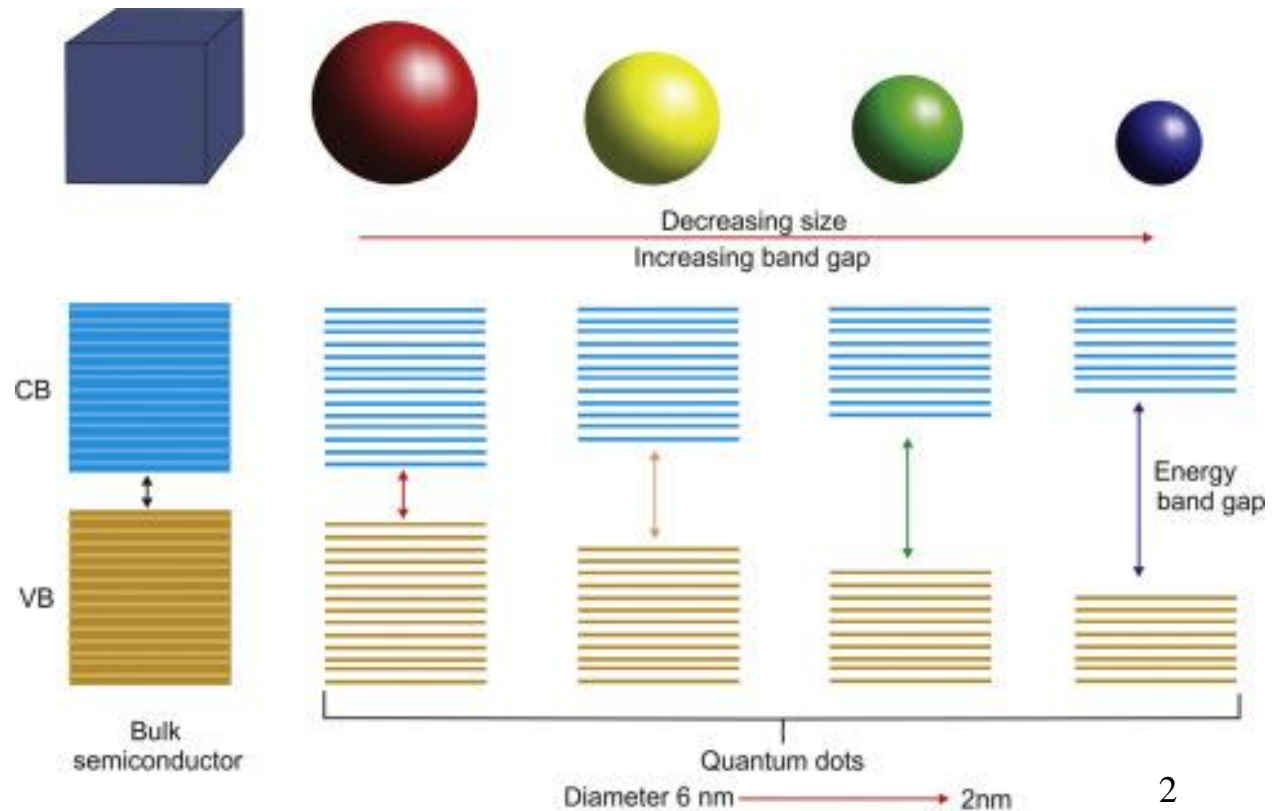# Nanophysics

(II - MSc PHYSICS - 3rd Semester)

Quantum Confinement

(Unit-I)

Course Teacher: Dr. K. JEGANATAN

Electronic or "quantum" confinement occurs as particle size becomes the same or smaller than the Bohr radius, mean free path length of electrons or the charging (Coulombic) behavior of the electrons. As a rule of thumb, "quantum" size effects appear in materials typically when the crystallite size becomes < 10 nm but can be important at several tens of nanometer.

