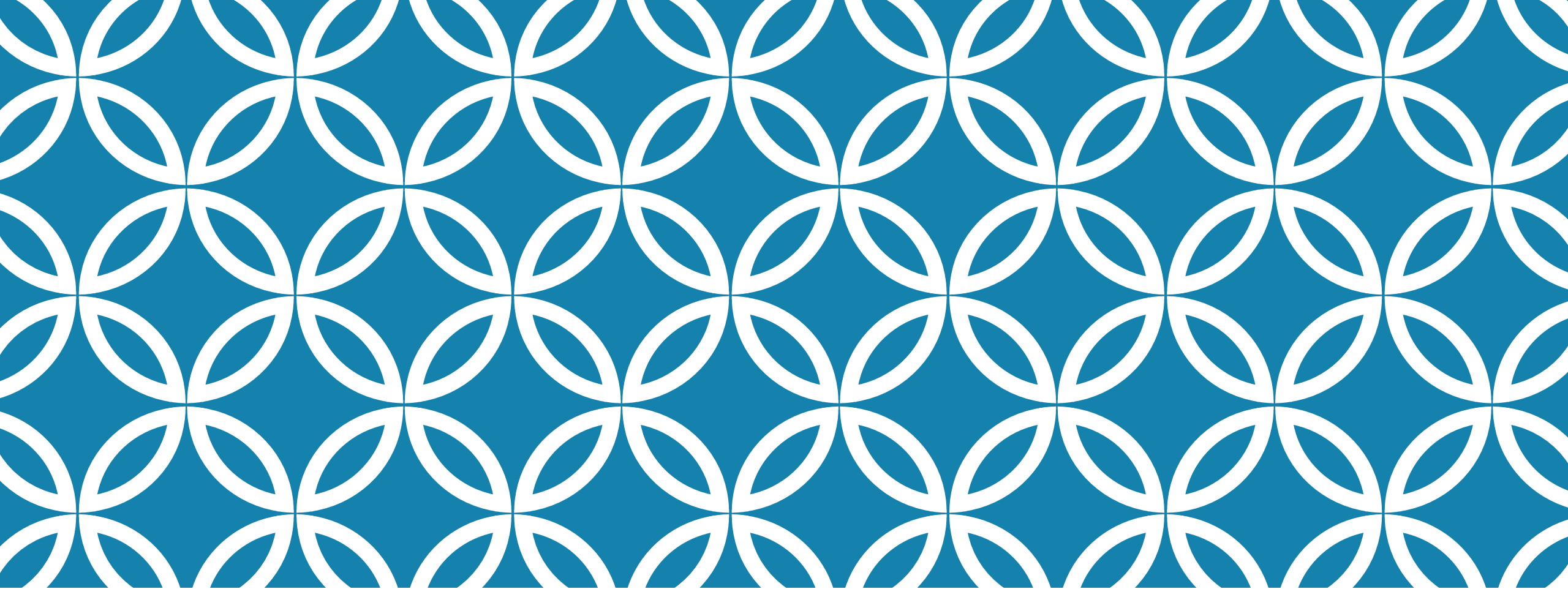




APPLICATIONS OF QUANTUM MECHANICS

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SYLLABUS AND REFERENCE BOOKS

Syllabus:

Eigenvalues and eigenfunction of particle confined in one dimensional box - Basics of nanophysics - Quantum confinement and nanostructures - Tunnel effect (qualitative) and scanning tunneling microscope.

Reference Books:

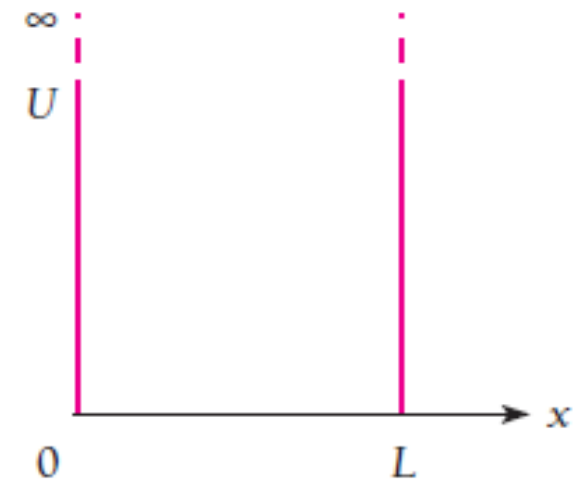
1. Arthur Beiser, Concepts of Modern Physics; Sixth Edition (2020), McGraw Hill Publication.
2. Raymond A. Serway, Clement J. Mosses, Curt A. Moyer Modern Physics, 2010, 3rd Indian Edition Cengage learning.

PARTICLE IN AN INFINITE SQUARE-WELL POTENTIAL (1-DIMENSIONAL BOX)

The simplest such system is a particle trapped in a 1-D box with infinitely hard walls that the particle cannot penetrate. This potential is called an infinite square well and is given by:

$$U(x) = \begin{cases} 0 & 0 < x < L \\ \infty & x \leq 0, x \geq L \end{cases}$$

- We may specify the particle's motion is restricted to traveling along the x axis between $x = 0$ and $x = L$ by infinitely hard walls.
- A particle does not lose energy when it collides with such walls, so that its total energy stays constant. The potential energy U of the particle is infinite on both sides of the box, while U is a constant-say 0 for convenience on the inside (Fig).
- As the particle cannot have an infinite amount of energy, it cannot exist outside the box, and so its wave function ψ is 0 for $x \leq 0$ and $x \geq L$.
- Our task is to find what is ψ within the box, namely, between $x = 0$ and $x = L$.



A square well potential with infinitely high barriers at each end corresponds to a box of infinitely hard walls

CONT'D....

Within the box Schrödinger's equation becomes
$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} \{E - U(x)\} \psi(x) = 0 \quad \text{————— (1)}$$

It is to be noted that in this problem potential energy does not depend on time. In fact we have assumed, $U=0$ inside the box, so Schrodinger's time independent equation would be applicable in this case.

Therefor equation (1) will reduce to:
$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} E \psi = 0$$

or
$$\frac{d^2\psi}{dx^2} + k^2 \psi = 0 \quad \text{————— (2)}$$

Where, $k^2 = \frac{2mE}{\hbar^2}$ or $k = \frac{\sqrt{2mE}}{\hbar}$

We can get this using de Broglie's formula, $\lambda = \frac{h}{mv} = \frac{h}{\sqrt{2mE}}$ and $k = \frac{2\pi}{\lambda}$

The general solution to the equation (2) is
$$\psi = A \sin kx + B \cos kx \quad \text{————— (3)}$$

Here A and B are constants and can be found using boundary conditions.

