• PROGRAM OF "PHYSICS"

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PHYSICS 4

(Wave and Modern Physics)

02 credits (30 periods)

Chapter 1 Mechanical Wave

Chapter 2 Properties of Light

Chapter 3 Introduction to Quantum Physics

Chapter 4 Atomic Physics

Chapter 5 Relativity and Nuclear Physics

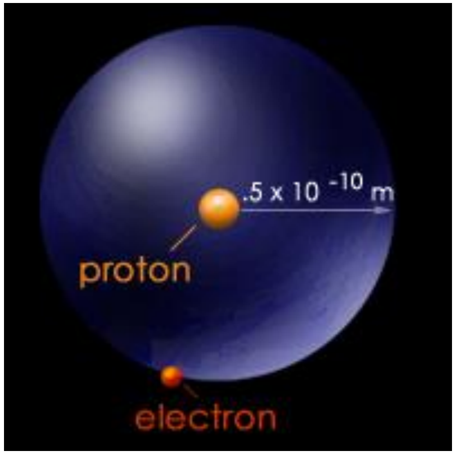
PHYSICS 4

Chapter 4 Atomic Physics

- The Bohr Atom
- The Schrödinger Equation for the Hydrogen Atom
- Many-Electron Atoms and the Exclusion Principle
- Quantum Computing
- X-Ray Production and Scattering
- The laser
- Semiconductivity

1. The Bohr Atom

1.1 The energy levels



The hydrogen atom consists of a single electron (charge – e) bound to its central nucleus, a single proton (charge + e), by an attractive Coulomb force

The electric potential energy is : $U = \frac{1}{4\pi\varepsilon_0}\frac{(e)(-e)}{r} = -\frac{e^2}{4\pi\varepsilon_0 r}$

We can demonstrate that the energies of the quantum electron is

$$E_n = -\left(\frac{me^4}{8\varepsilon_0^2 h^2}\right)\frac{1}{n^2} \longrightarrow \boxed{E_n = -\frac{13.6eV}{n^2}}$$

where *n* is an integer, that is <u>the principal quantum number</u>

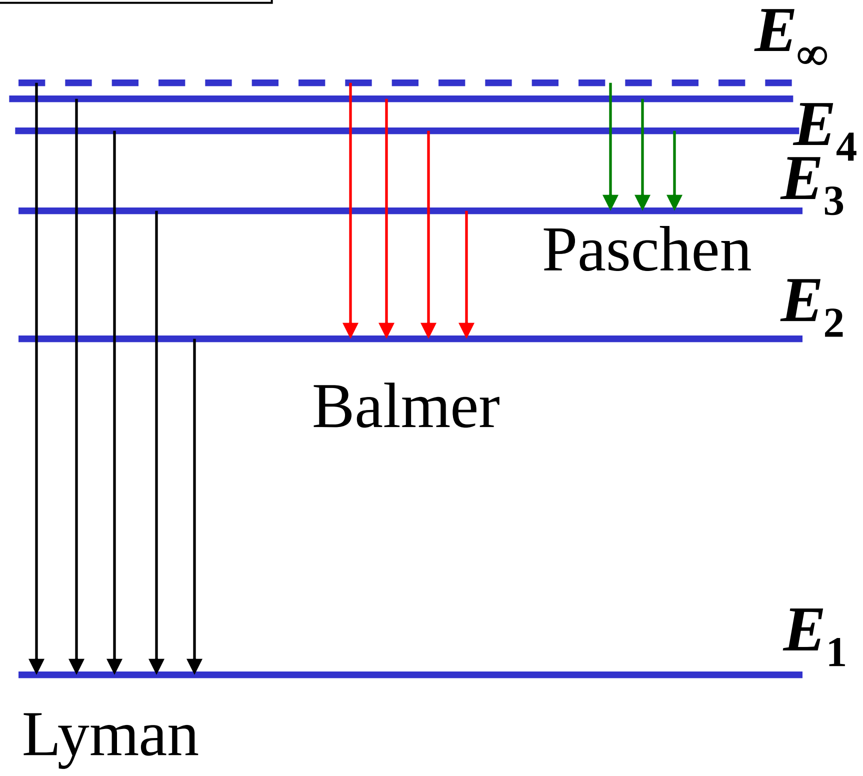
$\longrightarrow$ $\boxed{\text{The energies of the hydrogen atom is } \textbf{quantized}}$

