Chapter 5

ATOMIC PHYSICS

OBJECTIVES:

- To know about the quantum model of H-atom and its wave functions.
- To understand more about Visible and X ray spectra
- To explain basic interactions of radiation with matter.
- To understand the basic principles and requirements for working of laser.
- To recognize the various applications of laser.
- To apply and evaluate the above concepts by solving numerical problems

The Quantum Model of the Hydrogen Atom

The time-independent Schrödinger equation in 3-dimensional space is

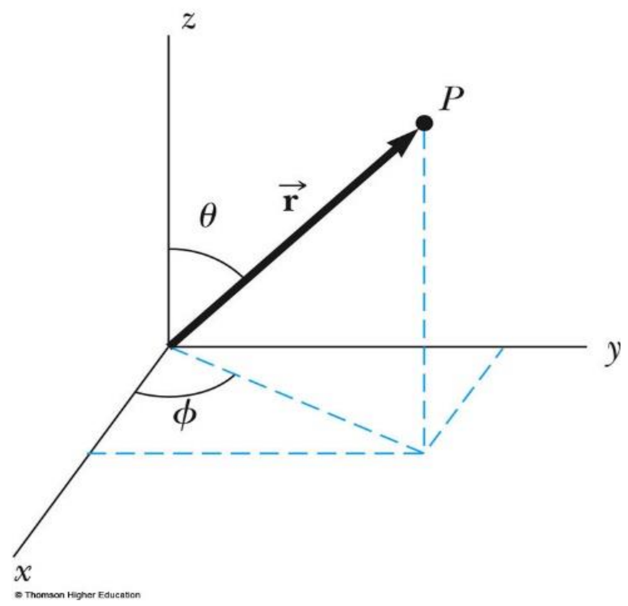
$$-\frac{\hbar^2}{2\,m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)+U\,\psi \;=\; E\,\psi$$

The potential energy function for the H-atom is

$$U(r) \;=\; -\frac{k_e e^2}{r}$$

Since the system is spherically symmetric, it is convenient to apply spherical coordinated system

$\psi(r,\ \theta,\ \phi) \;=\; R(r)\, f(\theta)\, g(\phi)$



The radial function $R(r)$ of ψ is associated with the **principal** quantum number $\boldsymbol{n}$. Solving $R(r)$, we get an expression for energy as,

$$E_n \;=\; -\left(\frac{k_e e^2}{2\,a_o}\right)\frac{1}{n^2} \;=\; -\frac{13.606\ eV}{n^2}, \qquad n = 1,\ 2,\ 3,\ \ldots$$

The polar function $f(\theta)$ is associated with the **orbital** quantum number ℓ. The azimuthal function $g(\phi)$ is associated with the **orbital magnetic** quantum number m_ℓ .

Allowed values:

n can range from 1 to ∞,

ℓ can range from 0 to $n-1$; [n allowed values].

m_ℓ can range from $-\ell$ to $+\ell$; [$(2\ell+1)$ allowed values].

$n = 1$	$\Rightarrow$	K	shell		$\ell = 0$	$\Rightarrow$	s	subshell
$n = 2$	$\Rightarrow$	L	shell		$\ell = 1$	$\Rightarrow$	p	subshell
$n = 3$	$\Rightarrow$	M	shell		$\ell = 2$	$\Rightarrow$	d	subshell
$n = 4$	$\Rightarrow$	N	shell		$\ell = 3$	$\Rightarrow$	f	subshell
$n = 5$	$\Rightarrow$	O	shell		$\ell = 4$	$\Rightarrow$	g	subshell
$n = 6$	$\Rightarrow$	P	shell		$\ell = 5$	$\Rightarrow$	h	subshell

Wave functions for hydrogen

- H-atom can be represented by wave functions that depend only on r (spherically symmetric function).
- The simplest wave function for H-atom is the 1s-state (ground state) wave function (n = 1, l = 0):

$$\psi_{1s}(r) = \frac{1}{\sqrt{\pi a_o^3}} e^{-\frac{r}{a_o}}$$

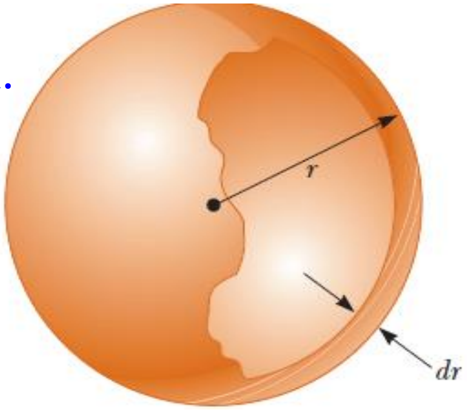
a_o = Bohr radius.

$$|\psi_{1s}|^2 = \left(\frac{1}{\pi a_o^3}\right) e^{-\frac{2r}{a_o}}$$

$|\psi_{1s}|^2$ is the probability density for H-atom in 1s-state.