CONT'D....

Boundary conditions of the potential dictate that the wave function, ψ must be zero at $x = 0$ and $x = L$.

Using 1st boundary condition, when $x = 0$ then $\psi = 0$

From equation (3), we get $0 = A \sin 0 + B \cos 0$

Which implies $B = 0$

Thus the wave function, ψ becomes $\psi = A \sin kx$

Using 2nd boundary condition, when $x = L$ then $\psi = 0$

From equation (4), we get $0 = A \sin kL$

This yields valid solutions for integer values of n such that:

$$kL = n\pi \quad (5) \quad \text{Where } n = 1, 2, 3, 4 \dots$$

Therefore the wave function is now

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

Expression of eigen function of the particle

CONT'D....

Still we have to find the constant A which can be found by normalizing the wave function

According to normalization condition in 1-dimension, $\int_{-\infty}^{\infty} |\psi|^2 dx = 1$

Now

$$|\psi_n|^2 = \psi_n \psi_n^* = A^2 \sin^2 \left(\frac{n\pi x}{L} \right)$$

(As given wave function is a real one so its multiplication with its complex conjugate will yield square of the function itself)

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

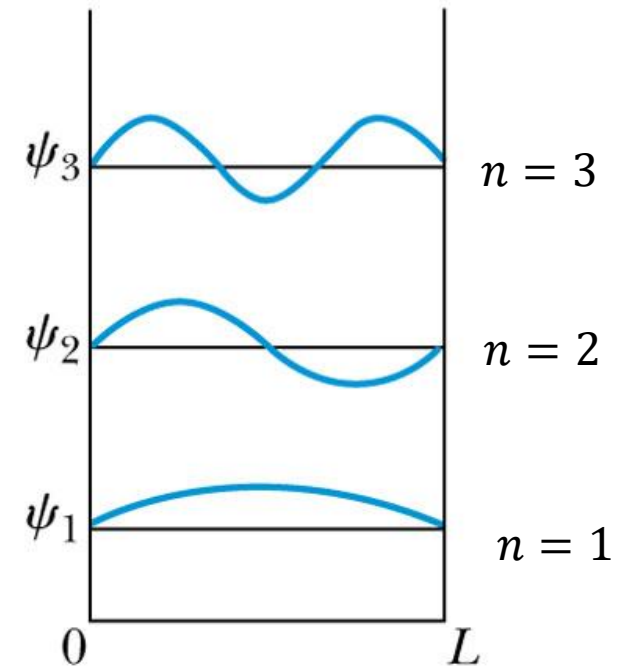
$$\therefore A^2 \int_0^L \sin^2 \left(\frac{n\pi x}{L} \right) dx = 1 \Rightarrow A^2 \int_0^L \frac{1 - \cos \left(\frac{2n\pi x}{L} \right)}{2} dx = 1 \Rightarrow \frac{A^2}{2} \int_0^L \left[1 - \cos \left(\frac{2n\pi x}{L} \right) \right] dx = 1$$

CONT'D....

On integrating w.r.t. x , we get $\frac{A^2}{2} \left[x - \frac{L}{2\pi n} \sin \left(\frac{2n\pi x}{L} \right) \right]_0^L = 1$

On substituting the limits, we get, $\frac{A^2}{2} L = 1 \Rightarrow A^2 = \frac{2}{L}$
 $\therefore A = \sqrt{\frac{2}{L}}$

Thus the normalized wave function becomes, $\psi_n = \sqrt{\frac{2}{L}} \sin \left(\frac{n\pi x}{L} \right)$



Expression for eigen function
of the particle

These functions are identical to those obtained for a vibrating string with fixed ends.

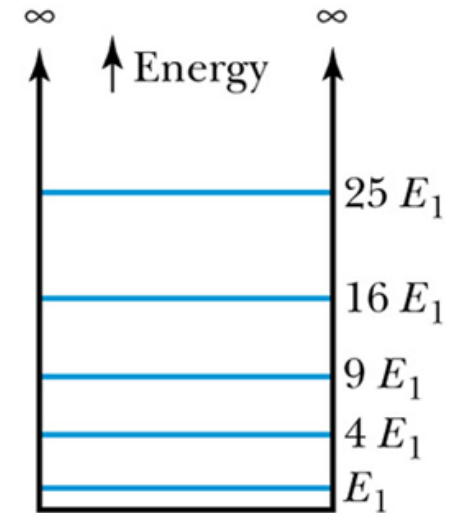
QUANTIZED ENERGY OF THE PARTICLE- ENERGY EIGEN VALUES

From equation (5), $kL = n\pi$

The quantized wave number and hence energy becomes

$$k_n = \frac{n\pi}{L} = \frac{\sqrt{2mE_n}}{\hbar} \Rightarrow E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

Expression for Energy Eigen Values



Note that the energy depends on the integer values of n . Hence the energy is quantized and non-zero.

The case of $n = 1$ is called the ground state energy.

$$E_1 = \frac{\pi^2\hbar^2}{2mL^2}$$

Which is very small however non-zero.

For $n = 2$,
1st excited state $E_2 = \frac{4\pi^2\hbar^2}{2mL^2}$ or $E_2 = 4E_1$

For $n = 3$,
2nd excited state $E_3 = 9E_1$ and so on...