1. 2 Spectral emission lines

When the electron jumps down from an energy level E_m to a lower one E_n , the hydrogen atom emits a photon of energy:

$$\varepsilon = hf_{mn} = \frac{hc}{\lambda_{mn}} = E_m - E_n$$

- If $E_n \equiv E_1$: Lyman series
- If $E_n \equiv E_2$: Balmer series
- If $E_n \equiv E_3$: Paschen series
- If $E_n \equiv E_4$: Brackett series
- .
- .
- .



PROBLEM 1

1/ What is the wavelength of light for the least energetic photon emitted in the Lyman series of the hydrogen atom spectrum lines?

2/ What is the wavelength of the line H_α in the Balmer series?

SOLUTION

1/ For the Lyman series: $\boxed{\varepsilon = hf_{m1} = \dfrac{hc}{\lambda_{m1}} = E_m - E_1}$

The least energetic photon is the transition between E_1 and the level immediately above it; that is E_2 . The energy difference is:

$$\Delta E = E_2 - E_1 = \left(-\frac{13.6eV}{2^2}\right) - \left(-\frac{13.6eV}{1^2}\right) = 10.2eV$$

$$\lambda = \frac{hc}{\Delta E} = \frac{(6.63\times10^{-34})\times(3\times10^{8})}{10.2\times1.6\times10^{-19}} = 1.22\times10^{-7}\,m = 0.122\,\mu\,m = 122nm$$

(in the ultraviolet range)

2/ The line H_α in the Balmer series corresponds to the transition between E_3 and E_2 .

The energy difference is:

$$\Delta E = E_3 - E_2 = \left(-\frac{13.6eV}{3^2}\right) - \left(-\frac{13.6eV}{2^2}\right) = 1.89eV$$

$$\lambda = \frac{hc}{\Delta E} = \frac{(6.63\times10^{-34})\times(3\times10^{8})}{1.89\times1.6\times10^{-19}} = 6.58\times10^{-7}m = 0.658\,\mu\,m = 658nm$$

(red color)

- The line H_α : $E_3 \rightarrow E_2$ (λ = 658 nm)
- The line H_β : $E_4 \rightarrow E_2$ (λ = 486 nm)
- The line H_γ : $E_5 \rightarrow E_2$ (λ = 434 nm)
- The line H_δ : $E_6 \rightarrow E_2$ (λ = 410 nm)

PROBLEM 2

An atom can be viewed as a numbers of electrons moving around a positively charged nucleus. Assume that these electrons are in a box with length that is the diameter of the atom (0.2 *nm*).
Estimate the energy (in eV) required to raised an electron from the ground state to the first excited state and the wavelength that can cause this transition.

SOLUTION

$$E_n = \frac{h^2}{8ma^2} \times n^2 \longrightarrow E_1 = \frac{h^2}{8ma^2} \times 1^2$$

$$= \frac{(6.625 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (0.2 \times 10^{-9})^2 \times 1.6 \times 10^{-19}} \times 1^2$$

$$= 9.40 eV$$

$$E_2 = \frac{h^2}{8ma^2} \times 2^2 = 4E_1 = 37.6 eV \longrightarrow \text{Energy required:}$$

$$\Delta E = E_2 - E_1 = 37.6 - 9.40 = 28.2 eV$$

The wavelength that can cause this transition: $\lambda = hc / \Delta E = 44.0 nm$

PROBLEM 3

According to the basic assumptions of the Bohr theory applied to the hydrogen atom, the size of the allowed electron orbits is determined by a condition imposed on the electron's orbital angular momentum: this quantity must be an integral multiple of $\hbar$:

$$mvr = n\hbar \quad ; n = 1, 2, 3, \ldots$$

1/ Demonstrate that the electron can exist only in certain allowed orbit determined by the integer *n*

2/ Find the formula for the wavelength of the emission spectra.