The 'quantum confinement effect' arises from the discretization of electronic energy states, confining the electrons in a material within a very small space
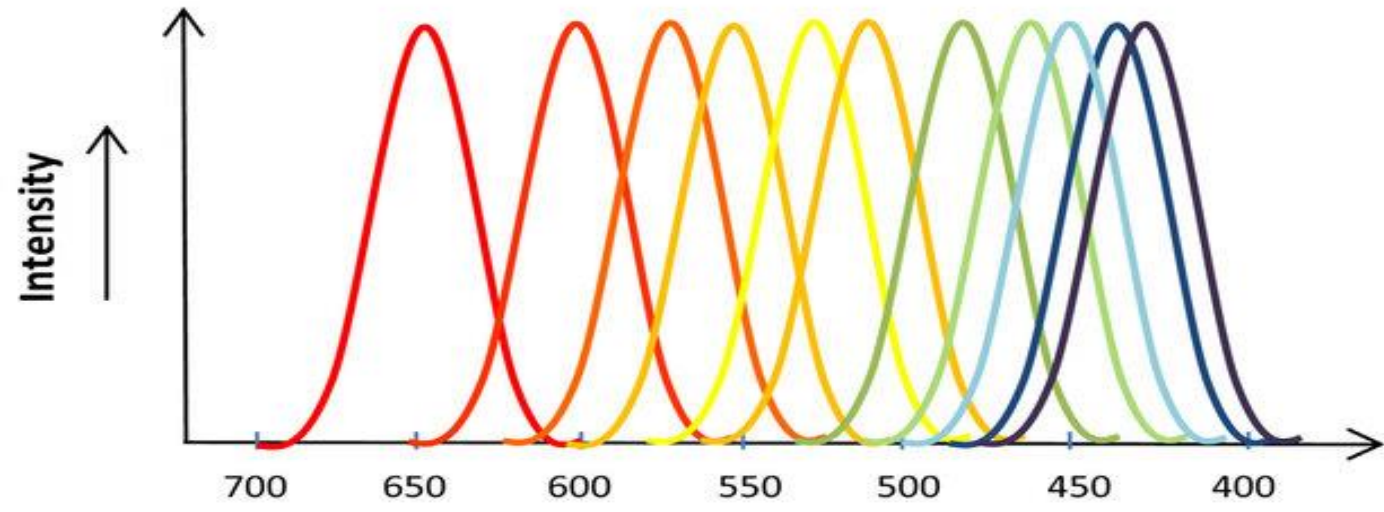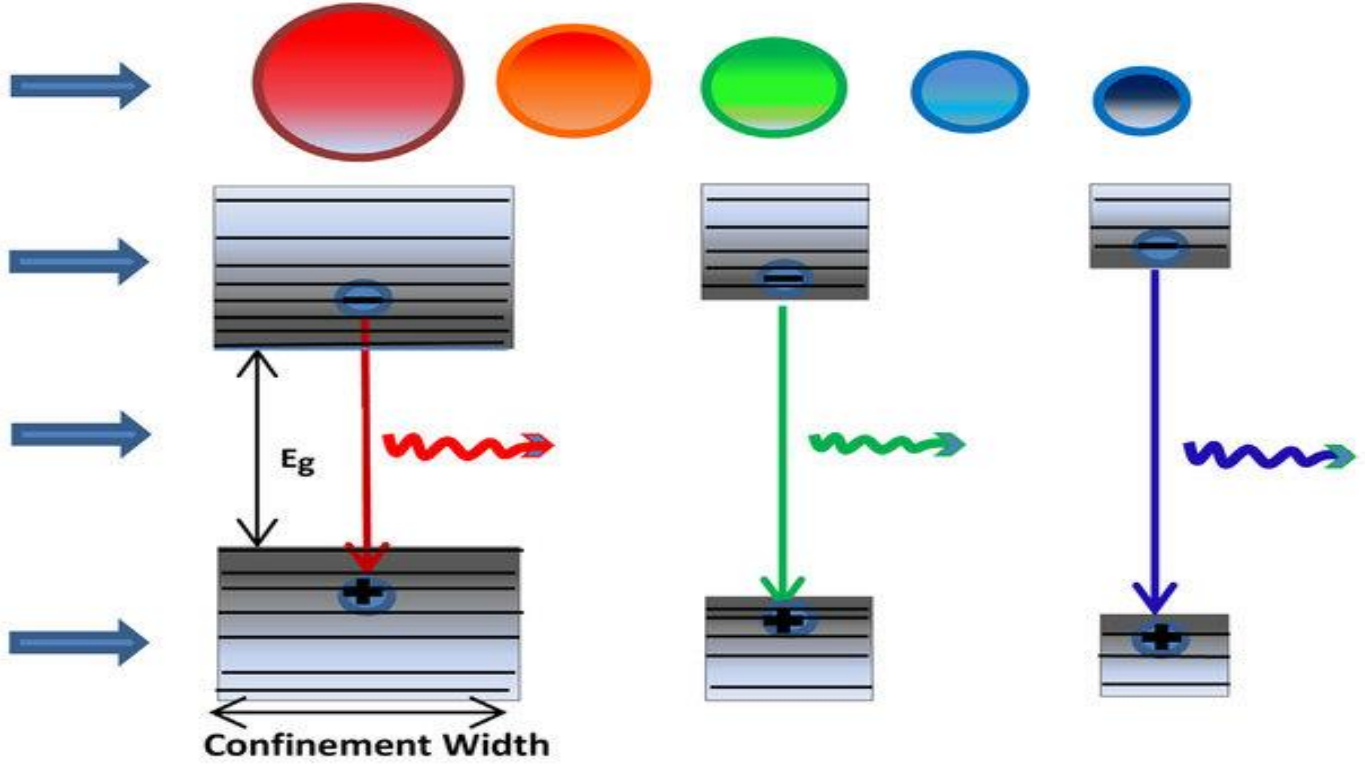