PLOTS OF PROBABILITY DENSITY OF THE PARTICLE

$$|\psi_n|^2 = \psi_n \psi_n^*$$

For $n = 1$, the ground state

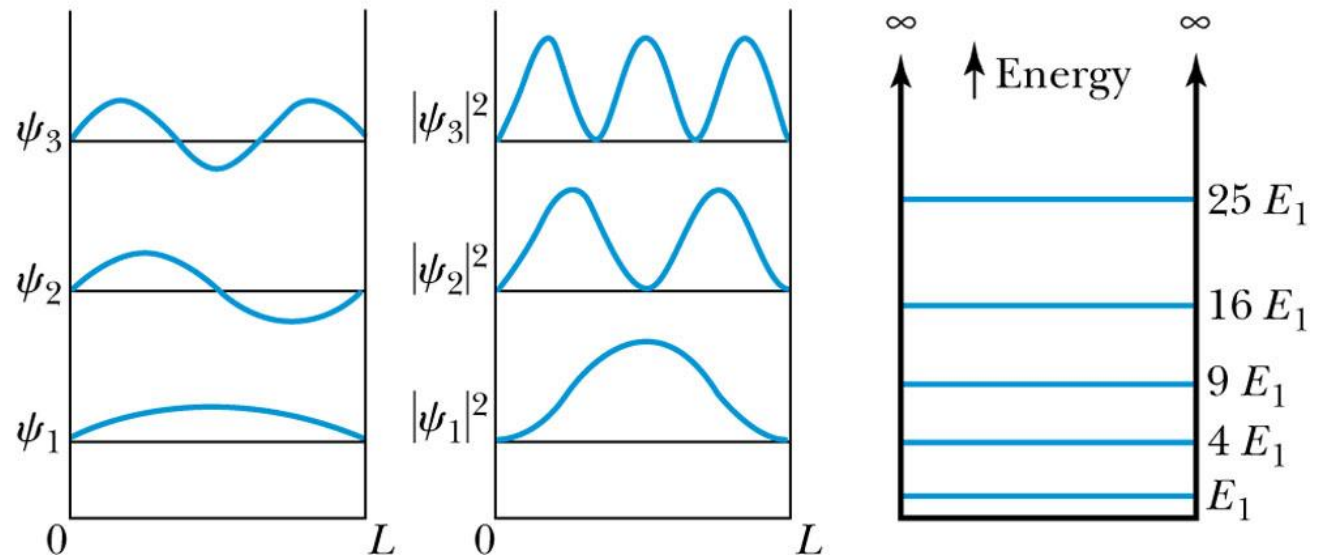
$$|\psi_1|^2 = \frac{2}{L} \sin^2\left(\frac{\pi x}{L}\right)$$

Probability density is maximum in the middle of the box

For $n = 2$, 1st excited state

$$|\psi_2|^2 = \frac{2}{L} \sin^2\left(\frac{2\pi x}{L}\right)$$

Probability density is zero in the middle of the box as well as at the boundaries and maximum at $L/4$ and $3L/4$



For $n = 3$, 2nd excited state

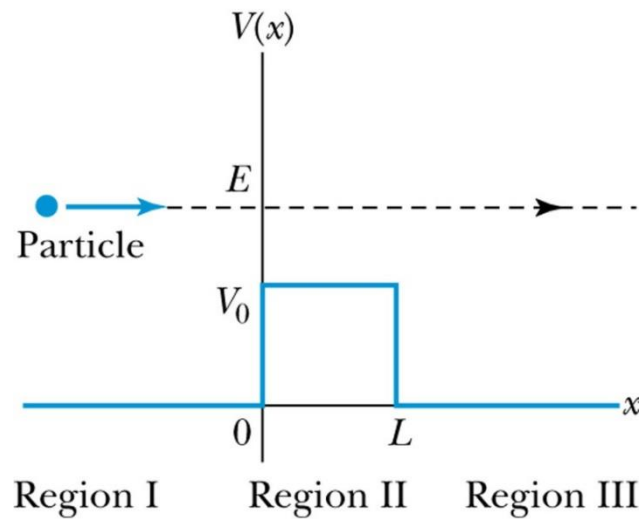
$$|\psi_3|^2 = \frac{2}{L} \sin^2\left(\frac{3\pi x}{L}\right)$$

Probability density is maximum at $L/6$, $L/2$ and $5L/6$.

BARRIERS AND QUANTUM TUNNELING

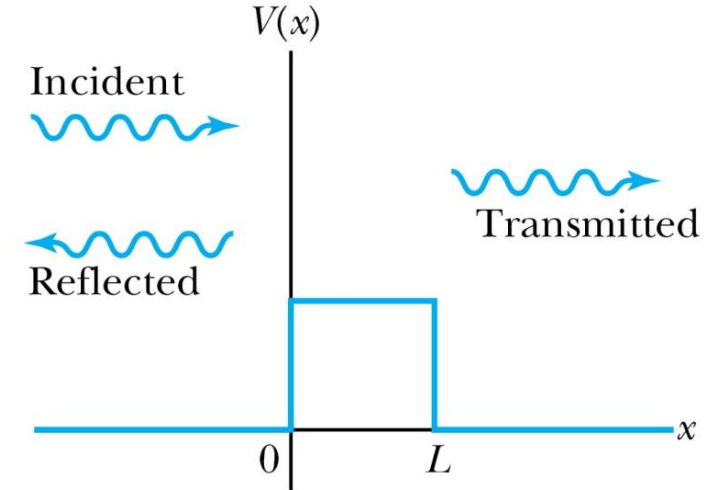
Consider a particle of energy E approaching a potential barrier of height V_0 and the potential everywhere else is zero.

We will first consider the case when the energy is greater than the potential barrier i.e. $E > V_0$



When $E > V_0$

Particle can comfortably go over the potential barrier, No tunnelling



CONT'D....

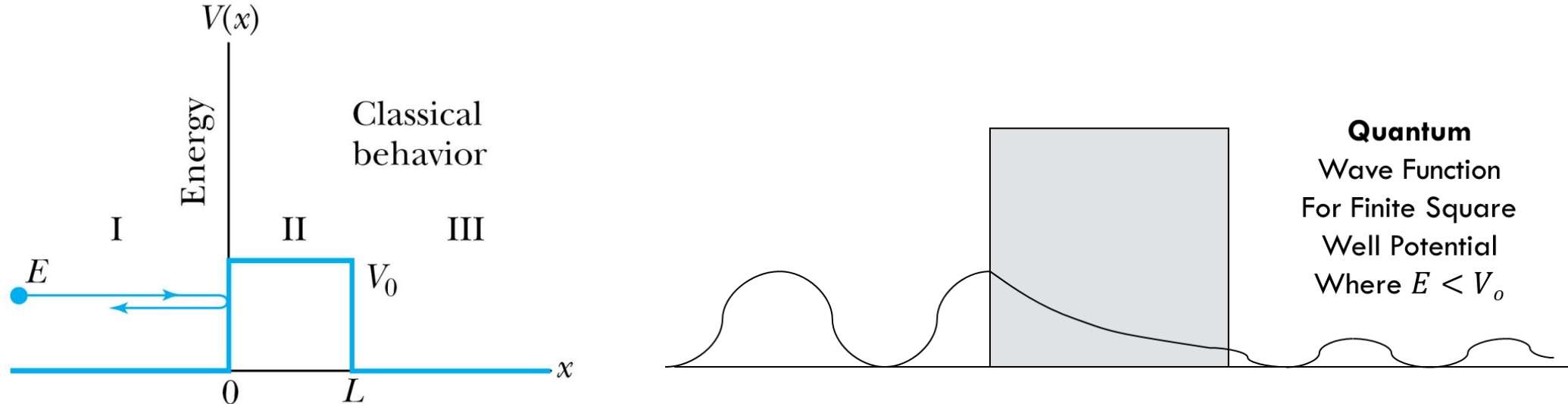


Classically, when an object hits a potential barrier that it doesn't have enough energy to pass, it will never go through that potential wall, it always bounces back.