SOLUTION

1/ $E = KE + PE = \frac{1}{2}mv^2 - k\frac{e^2}{r}$

Newton's second law: $F = ma; \quad k\frac{e^2}{r^2} = m\frac{v^2}{r} \longrightarrow KE = \frac{ke^2}{2r^2}$

The energy of the atom: $\boxed{E = -k\frac{e^2}{2r}}$

With: $v^2 = \frac{n^2\hbar^2}{m^2 r^2}$: $k\frac{e^2}{r^2} = m\frac{v^2}{r} \rightarrow \frac{ke^2}{r^2} = \frac{m}{r}\frac{n^2\hbar^2}{m^2 r^2}$; $ke^2 = \frac{n^2\hbar^2}{mr}$

We have: $\boxed{r_n = \frac{n^2\hbar^2}{mke^2}}$ (the electronic orbits are **quantized**)

With: $\boxed{a_0 = \frac{\hbar^2}{mke^2} = 0.0529nm}$ (Bohr radius), $\boxed{r_n = a_0 n^2}$

2/ We have : $E = -\frac{mk^2e^4}{2\hbar^2}\left(\frac{1}{n^2}\right)$ $\boxed{E_n = -\frac{13.6eV}{n^2}}$

The frequency of the emitted photon is given by: $f = \frac{E_i - E_f}{h}$

$\frac{1}{\lambda} = \frac{f}{c} = \frac{mk^2e^4}{4\pi c\hbar^3}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$ With: $R_H = \frac{mk^2e^4}{4\pi c\hbar^3} = 1.097\times 10^7 m^{-1}$

(Rydberg constant)

$$\boxed{\frac{1}{\lambda} = R_H\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)}$$

PROBLEM 4

The result of the Bohr theory of the hydrogen atom can be extended to hydrogen-like atoms by substituting Ze^2 for e^2 in the hydrogen equations.
Find the energy of the singly ionized helium He^+ in the ground state in eV and the radius of the ground-state orbit

SOLUTION

For He^+: $Z = 2$

$$E = -\frac{mk^2Z^2e^4}{2\hbar^2}\left(\frac{1}{n^2}\right) \qquad \boxed{E_n = -\frac{Z^2(13.6eV)}{n^2}}$$

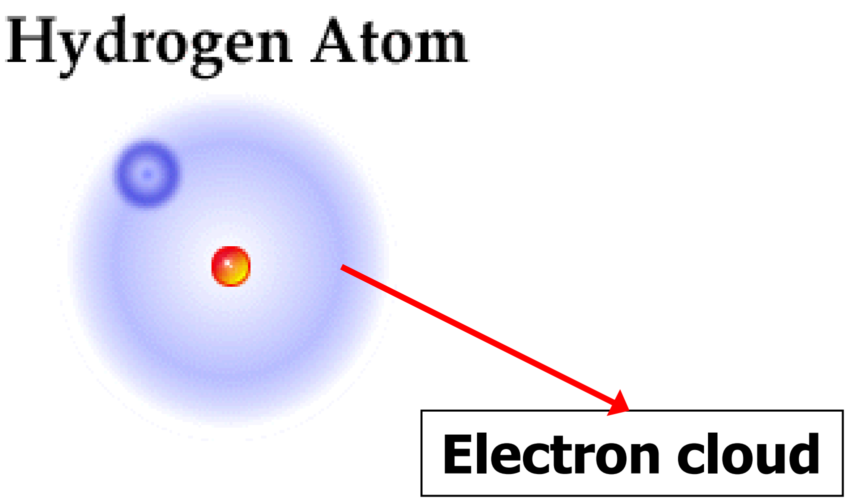
The ground state energy: $\boxed{E_1 = -4(13.6eV) = -54.4eV}$