Decreasing size
Increasing band gap

CB

VB

Energy band gap

Bulk semiconductor

Quantum dots

Diameter 6 nm ⟶ 2nm

2

Quantum Dot's Decreasing size

Conduction Band

Increasing energy gap and changing emission colours

E_g

Valance Band

Confinement Width

Intensity

700   650   600   550   500   450   400

Blue shift in wavelength(nm) with decreasing size

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Physics of Quantum Confinement

In 1970 Leo Esaki & Tsu proposed the fabrication of an artificial structure, consisting of alternating layers of 2 different semiconductors.

Layer Thickness

$$\approx 1 \text{ nm} = 10 \text{ Å} = 10^{-9} \text{ m} \equiv SUPERLATTICE$$

- The *main idea* was that introduction of an *artificial periodicity* will "fold" the Brillouin Zones into smaller BZ's ≡ "mini-zones".

⇒ The idea was that this would **raise the conduction band minima**, which is needed to observe novel physics and can be employed for some quantum and nano device applications.

- **Modern growth techniques** (starting in the 1980's), especially **MBE** & **MOCVD**, make fabrication of such structures possible!

- For the same reason, it is also possible to fabricate **many other kinds** of artificial structures on the scale of nm

(**nanometers**) ≡ **"Nanostructures"**

Superlattices   = **"2 dimensional"** structures
Quantum Wells   = **"2 dimensional"** structures
Quantum Wires   = **"1 dimensional"** structures
**Quantum Dots**   = *"0 dimensional"* structures!!

- Clearly, it is not only the electronic properties of materials which can be drastically altered in this way. Also, vibrational properties (phonons). Here, only electronic properties are considered

- For many years, quantum confinement has been a fast growing field in both theory & experiment! It is at the forefront of current research!

Quantum Confinement in Nanostructures: Overview

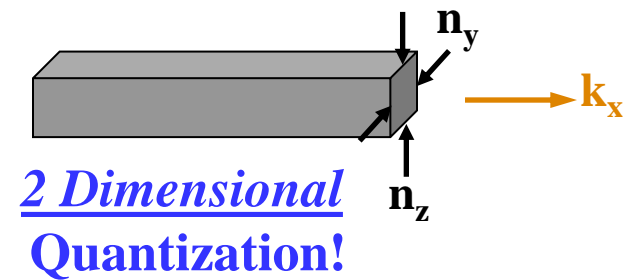**Electrons _Confined in 1 Direction_:**
 Quantum Wells (thin films)**:**
 $\Rightarrow$ **Electrons** can easily move in
 2 Dimensions!

n_z

k_y k_x

1 Dimensional **Quantization!**
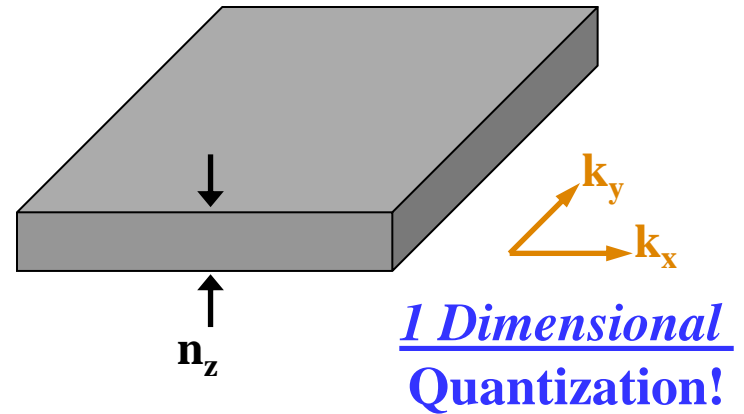
Electrons _Confined in 2 Directions_:
 Quantum Wires:
 $\Rightarrow$ **Electrons** can easily move in
 1 Dimension!

