

We have

$$\therefore \lambda = \frac{h}{\sqrt{2mE}} \qquad \therefore \lambda = \frac{h}{\sqrt{2meV}}$$

Putting the values,

h = 6.625 X 10^{-34} Js

m_o = 9.1 X 10^{-31} Kg

e = 1.6 X 10^{-19} C

we will get

$$\therefore \lambda = \frac{12.26}{\sqrt{V}} A^\circ$$

Properties of matter waves
(May-04,Dec-05)

1. $\lambda \propto 1/m$ lighter the particle greater is the wavelength associated with it.

2. $\lambda \propto 1/v$ greater the velocity of the particle, smaller is the associated wavelength.

3. If $v=\infty$ $\lambda=0$ not possible

4. If $v=0$ $\lambda=\infty$ no matter waves. i.e. matter waves are associated only with moving particles.

Properties of matter waves
(May-04,Dec-05)

5. λ is independent of charge of particle

6. Velocity of matter waves depends on velocity of particle generating it

Phase velocity (wave velocity)

The rate at which the phase of the wave propagates in space

Phase velocity, $v_p = \nu\lambda$------(1)

We know E= hע and Einstein mass energy relation $E = mc^2$

We can write $h\upsilon = mc^2$ Or $\upsilon = \dfrac{mc^2}{h}$..............(2)

Also de Broglie wavelength is given by

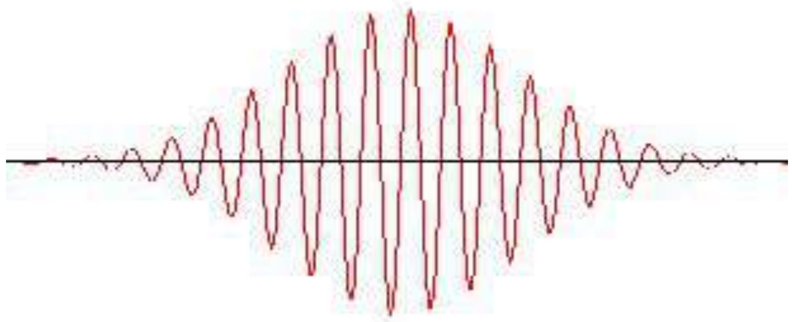
$\lambda = \dfrac{h}{mv}$................(3) Put equation (2) and (3) in (1)

$v_p = \dfrac{mc^2}{h} \times \dfrac{h}{mv} = \dfrac{c^2}{v}$ $v_p \times v = c^2$ $\Rightarrow v_p > c$

Which is not possible.

Hence phase velocity has no physical significance.

A “Wave Packet” or Wave group



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

Wave Packet

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

Group velocity(Vg) (May-07)

The rate at which the envelope of the wave packet propagates

Group velocity is given by $$v_g = \frac{d\omega}{dk}$$

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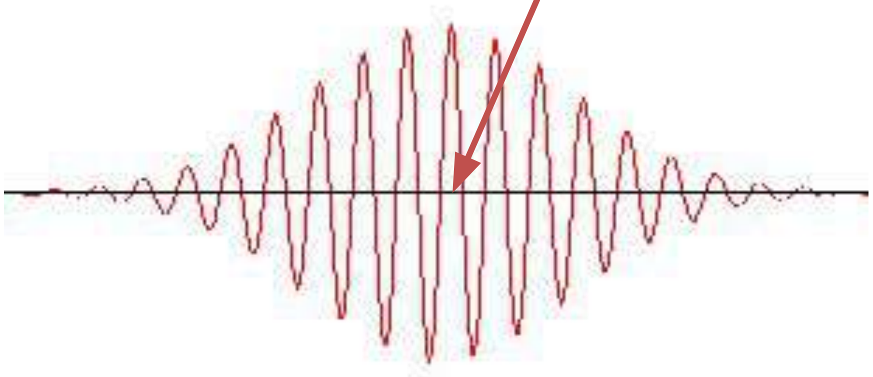
Where is the particle in Wave Packet?

Amplitude of wave in wave packet represents the probability of finding the particle.

Maximum probability



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Heisenberg's Uncertainty Principle

Statement: It is *impossible* to know both the *exact* position and the *exact* momentum of a particle *simultaneously*

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Mathematical expression

Let Uncertainty in Position be Δx

And uncertainty in Momentum be Δp_x

Then,

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

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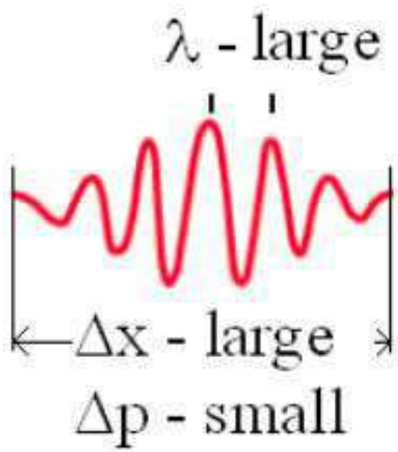
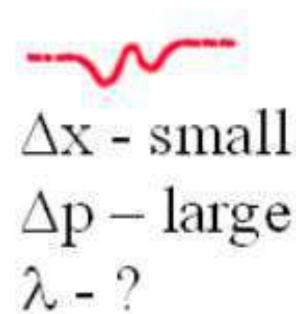
Uncertainty Principle and the Wave Packet