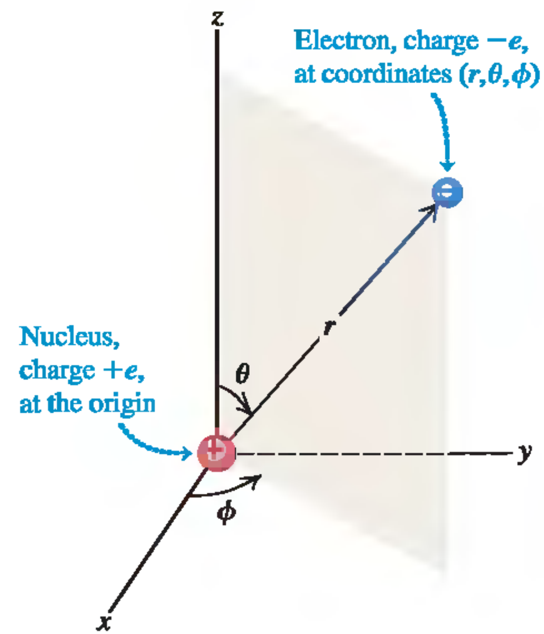
- The radius of the ground state : $r_n = \dfrac{n^2\hbar^2}{mkZe^2}$ $\qquad \boxed{r_n = a_0\dfrac{n^2}{Z}}$

$$\boxed{r_1 = a_0\frac{1^2}{2} = 0.0265nm}$$

(The atom is smaller; the electron is more tightly bound than in hydrogen atom)

2. The Schrödinger Equation for the Hydrogen Atom





In spherical coordinates (r, θ, φ), the hydrogen-atom problem is formulated as :

$$\psi(\vec{r}) \equiv \psi(r,\theta,\varphi) = R(r)Y(\theta,\varphi)\ ;\quad Y(\theta,\varphi) = \Theta(\theta)\Phi(\varphi)$$

The potential energy is : $U(r) = -\dfrac{1}{4\pi\varepsilon_0}\dfrac{e^2}{r}$

The Schrödinger equation in three dimensions :

$$\boxed{\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}+\frac{2m}{\hbar^2}[E-U(r)]\psi=0}$$

$$\longrightarrow \quad \frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}+\frac{2m}{\hbar^2}\left[E+\frac{1}{4\pi\varepsilon_0}\frac{e^2}{r}\right]\psi=0$$

2.1 Radial function of the hydrogen atom

If ψ depends only on r : $\psi \equiv \psi(r)$

$$r^2=x^2+y^2+z^2\,;\;\; 2r\frac{\partial r}{\partial x}=2x \longrightarrow \frac{\partial r}{\partial x}=\frac{x}{r}$$

$$\frac{\partial\psi}{\partial x}=\frac{d\psi}{dr}\frac{\partial r}{\partial x}=\frac{x}{r}\frac{d\psi}{dr}\,;\quad \frac{\partial^2\psi}{\partial x^2}=\frac{\partial}{\partial x}\frac{\partial\psi}{\partial x}=\frac{\partial}{\partial x}\left(\frac{x}{r}\frac{d\psi}{dr}\right)$$

$$\frac{\partial^2\psi}{\partial x^2}=\frac{1}{r}\frac{d\psi}{dr}-\frac{x}{r^2}\frac{\partial r}{\partial x}\frac{d\psi}{dr}+\frac{x}{r}\frac{d^2\psi}{dr^2}\frac{\partial r}{\partial x}=\frac{1}{r}\frac{d\psi}{dr}-\frac{x^2}{r^3}\frac{d\psi}{dr}+\frac{x^2}{r^2}\frac{d^2\psi}{dr^2}$$

$$\frac{\partial^2\psi}{\partial x^2} = \frac{1}{r}\frac{d\psi}{dr} - \frac{x^2}{r^3}\frac{d\psi}{dr} + \frac{x^2}{r^2}\frac{d^2\psi}{dr^2}$$