The radial probability density P(r) is the probability per unit radial length of finding the electron in a spherical shell of radius r and thickness dr.

P(r) dr is the probability of finding the electron in this shell.

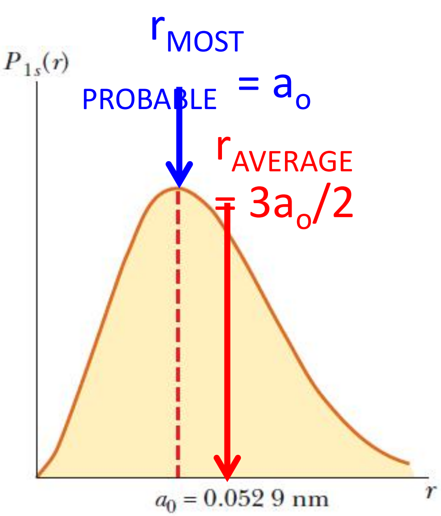


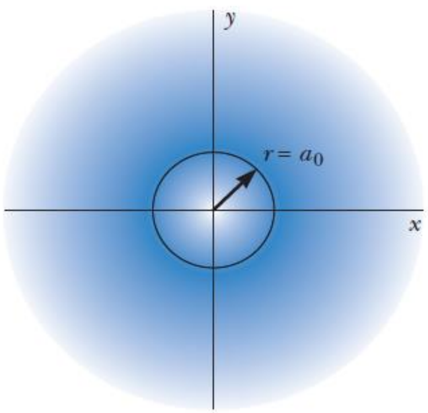
$$P(r)\,dr = |\psi|^2\,dv = |\psi|^2\,4\pi r^2\,dr$$

$$\therefore \quad P(r) = 4\pi r^2\,|\psi|^2$$

Radial probability density for H-atom in its ground state:

$$P_{1s}(r) = \left(\frac{4r^2}{a_o^3}\right)e^{-\frac{2r}{a_o}}$$

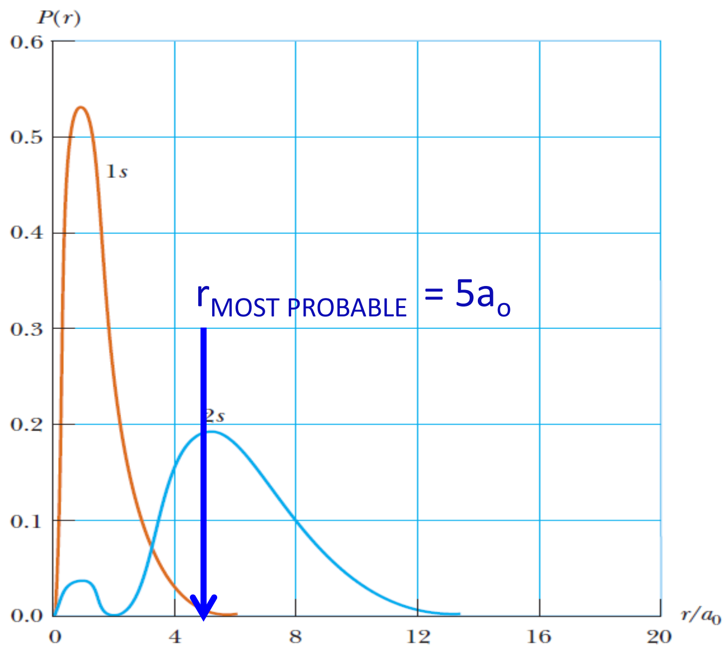




$P_{1s}(r)$ is maximum when

$r = a_o$ (Bohr radius).