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

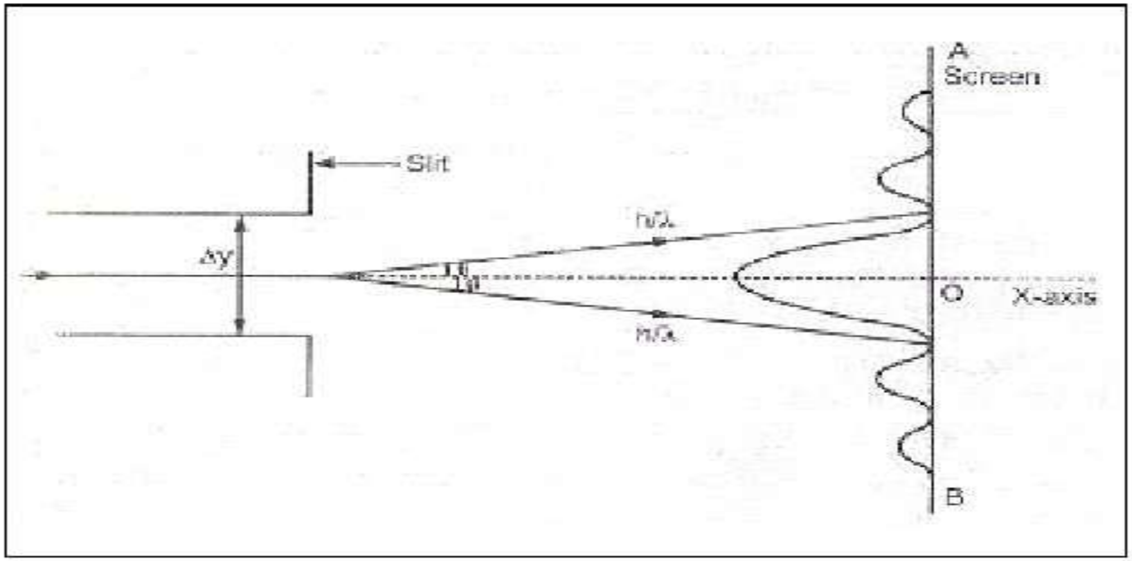


Wide wave packet



Narrow wave packet

Illustration of electron diffraction at a single slit…(May-04,05,08,09,10, Dec-04,06,07,09,10-6 Marks)



Single slit minima condition for m=1 is

a sin θ = λ

Here slit width =Δy=also uncertainty in position of electron along y direction

$$\Delta y \sin\theta = \lambda$$

$$\therefore \Delta y = \frac{\lambda}{\sin\theta} - - - (1)$$

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Uncertainty in momentum of electron along y direction after diffraction will be

$$\Delta p_y = p\sin\theta - (-p\sin\theta) \qquad \therefore \Delta p_y = 2p\sin\theta$$

$$\therefore \Delta p_y = 2\frac{h}{\lambda}\sin\theta ----(2) \qquad p = \frac{h}{\lambda}$$

From (1) and (2),

$$\therefore \Delta y \Delta p_y = 2\frac{h}{\lambda}\sin\theta \bullet \frac{\lambda}{\sin\theta}$$

$$\therefore \Delta y \Delta p_y = 2h \qquad i.e.\ \Delta y \Delta p_y \geq h \ or \ \frac{h}{2\pi}$$

Hence the proof.

Uncertainty principle applied to the pair of variables Energy and time.

K.E. of a particle is given by, $E = \frac{1}{2} mv^2 ----------(1)$

Differentiating equation (1), $\therefore \Delta E = \frac{1}{2} m 2v \Delta v$

$$\therefore \Delta E = m\Delta v . v ---(2)$$

Now velocity $v = \frac{\Delta x}{\Delta t}$ and $m\Delta v = \Delta p$

$\therefore \Delta E = \Delta p \frac{\Delta x}{\Delta t}$ $\therefore \Delta E \, \Delta t = \Delta p \, \Delta x$ $\therefore \Delta E \, \Delta t = \Delta x \, \Delta p --(3)$

By Heisenberg's uncertainty principle

$\Delta x \cdot \Delta t \geq h$ Equation (3) becomes $\Delta E \cdot \Delta t \geq h$

Hence the proof.

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Concept of wave function

What changes in electromagnetic wave is Electric field E, what changes in sound waves is Pressure P, similarly what changes in case of matter waves is wave function **ψ** (psi) (read as si)

The wave function represents probability amplitude for finding a particle at a given point in space at a given time.

All the information that can be obtained by making a measurement of a system (particle) is contained in a complex function called the wave function, ψ.

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Concept of wave function

Wave functions are generally *complex* functions

$$\Psi = A + iB$$

Complex Conjugate of it is

$$\Psi^* = A - iB$$

So $|\psi|^2 = \psi^* \psi$

$= A^2 - i^2 B^2$

$= A^2 + B^2$

$\psi^* \psi$ is always a positive real quantity and called as ***probability density***.

Physical significance of ψ

Ψ itself has no direct physical significance and hence is not experimentally measurable.

But $\psi^* \psi$ or $|\psi|^2$ represents **probability density** of finding the particle which is always positive

Ψ - May be positive/ negative . Negative probability is not possible.

Physical significance of ψ

The physical significance of the square of the *wavefunction,* ψ^2, is interpreted as the probability of finding a particle in a small region of space.

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Normalization of ψ

Although we do not know the precise location of the particle within a volume , we know that the particle is somewhere within it.
Then, the probability of finding the particle within that volume is 1
We can write

$$\int_{-\infty}^{+\infty} |\psi|^2 dV = 1 \quad ---(1)$$

A wavefunction that obeys equation (1) is called a "Normalized Wavefunction"

Normalization of ψ

If the particle does not exist at all

$$\int_{-\infty}^{+\infty} |\psi|^2 dV = 0$$

Well behaved wave functions (Conditions)

1. Ψ must be continuous and single valued everywhere

2. Ψ must be normalisable

3. Ψ must be finite.

4. $\frac{\partial \psi}{\partial x}, \frac{\partial \psi}{\partial y}, \frac{\partial \psi}{\partial z}$ must also be continuous and single valued

The Schrödinger wave equation

Which is the fundamental equation in quantum mechanics in the same sense as Newton's second law of motion is in classical mechanics.