The same result for *y* and *z* :

$$\frac{\partial^2\psi}{\partial y^2} = \frac{1}{r}\frac{d\psi}{dr} - \frac{y^2}{r^3}\frac{d\psi}{dr} + \frac{y^2}{r^2}\frac{d^2\psi}{dr^2}$$

$$\frac{\partial^2\psi}{\partial z^2} = \frac{1}{r}\frac{df\psi}{dr} - \frac{z^2}{r^3}\frac{d\psi}{dr} + \frac{z^2}{r^2}\frac{d^2\psi}{dr^2}$$

$$\longrightarrow \quad \frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} = \frac{d^2\psi}{dr^2} + \frac{2}{r}\frac{d\psi}{dr}$$

The Schrödinger equation :

$$\frac{d^2\psi}{dr^2} + \frac{2}{r}\frac{d\psi}{dr} + \frac{2m}{\hbar^2}\left[E + \frac{1}{4\pi\varepsilon_0}\frac{e^2}{r}\right]\psi = 0$$

- *Wave function for the ground state*

The wave function for the ground state of the hydrogen atom:

$$\boxed{\psi(r) = \frac{1}{a^{3/2}\sqrt{\pi}} e^{-r/a}}$$

Where a is the Bohr radius: $a = 0.529 \times 10^{-10} m = 52.9nm$

- *Wave function for the first excited state*

$$\boxed{\psi(r) = Ce^{-ar/2}(2 - ar)}$$

PROBLEM 5

Knowing that the wave function for the ground state of the hydrogen atom is

$$\psi(r) = Ae^{-r/a}$$

Where a is the Borh radius: $a = 0.529 \times 10^{-10} m = 52.9nm$

1/ What is the value of the normalization constant A ?

2/ What is the value of x at which the radial probability density has a maximum?

SOLUTION

1/ Because the electron moves in the three dimensional space, the probability of finding the electron in a volume dV is written:

$$|\psi|^2 dV = A^2 e^{-2r/a} dV$$

where: $dV = 4\pi\, r^2 dr$

Normalization condition: $$\boxed{\int_0^{+\infty} \left|\psi(r)\right|^2 dV = 1}$$

$$\longrightarrow \quad 4\pi\ A^2 \int_0^{+\infty} e^{-2r/a} r^2 dr = 1 \qquad (1)$$

We put: $I = \int_0^{+\infty} e^{-2r/a} r^2 dr$

By changing variable: $z = 2r/a \longrightarrow I = \left(\frac{a}{2}\right)^3 \int_0^{+\infty} e^{-z} z^2 dz$

By integration by parts, we can demonstrate the general formula:

$$\boxed{\int_0^{+\infty} e^{-z} z^n dz = n! = 1 \times 2 \times \ldots \times (n-1) \times n}$$

$$\longrightarrow \quad I = (a/2)^3 \int_0^{+\infty} e^{-z} z^2 dz = 2(a/2)^3 = a^3/4$$

Substituting the value of I into (1): $4\pi\ A^2 a^3 / 4 = 1 \longrightarrow A = \frac{1}{a^{3/2}\sqrt{\pi}}$