For example, if you throw a ball at a wall, it will bounce back at you.

QUANTUM TUNNELLING

Now we consider the situation where classically the particle does not have enough energy to surmount the potential barrier, $E < V_0$.



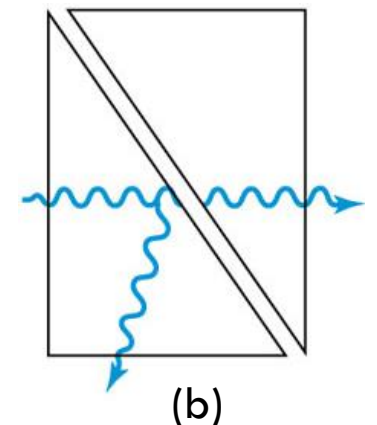
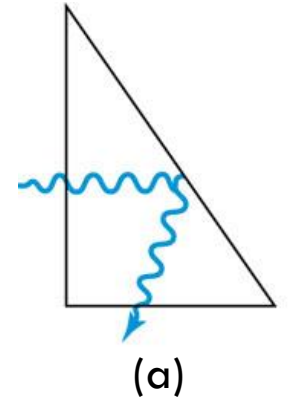
In quantum mechanics when a particle hits a potential that it doesn't have enough energy to pass, when inside the square well, the wave function dies off exponentially.

If the well is short enough, there will be a noticeable probability of finding the particle on the other side.

There is a small, but finite, probability that the particle can penetrate the barrier and even emerge on the other side.

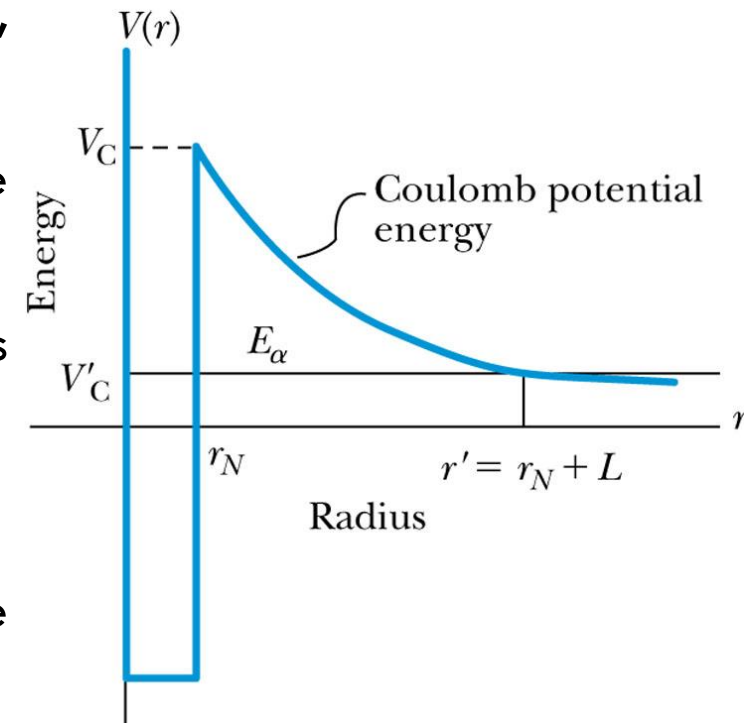
EXAMPLE 1: ANALOGY WITH WAVE OPTICS

- If light passing through a glass prism reflects from an internal surface with an angle greater than the critical angle, total internal reflection occurs.
- However, the electromagnetic field is not exactly zero just outside the prism.
- we bring another prism very close to the first one, experiments show that the electromagnetic wave (light) appears in the second prism.
- The situation is analogous to the tunneling described here. This effect was observed by Newton and can be demonstrated with two prisms and a laser.
- The intensity of the second light beam decreases exponentially as the distance between the two prisms increases.



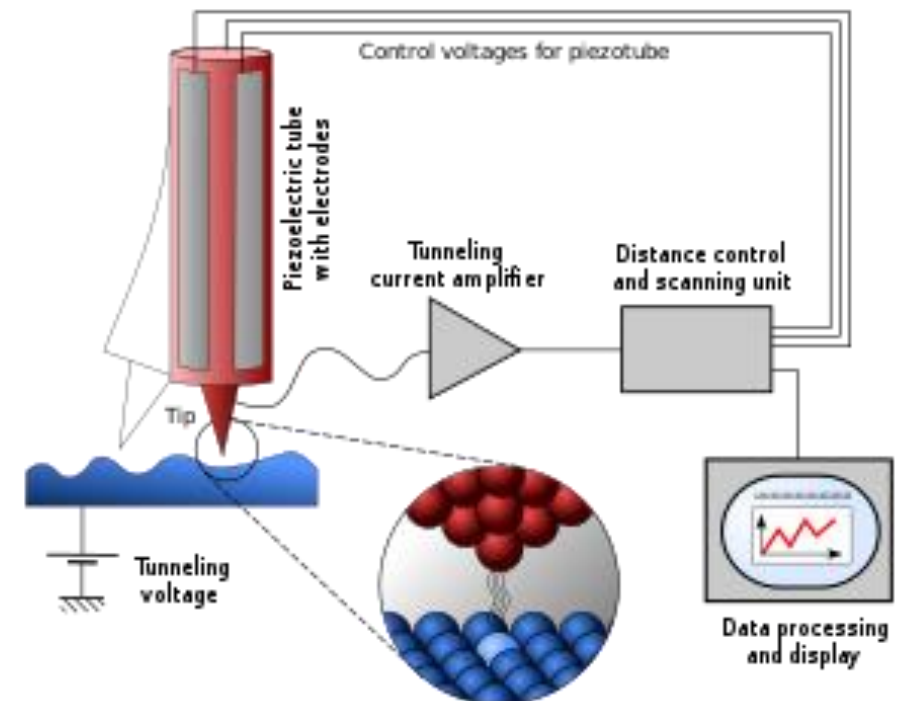
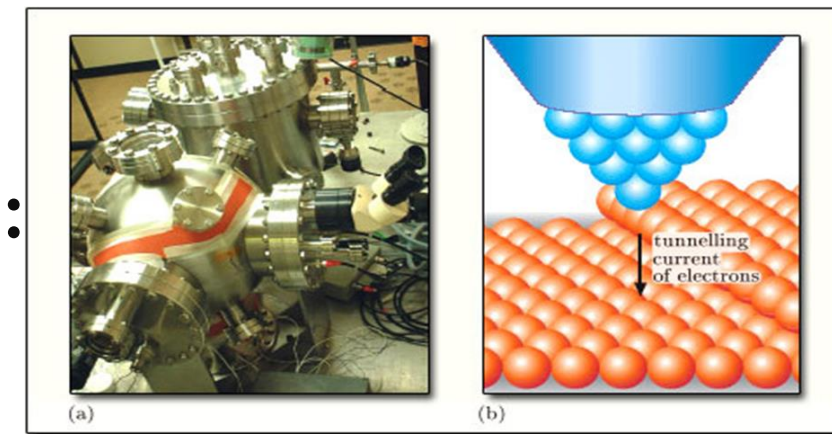
EXAMPLE 2: ALPHA-PARTICLE DECAY