Schrodinger's Time Independent wave equation

According to De-Broglie's hypothesis $\lambda = \frac{h}{p} = \frac{h}{mv}$

The usual wave equation is Cartesian coordinates is given by

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} = \frac{1}{u^2}\frac{\partial^2\psi}{\partial t^2} ----(1)$$

The solution of this equation is $\psi = \psi_0 e^{-i\omega t} ----(2)$

Differentiating equation (2) twice the respect to 't', we get,

$$\frac{\partial\psi}{\partial t} = -i\omega\psi_0 e^{-i\omega t}$$

$$\frac{\partial^2\psi}{\partial t^2} = -i^2\omega^2\psi_0 e^{-i\omega t} = \omega^2\psi_0 e^{-i\omega t} = \omega^2\psi$$

Substituting this value in equation (1)

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} = \frac{-\omega^2}{u^2}\psi$$

Time Independent wave equation

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Taking $$\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}=\nabla^2\psi$$

$$\therefore \nabla^2\psi = \frac{-\omega^2}{u^2}\psi \qquad \therefore \nabla^2\psi + \frac{\omega^2}{u^2}\psi = 0 - - - - (3)$$

We know, ω =2πυ and u = υλ

$$\therefore \frac{\omega^2}{u^2} = \frac{4\pi^2}{\lambda^2} = \frac{4\pi^2 p^2}{h^2} - - - - (4) \qquad \lambda = \frac{h}{p}$$

Total energy, $$E = K.E. + P.E. = \frac{1}{2}mv^2 + V$$

$$= \frac{m^2v^2}{2m} + V = \frac{p^2}{2m} + V$$

$$\therefore p^2 = 2m(E+V)$$ Put in (4)

Time Independent wave equation

$$\therefore \frac{\omega^2}{u^2} = \frac{8\pi^2 m(E-V)}{h^2} ----(5)$$

Put in (3)

$$\therefore \nabla^2\psi + \frac{8\pi^2 m(E-V)}{h^2}\psi = 0 ----(6)$$

This is Schrodinger's Time Independent Wave Equation

Schrodinger’s Time Dependent wave equation

According to De-Broglie’s hypothesis $\lambda = \frac{h}{p} = \frac{h}{mv}$

The usual wave equation is Cartesian coordinates is given by

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} = \frac{1}{u^2}\frac{\partial^2\psi}{\partial t^2} ----(1)$$

The solution of this equation is $\psi = \psi \,\square\, e^{-i\omega t} ----(2)$

Differentiating equation (2)with respect to ‘t’, we get,

$$\frac{\partial\psi}{\partial t} = -i\omega\psi \,\square\, e^{-i\omega t} \qquad \frac{\partial\psi}{\partial t} = -i\omega\psi ---(3)$$

We have, $\omega = 2\pi\upsilon$ and $\nu = \frac{E}{h}$

Time Dependent wave equation

$$\therefore \frac{\partial \psi}{\partial t} = -i2\pi \frac{E}{h}\psi$$

Multiplying both the sides by i we get

$$\therefore i\frac{\partial \psi}{\partial t} = 2\pi \frac{E}{h}\psi \qquad \therefore E\psi = \frac{ih}{2\pi}\frac{\partial \psi}{\partial t}$$

Schroedinher's time independent wave equation is

$$\therefore \nabla^2\psi + \frac{8\pi^2 m(E-V)}{h^2}\psi = 0 --- (4)$$

Putting value of Eψ in equation (4)

$$\therefore \nabla^2\psi + \frac{8\pi^2 m}{h^2}\left(\frac{ih}{2\pi}\frac{\partial \psi}{\partial t} + V\psi\right) = 0$$

Multipying both sides by $-\frac{h^2}{8\pi^2 m}$

Schrodinger's Time Dependent wave equation

$$\therefore -\frac{h^2}{8\pi^2 m}\nabla^2\psi - \frac{ih}{2\pi}\frac{\partial\psi}{\partial t} + V\psi = 0$$

$$\therefore -\frac{h^2}{8\pi^2 m}\nabla^2\psi + V\psi = \frac{ih}{2\pi}\frac{\partial\psi}{\partial t}$$

This is Schrodinger's Time Dependent Wave Equation

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Applications of Schrodinger' s time independent wave equations to problems of

(i) Particle in a rigid box (infinite potential well)

(ii) Particle in a non-rigid box (finite Potential Well)-Qualitative (results only)

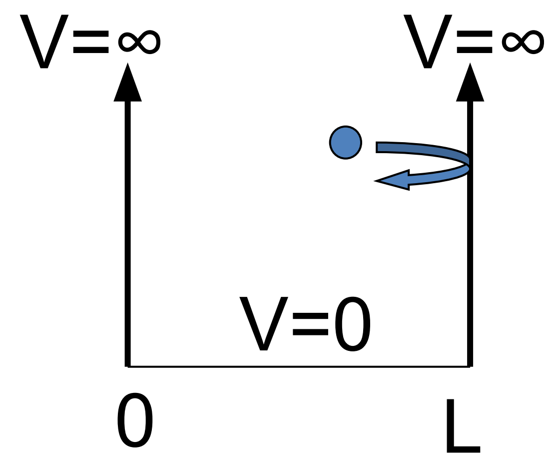
Particle in a rigid box (infinite potential well)

Consider a particle trapped in infinite potential well of width L.