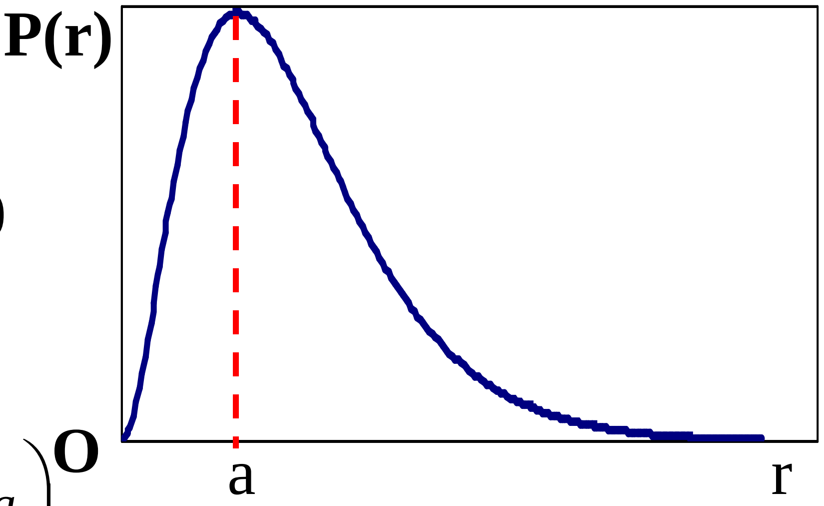
$$\boxed{\psi(r) = \frac{1}{a^{3/2}\sqrt{\pi}} e^{-r/a}}$$

2/ Because:

$$|\psi|^2 dV = A^2 e^{-2r/a} dV = \frac{1}{\pi a^3} e^{-2r/a} 4\pi r^2 dr = \frac{4}{a^3} e^{-2r/a} r^2 dr$$

the radial probability density is

$$P(r) = \frac{4}{a^3} e^{-2r/a} r^2$$



When $P\,(r)$ has a **maximum**: $\dfrac{dP(r)}{dr} = 0$

$$\frac{dP(r)}{dr} = \frac{4}{a^3}\frac{d}{dr}\left(e^{-2r/a} r^2\right)$$

$$= \frac{4}{a^3}\left(r^2(-\frac{2}{a})e^{-2r/a} + 2re^{-2r/a}\right)$$

$$= \frac{8}{a^4} r(a-r)e^{-2r/a} = 0 \longrightarrow \boxed{r = a}$$

(The value r = 0 corresponds to a minimum of $P(\,r)$)

<u>Physical meaning:</u> The position r = a is the **most probable** for the electron $\rightarrow$ **electronic clouds**

PROBLEM 6

Calculate the probability that the electron in the ground state of the hydrogen atom will be found outside the Bohr radius

SOLUTION

With: $\boxed{\psi(r) = \frac{1}{a^{3/2}\sqrt{\pi}} e^{-r/a}}$

The probability is found by: $\boxed{P = \int_a^{+\infty} \left|\psi(r)\right|^2 dV}$ where: $dV = 4\pi\, r^2 dr$

$$P = \frac{4}{a^3}\int_a^{+\infty} r^2 e^{-2r/a} dr$$ By changing variables: $z = 2r/a$,

$$P = \frac{1}{2}\int_2^{+\infty} z^2 e^{-z} dz = -\frac{1}{2}\{z^2 + 2z + 2\}e^{-z}\Big|_2^{\infty} = 5e^{-2} = 0.677 \boxed{\rightarrow P = 67.7\%}$$

PROBLEM 7

The wave function of a particle is given as: $\psi(r) = Ce^{-|x|/a}$

1/ Find C in terms of a such that the wave function is normalized in all space

2/ Calculate the probability that the particle will be found in the interval $-a \le x \le a$

SOLUTION

1/ With: $C^2 \int_{-\infty}^{+\infty} e^{-2|x|/a} dx = 1 \longrightarrow 2C^2 \int_0^{+\infty} e^{-2x/a} dx = 1$

$$\longrightarrow 2C^2\left(\frac{a}{2}\right) = 1 \longrightarrow \boxed{C = \frac{1}{\sqrt{a}}}$$

2/ $P = \int_{-a}^{+a} |\psi(x)|^2 dx = 2\int_0^{+a} |\psi(x)|^2 dx = 2C^2 \int_0^{+a} e^{-2x/a} dx$

$$P = 2C^2(a/2)(1-e^{-2}) = 2(1/\sqrt{a})^2(a/2)(1-e^{-2}) = 86.5\%$$

2.2 Quantization of Orbital Angular Momentum

NOTES : In classical mechanics :