n_y k_x

2 Dimensional **Quantization!**

n_z

Electrons _Confined in 3 Directions_:
 Quantum Dots:
 $\Rightarrow$ **Electrons** can easily move in
 0 Dimensions!

n_z n_x n_y

3 Dimensional **Quantization!**
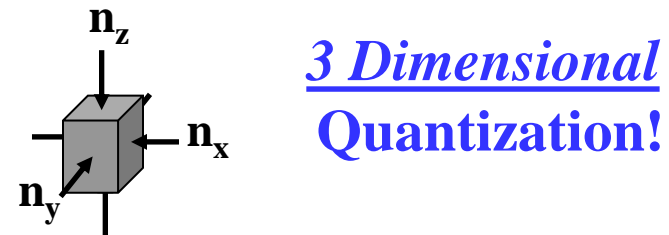
Each further confinement direction changes a continuous k component to a discrete component characterized by a quantum number n.

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- **<u>PHYSICS</u>:** Revisit the band structure
  - Consider the 1st Brillouin Zone for the infinite crystal. The maximum wave vectors are of the order

$$k_m \approx (\pi/a)$$

  a = lattice constant. The potential V is periodic with period a. In the almost free e⁻ approximation, the bands are free e⁻ like except near the Brillouin Zone edge. That is, they are of the form:

$$E \approx (\hbar k)^2/(2m_o)$$

  So, the <u>energy at the Brillouin Zone edge</u> has the form:

$$E_m \approx (\hbar k_m)^2/(2m_o)$$

  or

$$E_m \approx (\hbar\pi)^2/(2m_o a^2)$$

A Brillouin zone is defined as a Wigner-Seitz primitive cell in the reciprocal lattice. The first Brillouin zone is the smallest volume entirely enclosed by planes that are the perpendicular bisectors of the reciprocal lattice vectors drawn from the origin

a)

Brillouin zone

b)