Boundary conditions:

Inside the well $V=0$ for $0 \leq x \leq L$

Outside the well $V=\infty$ for $x<0$, $x>L$



Particle in a rigid box (infinite potential well)

We have Schrödinger's time independent wave equation

$$\nabla^2\psi + \frac{2m}{\hbar^2}(E - V)\psi = 0 \text{ - - - - } (1)$$

In one dimension for $0 \leq \mathbf{x} \leq L$, $V=0$

The equation becomes

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E)\psi = 0$$

$$\therefore \frac{d^2\psi}{dx^2} + k^2\psi = 0 \text{ - - - - - - - - - } (2)$$

where

$$k^2 = \frac{2mE}{\hbar^2} \text{ - - - - - - - - - } (3)$$

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Particle in a rigid box (infinite potential well)

General solution of (2) can be given as

$\psi(x) = A \sin kx + B \cos kx$ ------------------------ (4)

We apply the Boundary conditions

condition 1. $\psi = 0$ at $x=0$

This gives us $B = 0$ from eq (4), then the solution becomes

$\psi(x) = A \sin kx$ -------------------(5)

condition 2. $\psi = 0$ at $x = L$ or $\psi(L) = 0$

Putting in (5) gives, $\sin kL = 0$ i.e. $kL = n\pi$ where $n = 1, 2, 3, \ldots$

Then $k = \frac{np}{L}$ --------(6)

Particle in a rigid box (infinite potential well)

From eq (3)

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2mL^2} = \frac{n^2 h^2}{8mL^2} \quad \text{-------(7)}$$

where n =1,2,3,…..

The lowest energy : ground level

$$E_1 = \frac{h^2}{8mL^2}$$

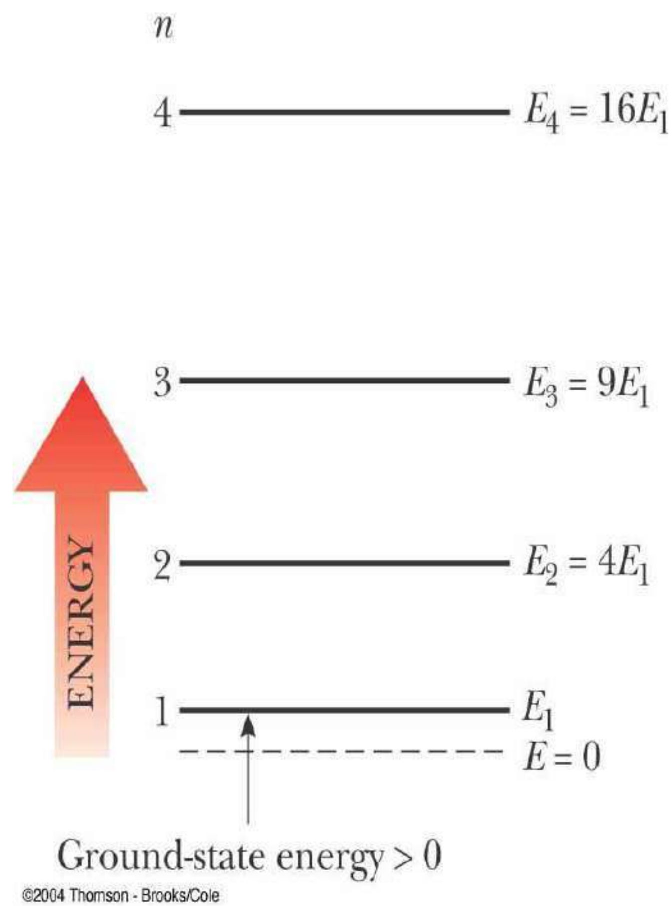
$$\text{and}$$

$$E_n = n^2 E_1 \quad \text{--------(8)}$$

Energy Level Diagram – Particle in a rigid Box

From (8) energy of the particle has not any arbitrary value but specific values i.e. energy of the particle is *quantised*.

E = 0 is not allowed
i.e. the particle can never be at rest



Wave function for the particle

We have ψ (x) = A sin kx and $k = \frac{n\pi}{L}$

$$\therefore \ \psi_n(x) = A \sin\left(\frac{n\pi x}{L}\right) \quad - - - \quad (9)$$

Using normalsation condition, $\int_{-\infty}^{\infty} |\psi|^2 dx = 1$

We can write, $A^2 \int_0^L \sin^2 \frac{n\pi x}{L} dx = 1$

solving, *or*

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

Wave function for the particle

Putting value of A in (9) we get the wave function for the particle,

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right).$$

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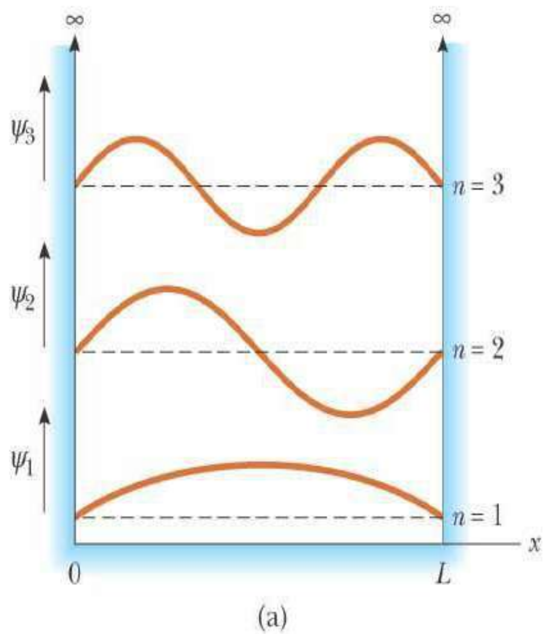
Graphical Representations for a Particle in a rigid box



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Analysis of graphs

$|\psi|^2$ i.e. probability density is zero at the boundaries

$|\psi|^2$ is zero at other locations as well, depending on the values of n

The number of zero points increases by one each time the quantum number increases by one

For higher n, problem becomes classical

Comparison of predictions of classical mechanics with quantum mechanics

Classically probability of finding the particle is equal everywhere while from quantum mechanical point of view probability of finding the particle is different at different places and for different quantum number.