- The phenomenon of tunneling explains the alpha-particle decay of heavy, radioactive nuclei.
- Inside the nucleus, an alpha particle feels the strong, short-range attractive nuclear force as well as the repulsive Coulomb force.
- The nuclear force dominates inside the nuclear radius where the potential is approximately a square well.
- The Coulomb force dominates outside the nuclear radius.
- The potential barrier at the nuclear radius is several times greater than the energy of an alpha particle.
- According to quantum mechanics, however, the alpha particle can “tunnel” through the barrier.
- Hence this is observed as radioactive decay.



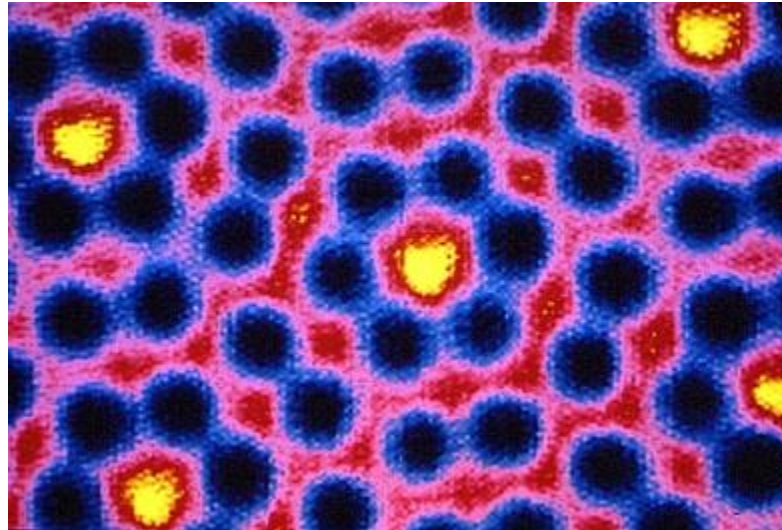
APPLICATIONS OF QUANTUM TUNNELLING: SCANNING TUNNELLING MICROSCOPE

- Scanning Tunneling Microscopy, or STM, is an imaging technique used to obtain ultra-high resolution images at the atomic scale, without using light or electron beams.
- It is used to study the 3-D topography of conducting surfaces
- STM was invented in 1981 by two IBM scientists named **Gerd Binnig and Heinrich Rohrer**.
- [Five years later, the invention earned them the Nobel Prize in Physics.](#)

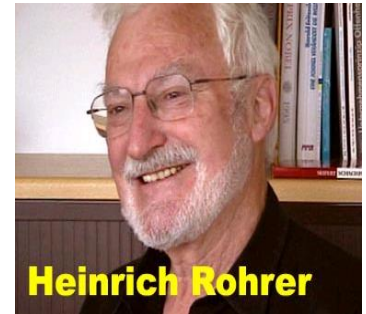


Schematic of a Scanning Tunnelling Microscope

STM IMAGE



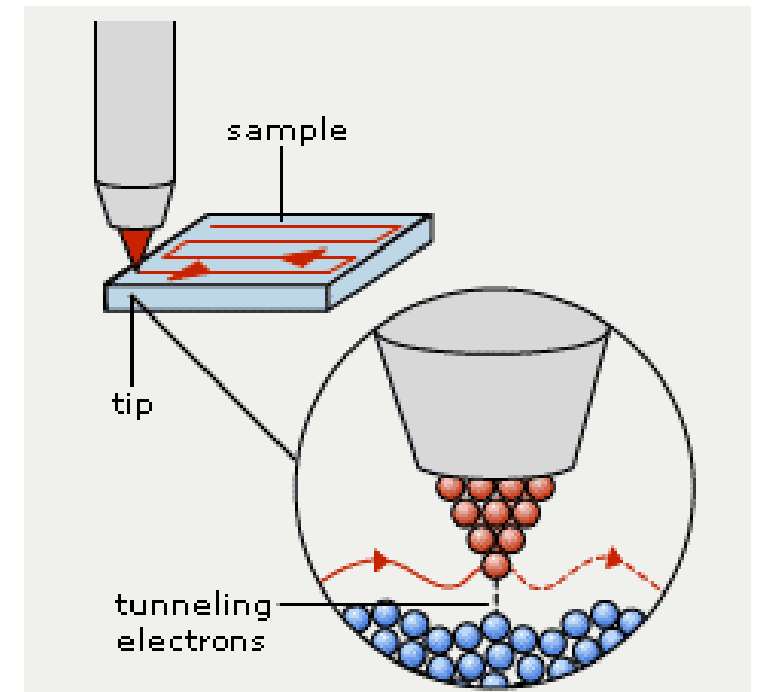
Resolution: ~ 0.01 nm.



- Silicon surface atoms enlarged 20 million times, color-enhanced by computer.
- The world's first images of individual surface atoms and the bonds that hold them in place were produced by a research technique developed by IBM -- scanning tunneling microscopy

WORKING PRINCIPLE OF STM

- Scanning tunneling microscope (STM) is a powerful technique for *viewing surfaces at the atomic level*.
- STM probes the electronic density of states of a material using tunneling current.
- The STM is based on the concept of Quantum Tunneling.
- An extremely fine conducting probe is held about an atom's diameter from the sample.
- Electrons tunnel between the surface and the tip, producing an electrical signal.
- While it slowly scans across the surface, the tip is raised and lowered in order to keep the signal constant and maintain the distance.
- This enables it to follow even the smallest details of the surface it is scanning.



CONT'D....

- A STM does not measure nuclear position directly. Rather it measures the electron density clouds on the surface of the sample.
- In some cases, the electron clouds represent the atom locations pretty well, but not always.