$$\psi_{2s}(r) = \frac{1}{4\sqrt{2\pi}}\left(\frac{1}{a_o}\right)^{\frac{3}{2}}\left(2 - \frac{r}{a_o}\right)e^{-\frac{r}{a_o}}$$



ψ_{2s} is spherically symmetric (depends only on r)

$E_2 = E_1/4 = -3.401$ eV (1^{ST} excited state)

More on Atomic Spectra: Visible and X-Ray

- The frequency of this photon is $f = \Delta E/h$
- The **selection rules** for the *allowed transitions* are

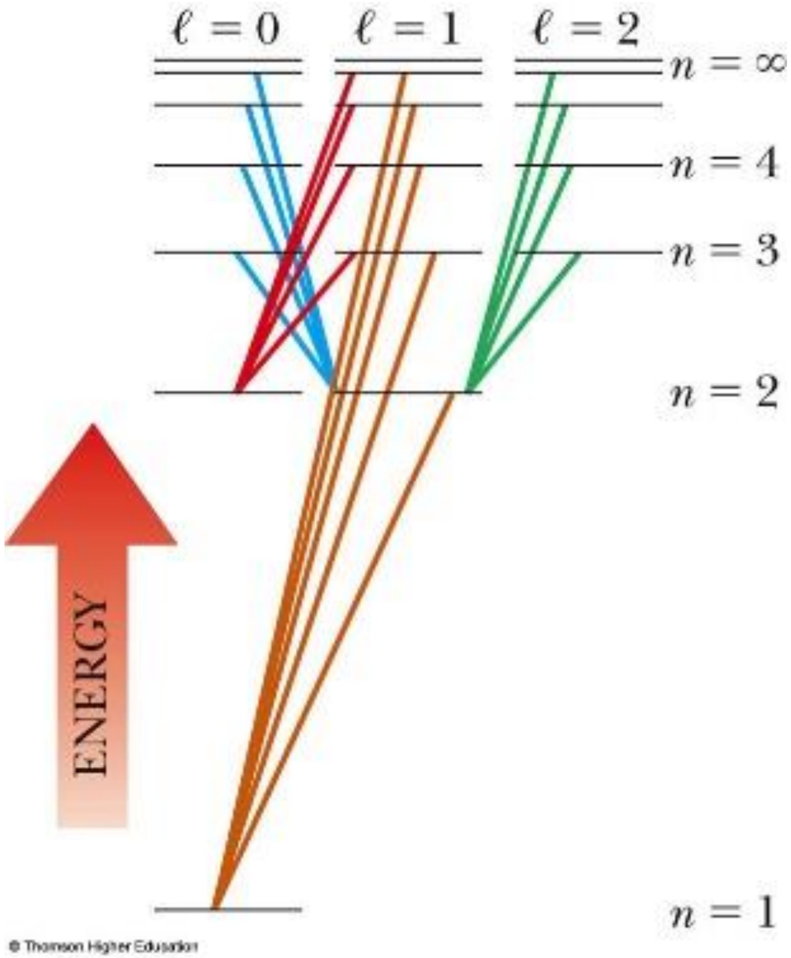
$$\Delta\ell = \pm 1 \quad \text{and} \quad \Delta m_\ell = 0, \pm 1$$

- The allowed energies for one-electron atoms and ions, such as hydrogen and He, are

$$E_n = -\frac{k_e e^2}{2a_0}\left(\frac{Z^2}{n^2}\right) = -\frac{(13.6\,\text{eV})Z^2}{n^2}$$

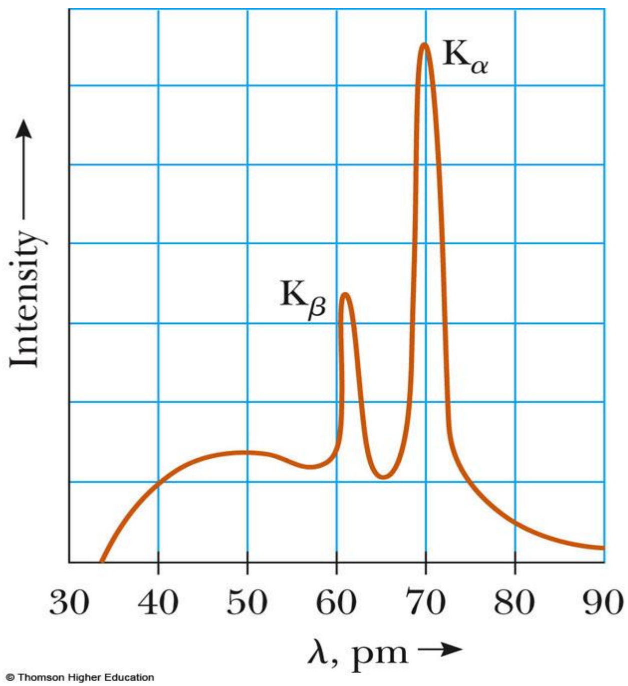
- For multi-electron atoms, the positive nuclear charge *Ze* is largely shielded by the negative charge of the inner-shell electrons.