- Force and linear momentum in translational motion :

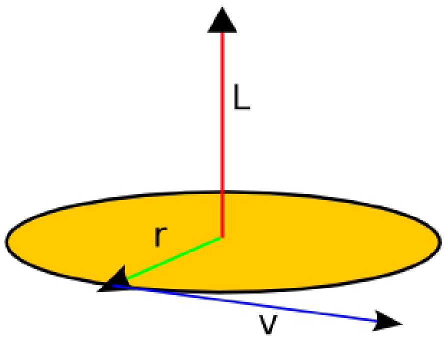
$$\vec{F} = m\vec{a} = m\frac{d\vec{v}}{dt} = \frac{d(m\vec{v})}{dt} = \frac{d\vec{p}}{dt}$$

- Torque and angular momentum in rotational motion

$$\tau = Fd \longrightarrow L = pr$$

$$\vec{\tau} = \vec{F} \times \vec{r} \longrightarrow \vec{L} = \vec{r} \times \vec{p}$$

$$L = mvr = m(r\omega)r = (mr^2)\omega = I\omega$$



In quantum mechanics :

- In the wave function of electron in hydrogen atom :

$$\psi(\vec{r}) \equiv \psi(r,\theta,\varphi) = R(r)Y(\theta,\varphi)\ ;\ Y(\theta,\varphi) = \Theta(\theta)\Phi(\varphi)$$

The requirement that the $\Theta(\theta)$ function must be finite at $\theta = 0$ and $\theta = \pi$ gives the result : L can take some possible values :

$$\boxed{L = \sqrt{l(l+1)}\,\hbar}$$

$$(\ l = 0\ ;1\ ;2\ ;3\ ;...;\ n-1\ )$$

The number ***l*** is called : the **orbital angular-momentum quantum number** or the **orbital quantum number** for short.

In quantum mechanics : $\boxed{L = \sqrt{l(l+1)}\,\hbar}$

$$(l = 0\,;1\,;2\,;3\,;...;\,n-1\,)$$

• On the other hand, the permitted values of the component of $\boldsymbol{L}$ in a given direction, say the z-component L_z are determined by the requirement that the $\Phi(\varphi)$ function must equal $\Phi(\varphi + 2\pi)$.

The possible values of L_z are

$$\boxed{L_z = m_l\hbar}$$

$$(m_l = 0\,;\pm1\,;\pm2\,;\pm3\,;...;\pm l\,)$$

$$\Downarrow$$

$$(m_l = -l\,;-l+1\,;-l+2\,;...-1\,;0\,;1\,;...;\,l-1\,;\,l)$$

We call $\boldsymbol{m_l}$ the **orbital magnetic quantum number**

$$\boxed{L = \sqrt{l(l+1)}\,\hbar} \quad (\, l = 0\,;1\,;2\,;3\,;...;\,n-1\,)$$

$$\boxed{L_z = m_l \hbar} \quad (\, m_l = 0\,;\pm 1\,;\pm 2\,;\pm 3\,;...;\pm l\,)$$

$$(\, m_l = -l\,;-l+1\,;-l+2\,;...-1\,;0\,;1\,;...;\,l-1\,;\,l)$$

EXAMPLE : For ***n*** = 3; the possible values of ***l*** are : **0 ; 1 ; 2**

With ***l*** = 2; the possible values of $\boldsymbol{m_l}$ are : **-2 ; -1 ; 0 ; +1 ; +2**