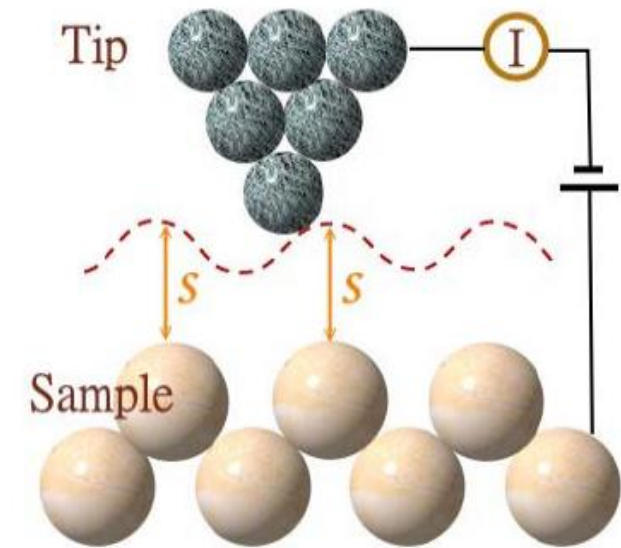
OPERATING MODES OF STM

The STM operates in two distinct modes: constant height mode and constant current mode.

- Constant height mode is generally used when the sample surface is very smooth.
- In this mode, the probe tip stays at a set height while it quickly raster scans across the sample.
- By measuring changes in the intensity of the tunneling current as a function of (x, y) position and bias voltage, researchers can construct an image of the electronic density of states of the sample surface, defects, frontier molecular orbitals, and more.

CONSTANT CURRENT MODE

- The more popular mode is known as the constant current mode.
- In this mode, the tunneling current is held constant by the use of a feedback loop system that adjusts the distance between the tip and the surface.
- That is to say, if the tunneling current exceeds the target value, the feedback control system will increase the distance between the tip and the sample; if the tunneling current is less than the target current value, the feedback control system will bring the tip closer to the surface of the sample.
- The resulting three-dimensional distance profile as a function of (x, y) position can help researchers measure a wide array of characteristics, including surface roughness, defects, and the size and conformation of molecules on the surface.



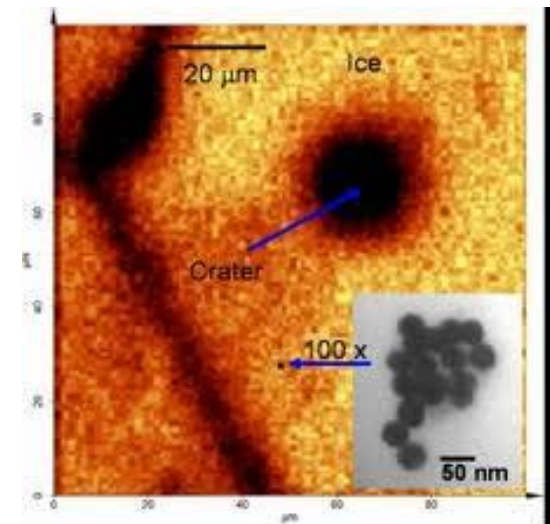
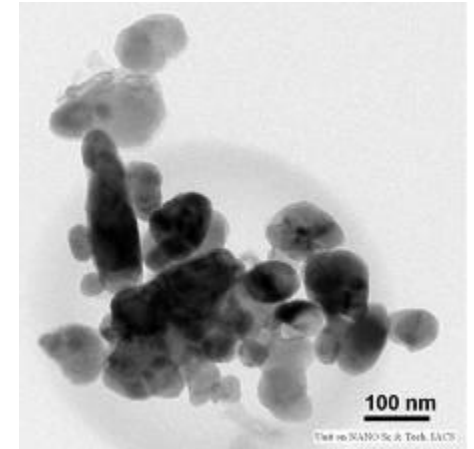
Constant Current Mode

NANOMATERIALS

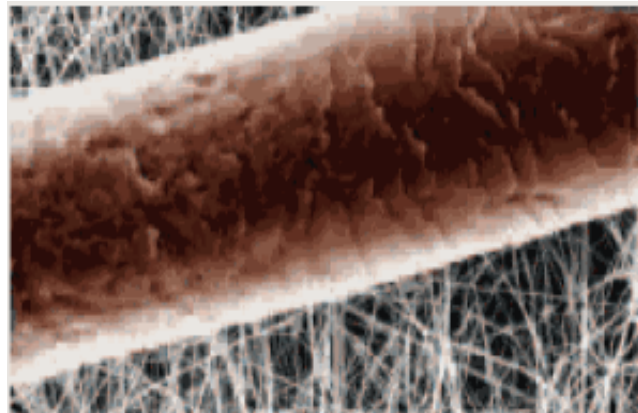
- Top-down Science
- Bottom-up Science

Nanomaterials are the materials possessing grain sizes of the order of a billionth of a meter (10^{-9}m).