For higher n, problem becomes classical

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Particle in a non-rigid box (finite Potential Well)- Qualitative (results only)

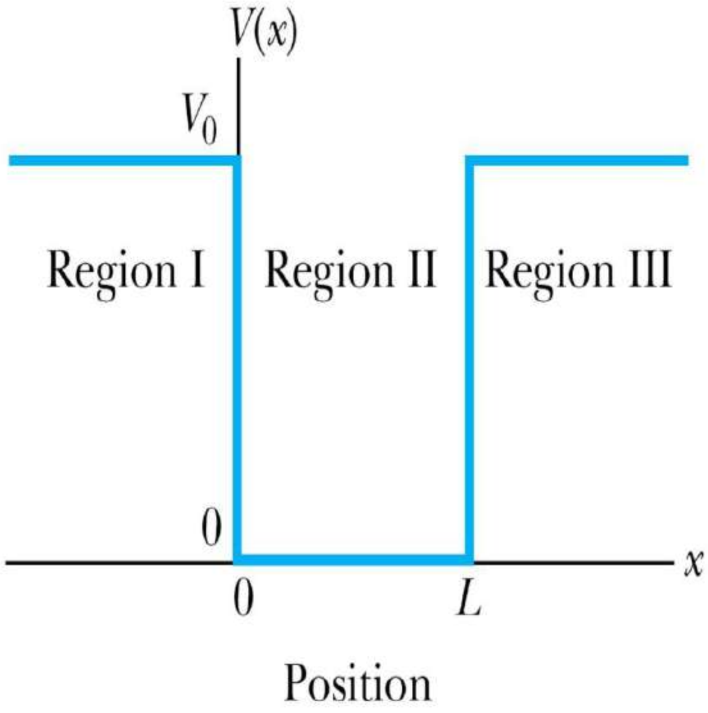
Consider a particle of mass m trapped in a finite potential well of width L. The boundary conditions are

$V=V_0$ for $x \leq 0$

$=0$ for $x<0<L$

$=x \geq L$

Let $E < V_0$



Particle in a non-rigid box

As the particle exist in 3 regions, we have 3 wave functions for the particle i.e. $\Psi_I \Psi_{II} \Psi_{III}$. The Schrödinger equation for regions I, II and III can be written as:

$$\frac{d^2y_I}{dx^2} + \frac{2m}{h^2}(E - Vo)y_I = 0 \qquad \frac{d^2y_{II}}{dx^2} + \frac{2m}{h^2}(E)y_{II} = 0$$

$$\frac{d^2y_{III}}{dx^2} + \frac{2m}{h^2}(E - Vo)y_{III} = 0$$

Let

$$k^2 = \frac{2m}{h^2}E$$

and

$$-k'^2 = \frac{2m}{h^2}(E - Vo)$$

Particle in a non-rigid box

Then equations becomes

$$\frac{d^2 y_I}{dx^2} - k'^2 y_I = 0$$

$$\frac{d^2 y_{II}}{dx^2} + k^2 y_{II} = 0$$

$$\frac{d^2 y_{III}}{dx^2} - k'^2 y_{III} = 0$$

The solutions of above differential equations in second order can be written using two constants as,

$$y_I(x) = Ae^{k'x} + Be^{-k'x}$$

$$y_{II}(x) = Pe^{ikx} + Qe^{-ikx}$$

$$y_{III}(x) = Ce^{k'x} + De^{-k'x}$$

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Particle in a non-rigid box

As $x \to \pm\infty$, $\psi \neq 0$

Therefore constants, B=0 and C=0

Therefore equations becomes,

$$y_I(x) = Ae^{k'x}$$

$$y_{II}(x) = Pe^{ikx} + Qe^{-ikx}$$

$$y_{III}(x) = De^{-k'x}$$

Using boundary conditions we can write four equations and we can solve these equations to find four constants and hence the wave functions for the three regions.