$$E_n = -\frac{(13.6\,\text{eV})Z_{\text{eff}}^2}{n^2}$$



Some allowed electronic transitions for hydrogen, represented by the colored lines

X-Ray Spectra



The x-ray spectrum of a metal target. The data shown were obtained when 37-keV electrons bombarded a molybdenum target.

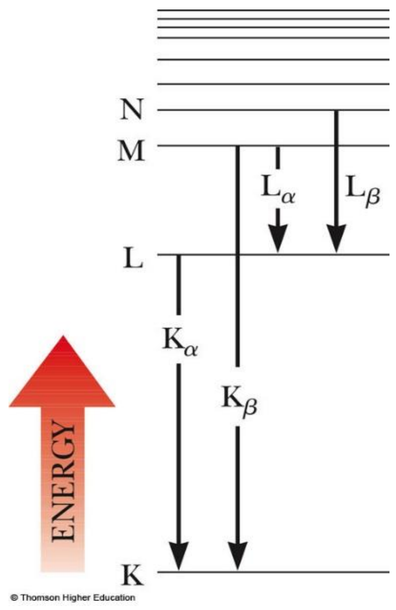
X-ray spectrum has two parts:

Continuous spectrum

Characteristic spectrum

$$e\Delta V = hf_{MAX} = \frac{hc}{\lambda_{MIN}}$$

$$hf = \frac{hc}{\lambda} = E_{ni} - E_{nf}$$

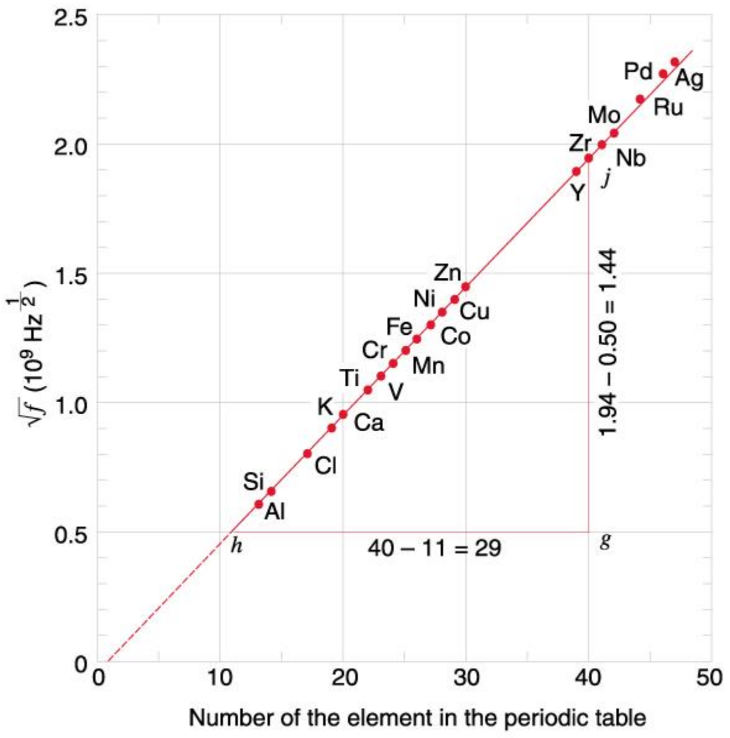


Moseley's observation on the characteristic K_α x-rays shows a relation between the frequency (f) of the $K\alpha$ x-rays and the atomic number (Z) of the target element in the x-ray tube:

$$\sqrt{f} = C\left(Z-1\right)$$

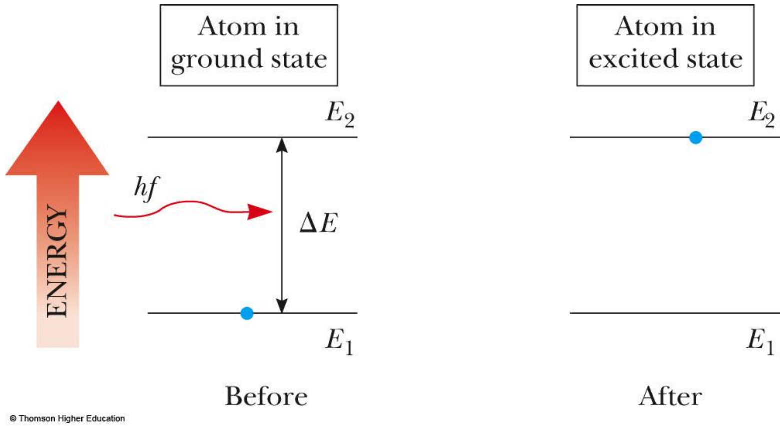
C is a constant.

Note: Based on this observation, the elements are arranged according to their atomic numbers in the periodic table

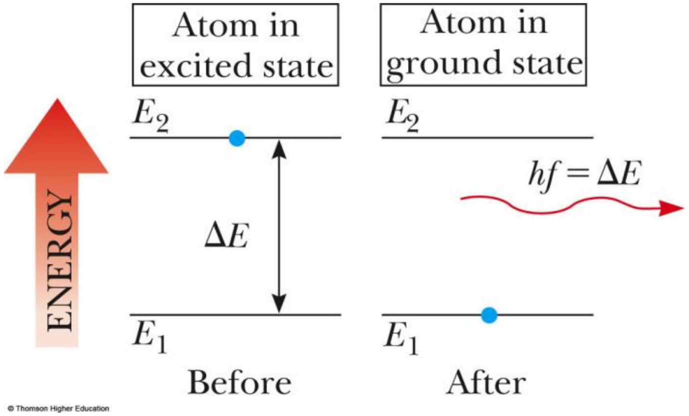


Spontaneous and Stimulated transitions

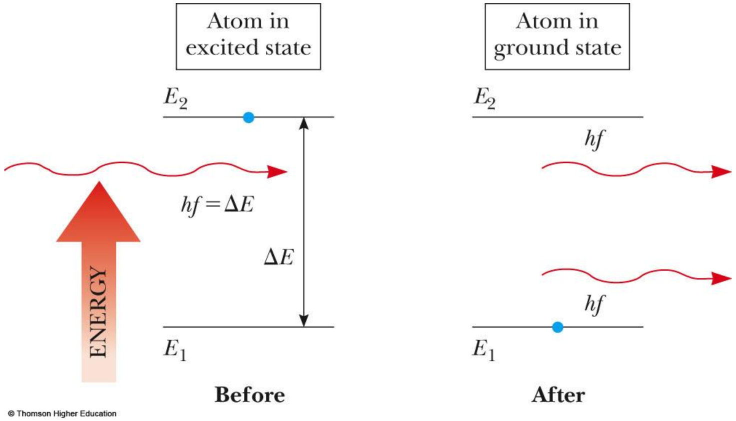
Stimulated Absorption:



Spontaneous Emission:



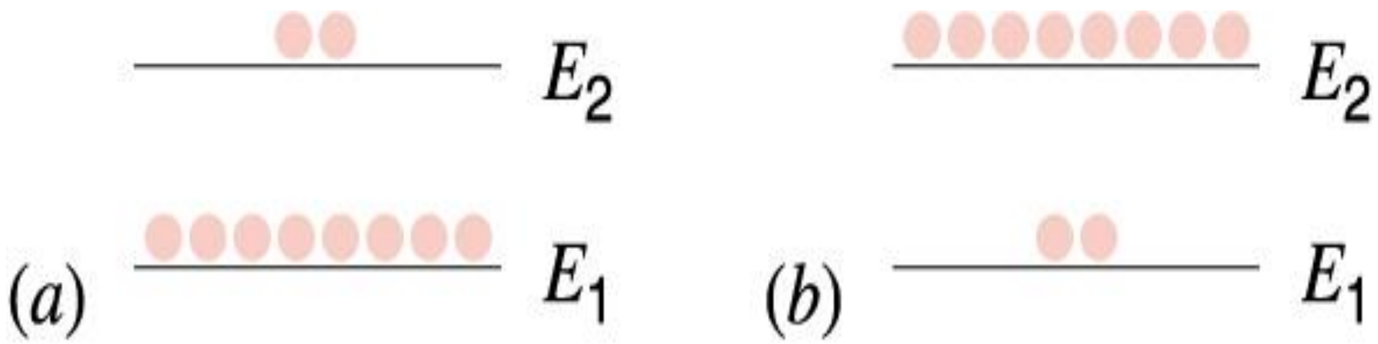
Stimulated Emission:



Boltzmann statistics, the ratio of population of atoms in two energy states E_1 and E_2 at equilibrium temperature T is,

$$\frac{n(E_2)}{n(E_1)} = exp\left(-\frac{E_2 - E_1}{kT}\right)$$

Population inversion:



LASER

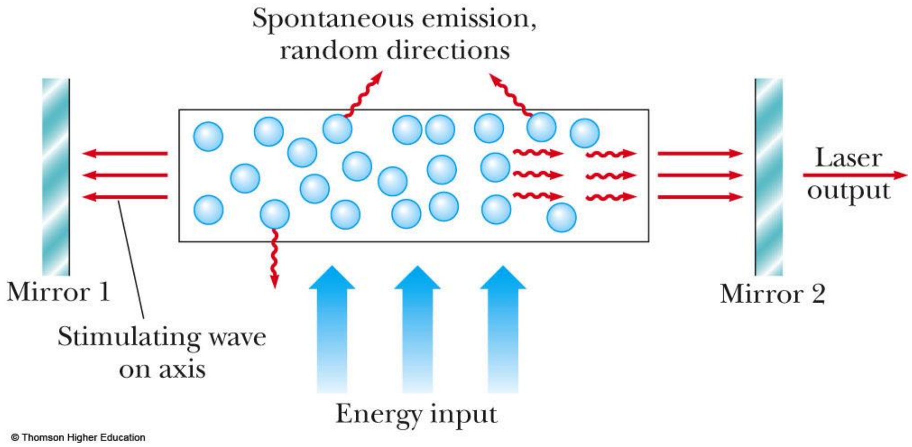
(Light Amplification by Stimulated Emission of Radiation)

Essential conditions:

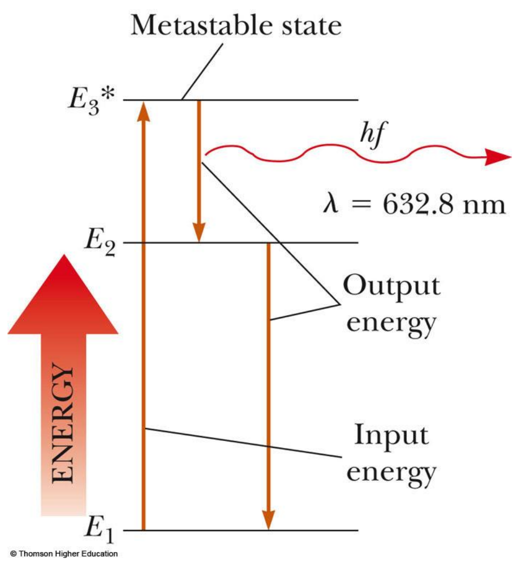
Population inversion: The number of photons emitted must be greater than the number absorbed. This can be achieved by population inversion.

Metastable states: The average life time of the atom is 10^{-3} s which is much longer than that of the ordinary excited state ($\approx 10^{-8}$s). In this case, the population inversion can be established and stimulated emission is likely to occur before spontaneous emission.

The **emitted photons must be confined** in the system long enough to enable them to stimulate further emission from other excited atoms. That is achieved by using **reflecting mirrors** at the ends of the system.



Schematic diagram of a laser design.



Energy-level diagram for a neon atom in a helium–neon laser.

Applications of laser

- In investigating the basic laws of interaction of atoms and molecules with electromagnetic wave of high intensity.
- Laser is widely used in engineering applications like optical communication, micro-welding and sealing etc.
- In medical field: Bloodless and painless surgery, treating dental decay, tooth extraction, cosmetic surgery.