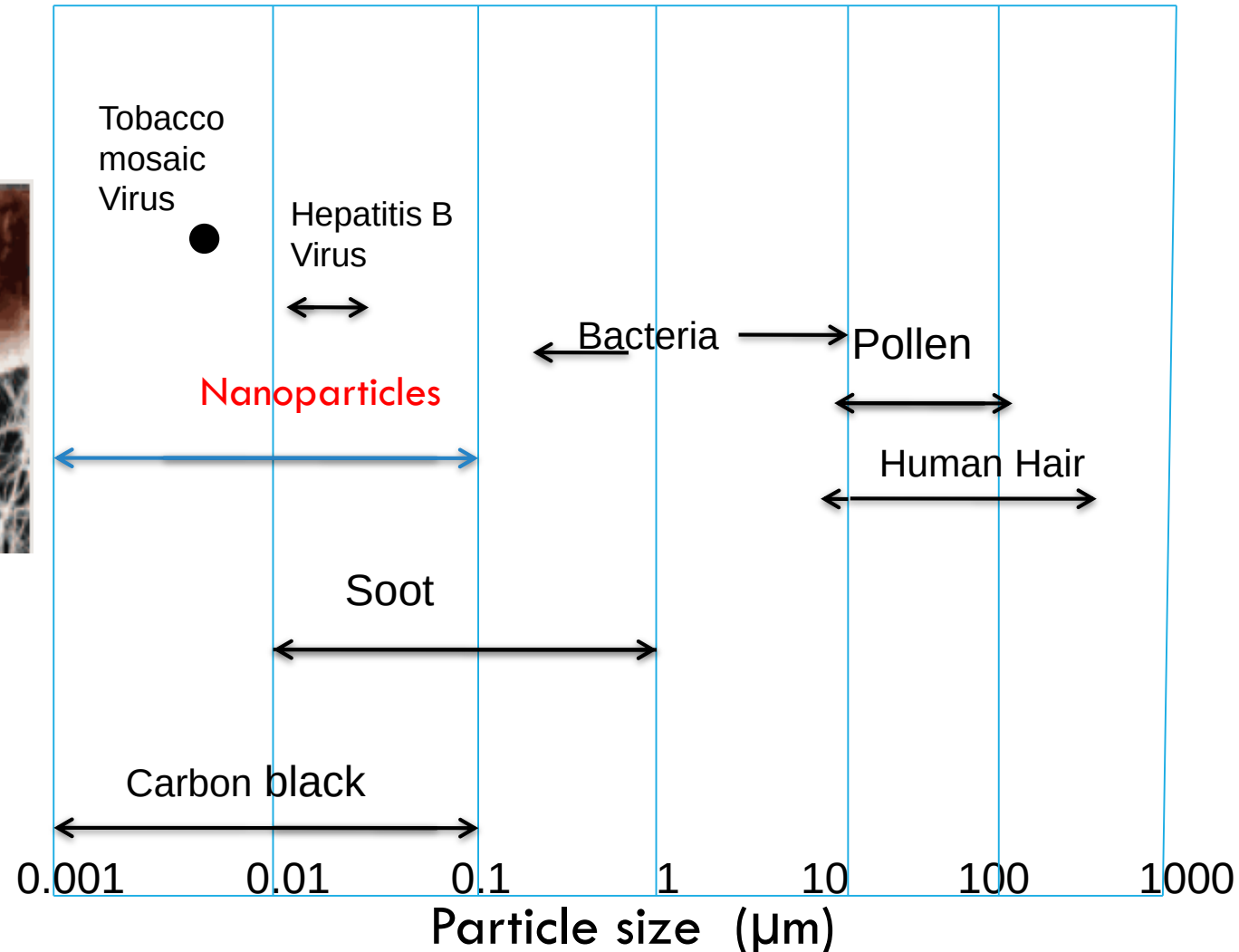
Nanomaterial research literally exploded in mid -1980's



TYPICAL SIZE OF SMALL PARTICLES



A Scanning
electron
microscope
image of a hair
strand



CONT'D....

- ❖ Conventional material have grain size anywhere from 100 μm to 1 mm and more
- ❖ Particles with size between 1-100 nm are normally regarded as Nanomaterials
- ❖ The average size of an atom is of the order of 1-2 Angstroms in radius.
- ❖ 1 nanometer = 10 Angstroms
- ❖ 1 nm there may be 3-5 atoms

WHAT MAKES A NANOMATERIAL DIFFERENT FROM BULK?

Two principal factors cause the properties of nanomaterials to differ significantly from Bulk materials:

- Increased relative surface area
- Quantum effects

These factors can change or enhance properties such as chemical reactivity, strength, magnetic, thermal and electrical properties.

Surface Effects:

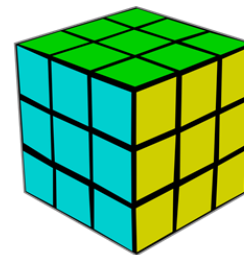
As a particle decreases in size, a greater proportion of atoms are found at the surface compared to those inside. For example, a particle of

Size-30 nm → 5% of its atoms on its surface

Size-10 nm → 20% of its atoms on its surface

Size-3 nm → 50% of its atoms on its surface

Nanoparticles are more reactive than large particles.



$$\begin{aligned}\text{sides} &= 3 \\ \text{surface} &= 3^2 \times 6 = 54 \\ \text{volume} &= 3^3 = 27\end{aligned}$$

$$\text{surface/volume} = 2$$



$$\begin{aligned}\text{sides} &= 2 \\ \text{surface} &= 2^2 \times 6 = 24 \\ \text{volume} &= 2^3 = 8\end{aligned}$$

$$\text{surface/volume} = 3$$



$$\begin{aligned}\text{sides} &= 1 \\ \text{surface} &= 1^2 \times 6 = 6 \\ \text{volume} &= 1^3 = 1\end{aligned}$$

$$\text{surface/volume} = 6$$

CLASSIFICATION OF NANOMATERIALS

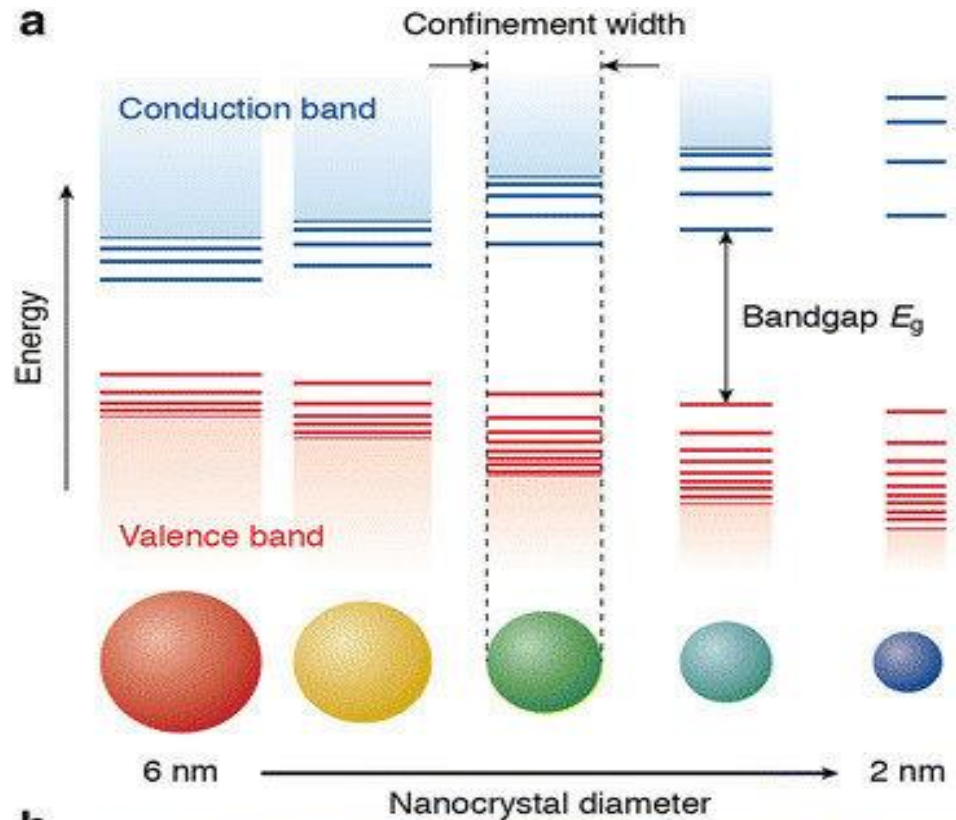


- ❖ Nanomaterials are those materials which have structured components with at least one dimension less than 100 nm.
- ❖ One dimension in nanoscale (Other two dimensions are extended) (2-D) e.g. Thin films, Surface Coatings, Computer chips
- ❖ Two dimensions in nanoscale (Other one dimension is extended) (1-D) e.g. Nanowires, Nanotubes
- ❖ Three dimensions squeezed to nanoscale (0-D) e.g. Nanoparticles, Precipitates, Colloids, Quantum dots (tiny particles of semiconductor material)