$$y_I(0) = y_{II}(0)$$

$$\frac{dy_I(0)}{dx} = \frac{dy_{II}(0)}{dx}$$

$$y_{II}(L) = y_{III}(L)$$

$$\frac{dy_{II}(L)}{dx} = \frac{dy_{III}(L)}{dx}$$

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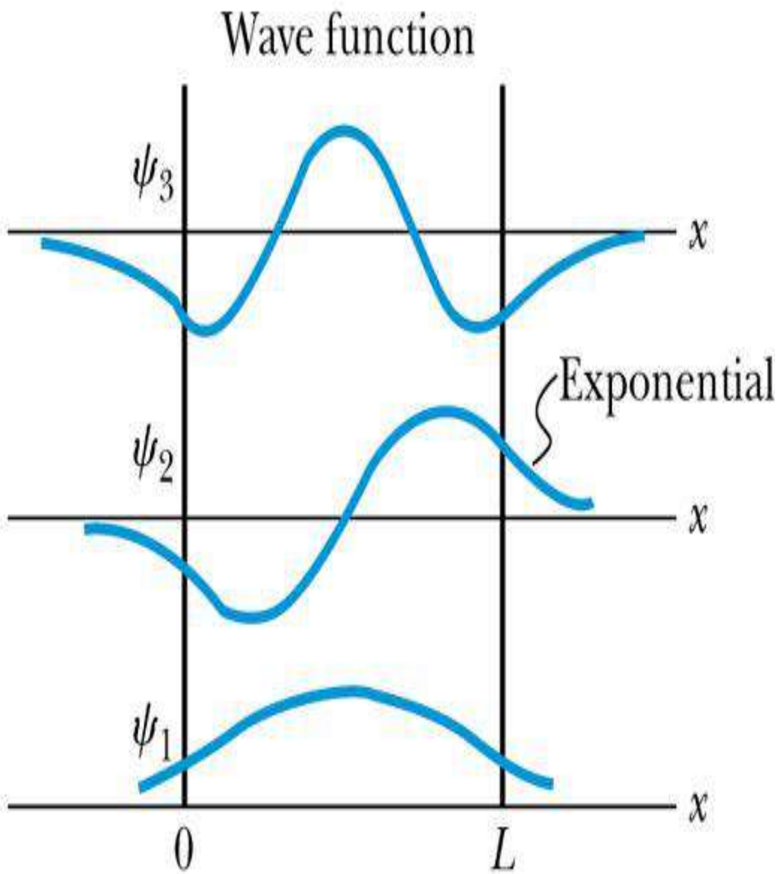
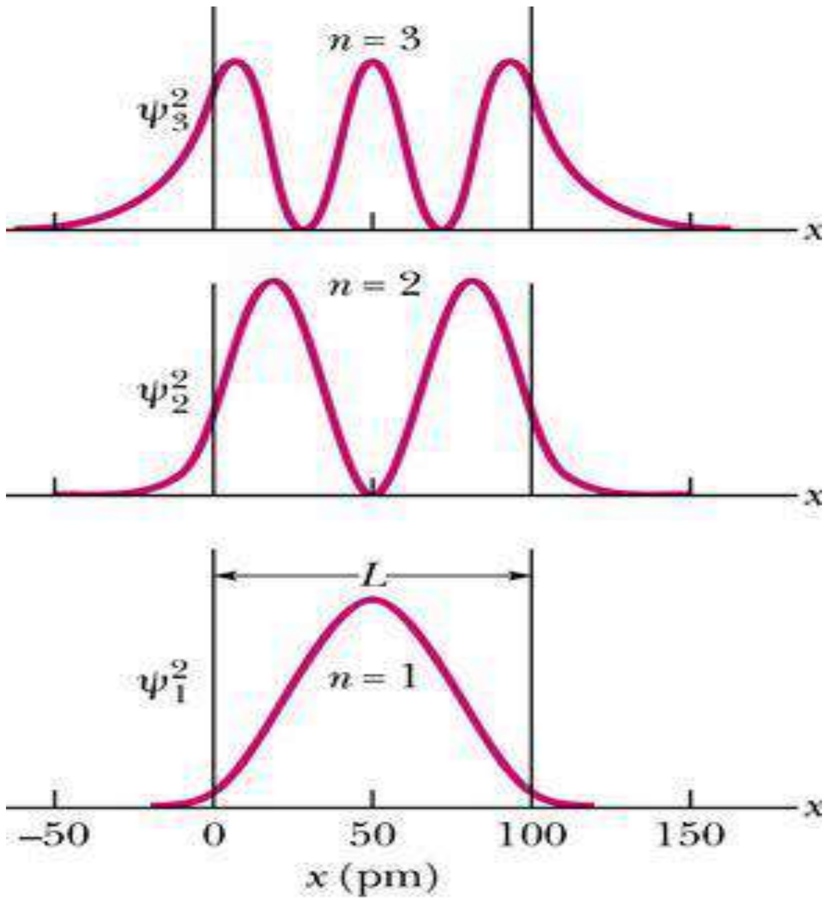
Wave functions

Probability density





Particle in a non-rigid box (Analysis)

From the graph of probability density it is clear that particle has non zero probability outside the box. Other things are like rigid box.

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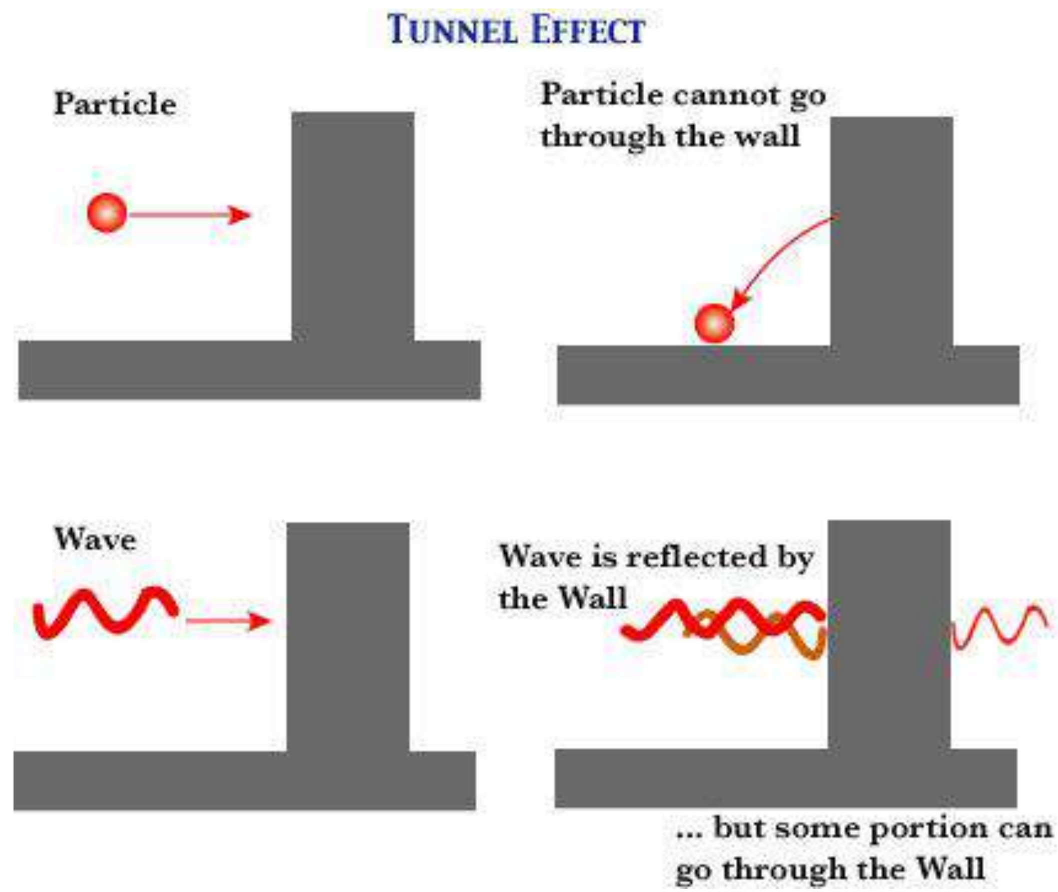
Tunneling Effect