Brillouin zone
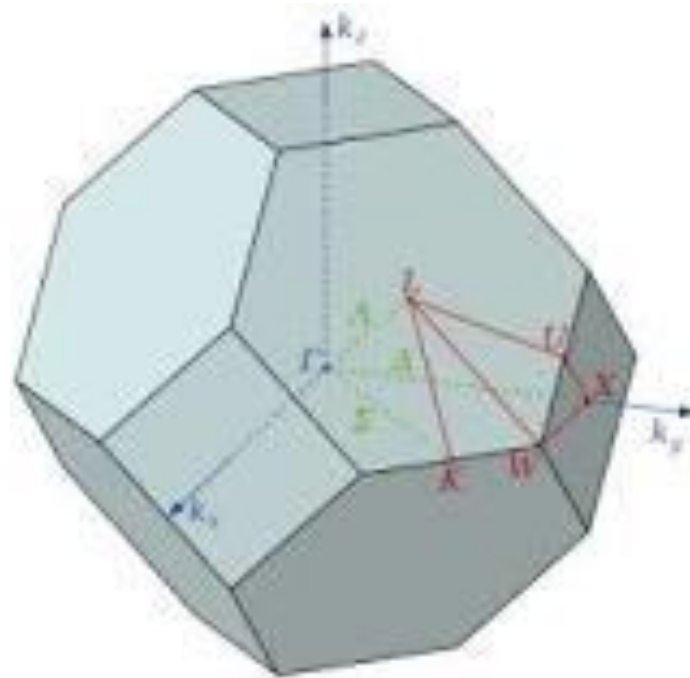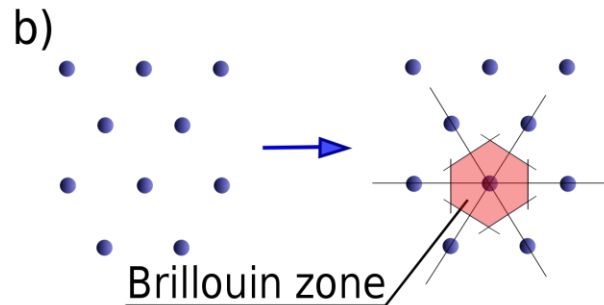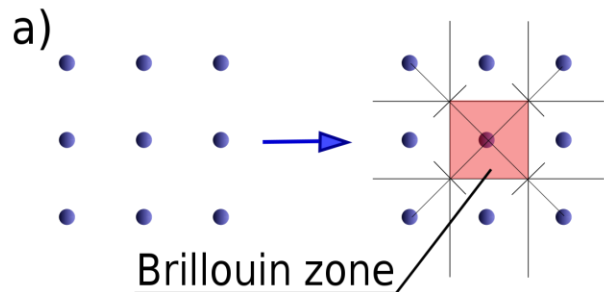
In reciprocal space, a reciprocal lattice is defined as the set of wavevectors of plane waves in the Fourier series of any function whose periodicity is compatible with that of an initial direct lattice in real space.
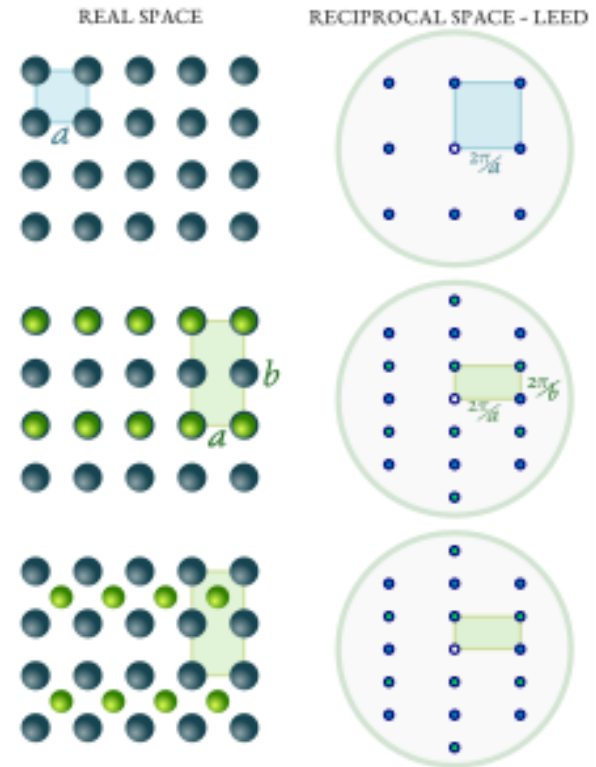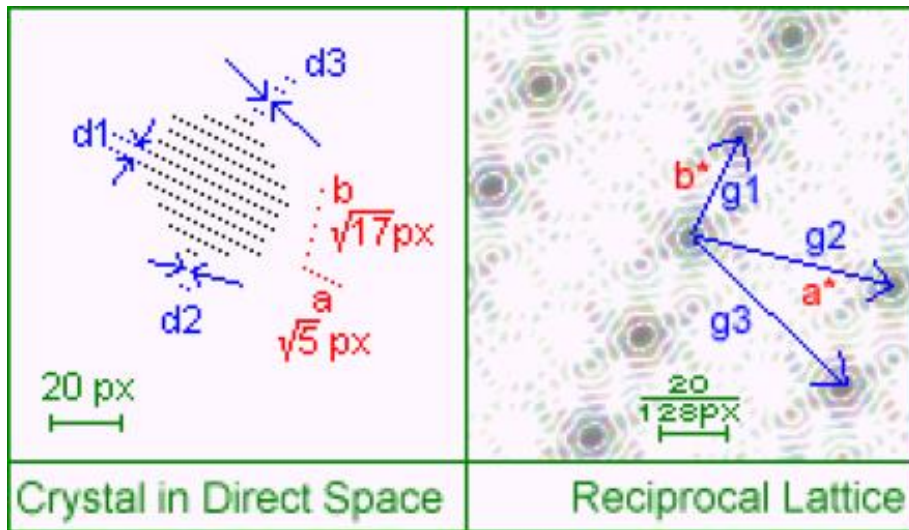
- *SUPERLATTICES* ≡ Alternating layers of material. Periodic, with periodicity **L** (layer thickness). Let $k_z =$ wavevector perpendicular to the layers.

- In a superlattice, the potential **V** has a *new periodicity* in the **z** direction with periodicity **L >> a**

  ⇒ In the **z** direction, the Brillouin Zone is much smaller than that for an infinite crystal. The maximum wavevectors are of the order: $k_s \approx (\pi/L)$

  ⇒ At the BZ edge in the **z** direction, the energy has the form:

  $$E_s \approx (\hbar\pi)^2/(2m_oL^2) + E_2(k)$$

  $E_2(k) =$ the 2 dimensional energy for **k** in the **x,y** plane.