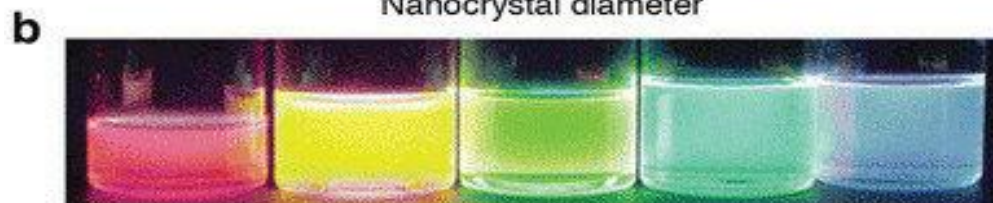
QUANTUM CONFINEMENT

- Quantum confinement can be observed once the diameter of a material is of the same magnitude as the de Broglie wavelength of the electron wave function.
- When materials are this small, their electronic and optical properties deviate substantially from those of bulk materials.
- A particle behaves as if it was free when the confining dimension is large compared to the wavelength of the particle.
- During this state, the band gap remains at its original energy due to a continuous energy state. However, as the confining dimension decreases and reaches a certain limit, typically in nano scale, energy spectrum becomes discrete.
- As a result, the band gap becomes size-dependent. This ultimately results in a blue shift in light emission as the size of the particles decreases.

EXAMPLE: GOLD NANO PARTICLES



Different sizes gold nano particles appear of different colors. As the size of the particle is reduced, the wavelength of the light emitted by the particle decreases due to increase in energy band gap.



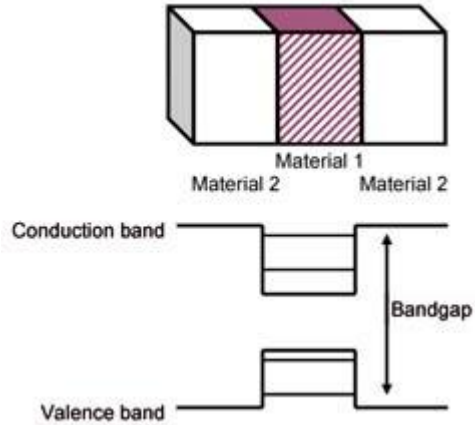
DENSITY OF STATES IN 3-D, 2-D, 1-D, 0-D NANO MATERIALS

The density of states function describes the number of states that are available in a system and is essential for determining the carrier concentrations and energy distributions of carriers within a semiconductor.

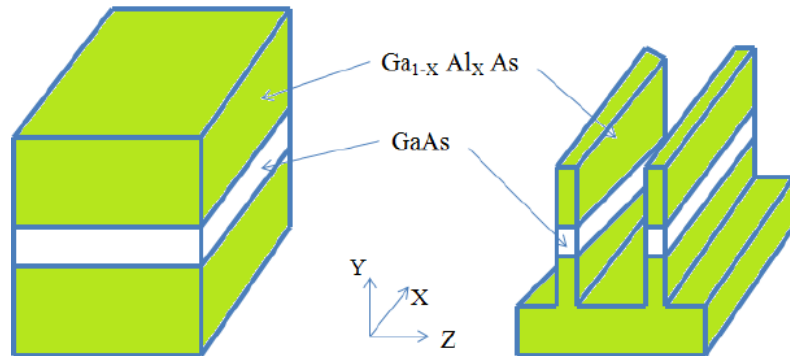
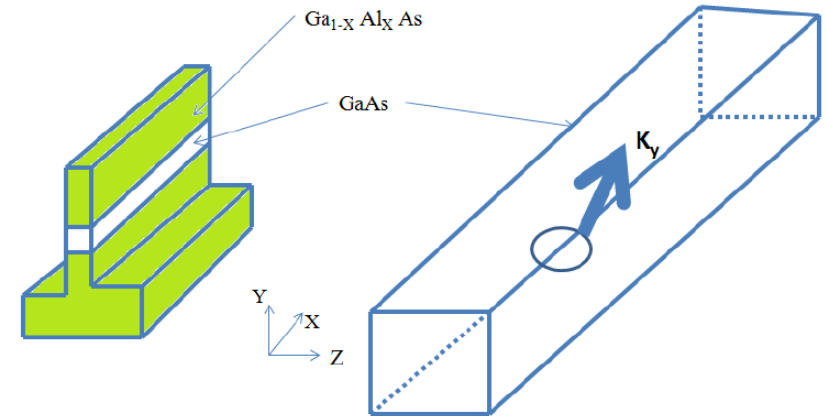
In semiconductors, the free motion of carriers is limited to two, one, and zero spatial dimensions. When applying semiconductor statistics to systems of these dimensions, the density of states in quantum wells (2D), quantum wires (1D), and quantum dots (0D) must be known.

HOW TO MAKE QUANTUM WELL, WIRE AND DOT STRUCTURES?

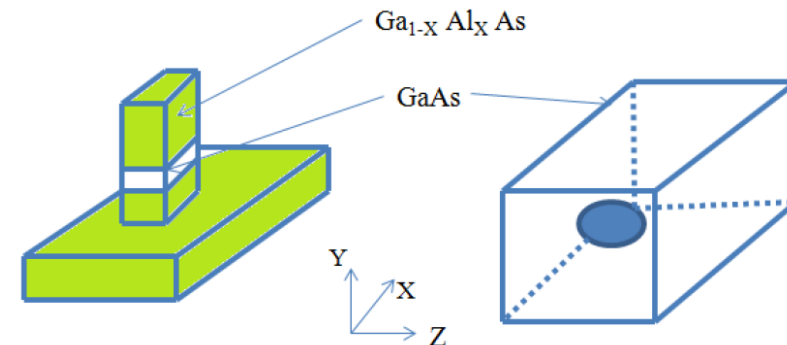
Quantum well



Quantum wire



Quantum dot



DENSITY OF STATES AS A FUNCTION OF ENERGY