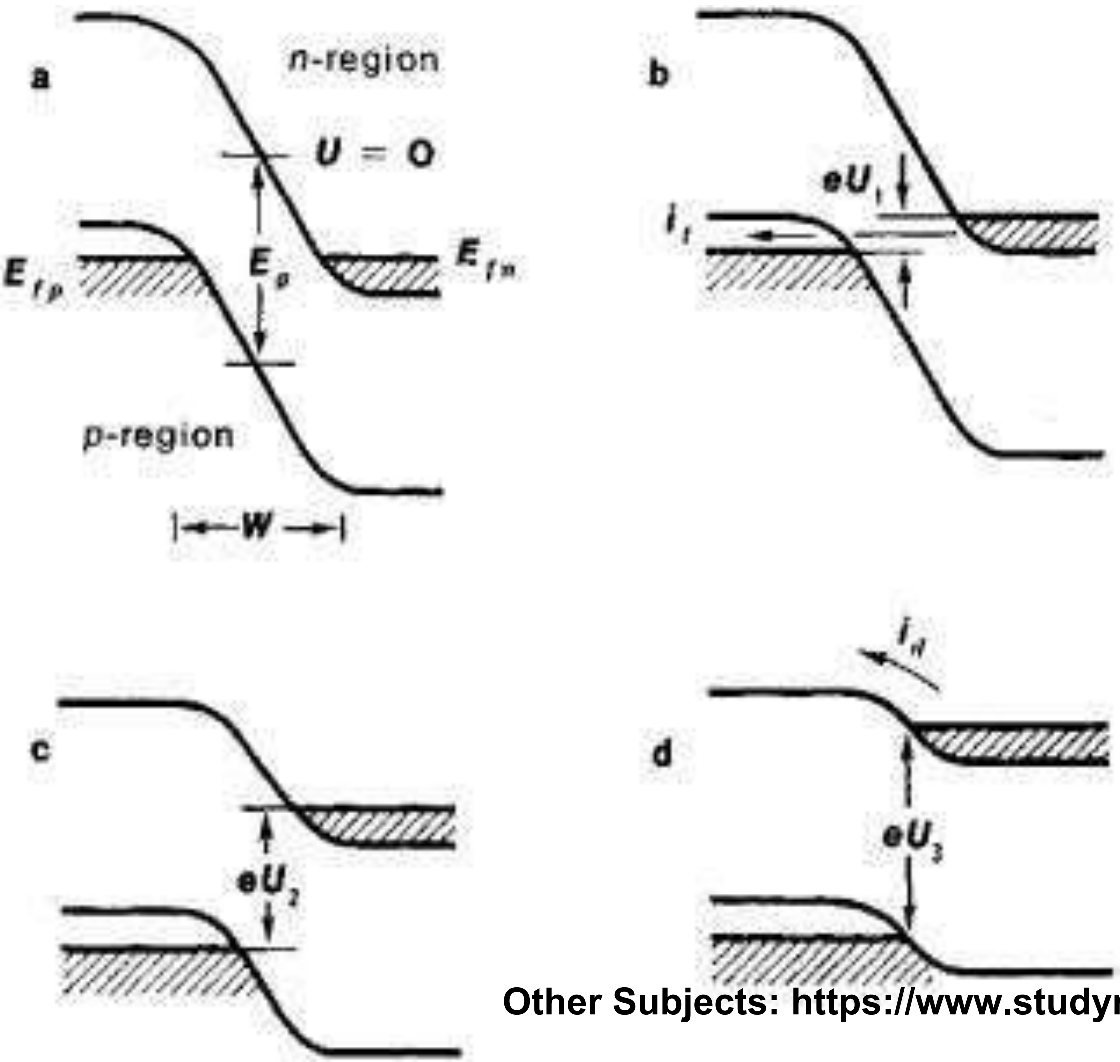
Classically a particle having less energy than the potential barrier cannot overcome it.

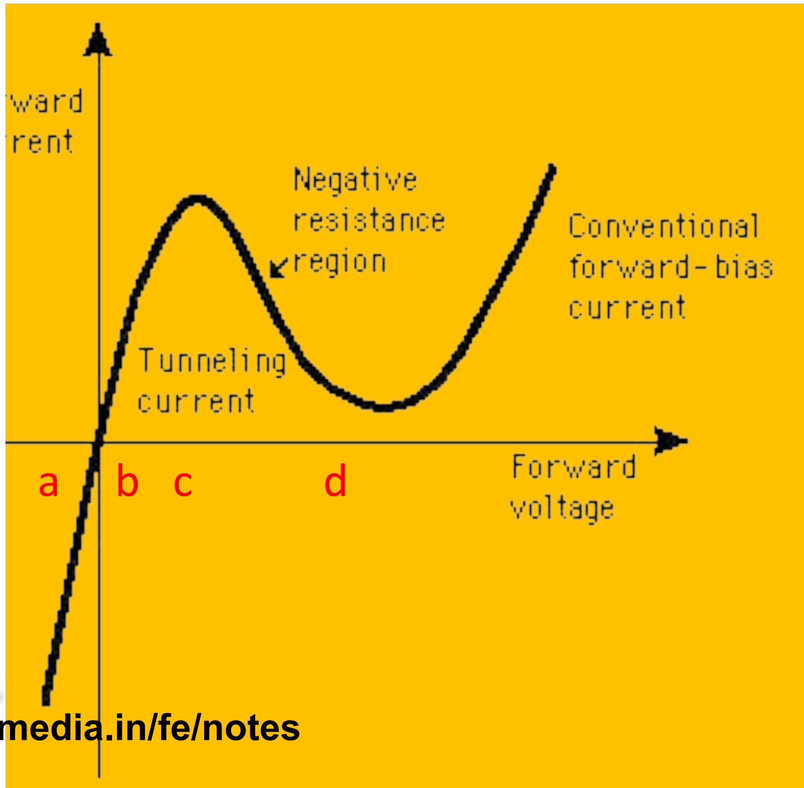
But in quantum mechanics it can. This effect of passing the particle through the barrier is called tunnel effect.