  Note that: $(\hbar\pi)^2/(2m_oL^2) \ll (\hbar\pi)^2/(2m_oa^2)$

Primary Qualitative Effects of Quantum Confinement

- Consider *electrons confined along 1 direction* (say, **z**) to a layer of width **L:**

Energies

- The *energy bands are quantized* (instead of continuous) in k_z & shifted **upward. So k_z is quantized:**

$$k_z = k_n = [(n\pi)/L], \ n = 1, 2, 3$$

- So, in the effective mass approximation (**m***), *the bottom of the conduction band is quantized* (like a particle in a **1 d** box) & shifted:

$$E_n = (n\hbar\pi)^2/(2m^*L^2)$$

- *Energies are quantized!* Also, the *wavefunctions are 2 dimensional Bloch functions* (*traveling waves*) for **k** in the **x,y** plane & *standing waves in the z direction*.

Quantum Confinement Terminology

Quantum Well ≡ QW

= A single layer of material **A** (layer thickness **L**), sandwiched between 2 **macroscopically large layers** of material **B**. Usually, the bandgaps satisfy:

$$E_{gA} < E_{gB}$$

Multiple Quantum Well ≡ MQW

= Alternating layers of materials **A** (thickness **L**) & **B** (thickness **L′**). In this case:

$$L' \gg L$$

So, the e⁻ & e⁺ in one **A** layer are independent of those in other **A** layers.

Superlattice ≡ SL

= Alternating layers of materials **A** & **B** with similar layer thicknesses.

Brief Elementary Quantum Mechanics & Solid State Physics Review

- **Quantum Mechanics of a Free Electron:**
  - The **energies are continuous**: $E = (\hbar k)^2/(2m_o)$ (1d, 2d, or 3d)
  - The **wavefunctions are traveling waves**:

$$\psi_k(x) = A\,e^{ikx} \quad (1d) \qquad\qquad \psi_k(r) = A\,e^{ik \bullet r} \quad (2d\ or\ 3d)$$

- **Solid State Physics: Quantum Mechanics of an Electron in a Periodic Potential in an infinite crystal :**
  - The **energy bands are (approximately) continuous**: $E = E_{nk}$
  - At the bottom of the conduction band or the top of the valence band, in the effective mass approximation, **the bands can be written:**

$$E_{nk} \cong (\hbar k)^2/(2m^*)$$

  - The **wavefunctions are Bloch Functions** = *traveling waves*:

$$\Psi_{nk}(r) = e^{ik \bullet r}\,u_{nk}(r); \ \ u_{nk}(r) = u_{nk}(r+R)$$

Some Basic Physics

- **Density of states** (DoS)

$$DoS = \frac{dN}{dE} = \frac{dN}{dk}\frac{dk}{dE}$$

in 3D:

$$N(k) = \frac{\text{k space vol}}{\text{vol per state}}$$
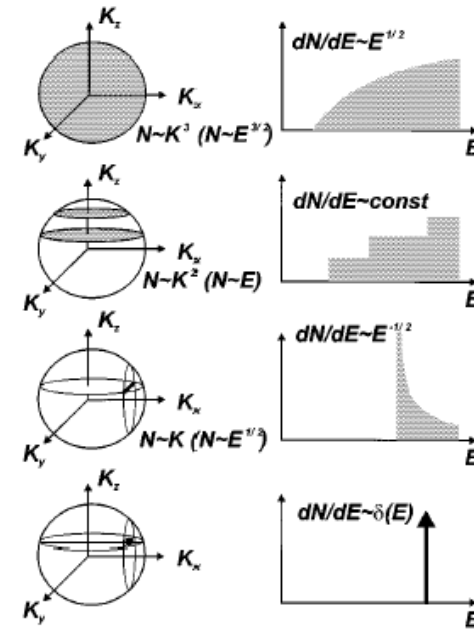
$$= \frac{4/3\,\pi k^3}{(2\pi)^3/V}$$

Fig. 1. Density of states for charge carriers in structures with different dimensionalities.

Structure	Degree of Confinement	$\dfrac{dN}{dE}$
Bulk Material	0D	$\sqrt{E}$
Quantum Well	1D	1
Quantum Wire	2D	$1/\sqrt{E}$
Quantum Dot	**3D**	**δ(E)**