Applications of tunnel diode

Tunnel diode





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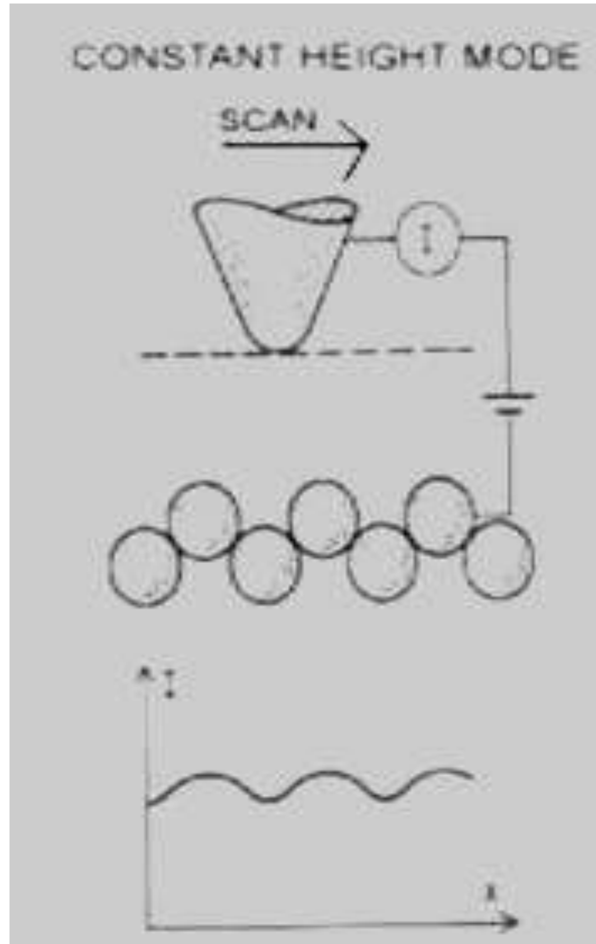
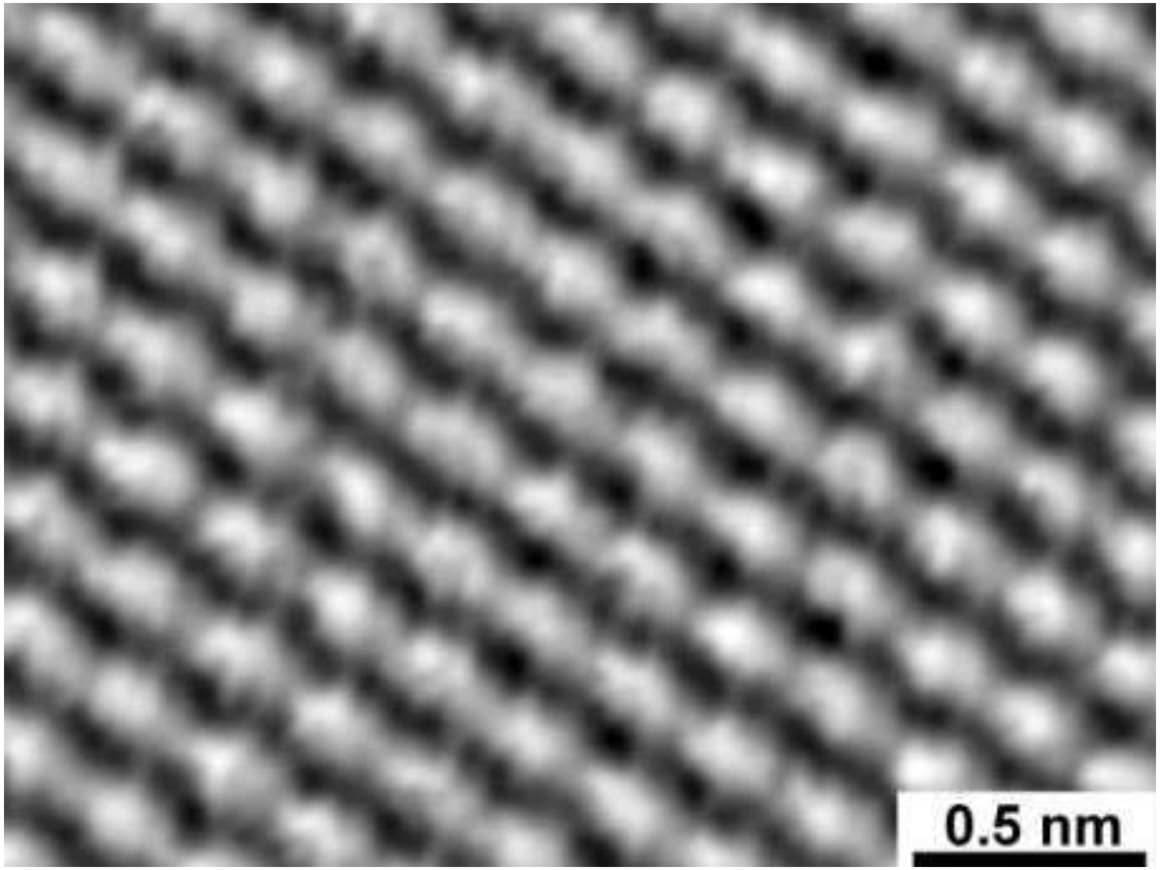
Scanning Tunneling Microscope





Graphite surface at atomic scale by STM