$$L = \sqrt{2(2+1)}\,\hbar = \sqrt{6}\,\hbar = 2.45\,\hbar$$

$$L_z = 0\,;\pm 1\hbar\,;\pm 2\hbar$$

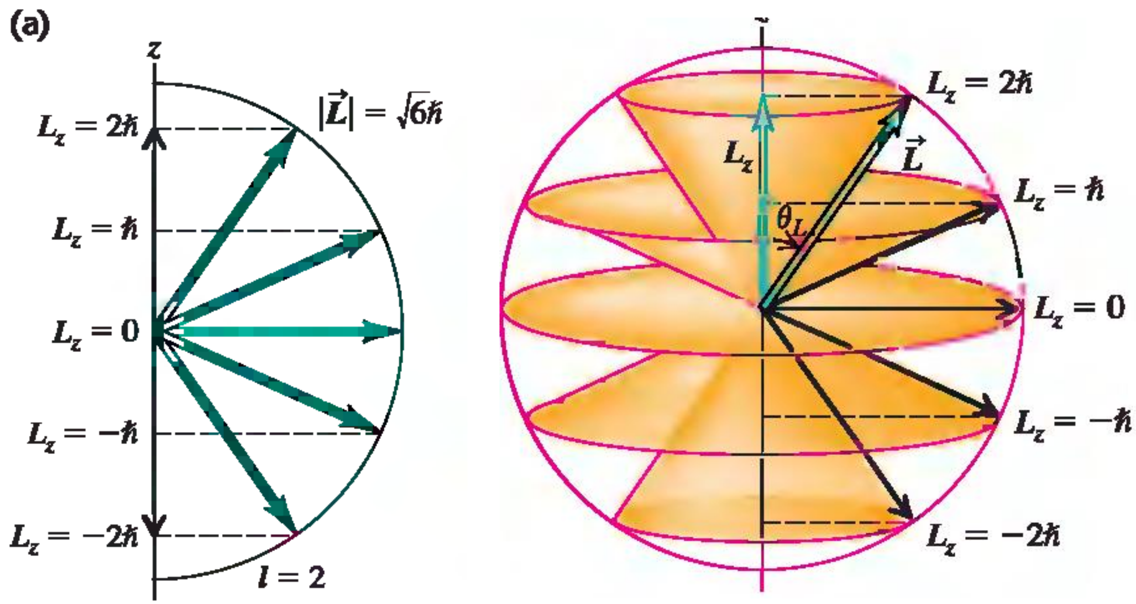


TABLE 28.2 Three Quantum Numbers for the Hydrogen Atom

Quantum Number	Name	Allowed Values	Number of Allowed States
n	Principal quantum number	$1, 2, 3, \ldots$	Any number
ℓ	Orbital quantum number	$0, 1, 2, \ldots, n - 1$	n
m_ℓ	Orbital magnetic quantum number	$-\ell, -\ell + 1, \ldots, 0, \ldots, \ell - 1, \ell$	$2\ell + 1$

PROBLEM 8

How many distinct (n, l, m_l) states of the hydrogen atom with n = 3 are there? Find the energy of these states.

SOLUTION

For n = 3; the possible values of l are : **0 ; 1 ; 2**

With l = 0 ; the possible value of m_l is : **0**

With l = 1 ; the possible values of m_l are : **-1 ; 0 ; +1**

With l = 2 ; the possible values of m_l are : **-2 ; -1 ; 0 ; +1 ; +2**

The total number of (n , l , m_l) states with n = 3 is therefore
1 + 3 + 5 = 9.

$$\boxed{E_n = -\frac{13.6eV}{n^2}} \longrightarrow E_3 = -\frac{13.6\ eV}{3^2} = -1.51\ eV$$

PROBLEM 9

Consider the n = 4 states of hydrogen.
(a) What is the maximum magnitude L of the orbital angular momentum?
(b) What is the maximum value of L_z?
(c) What is the minimum angle between $\boldsymbol{L}$ and the z-axis?

SOLUTION

(a)

When n = 4, the maximum value of the orbital angular-momentum quantum number l is $(n-1)=(4-1)=3$

$$L=\sqrt{l(l+1)}\,\hbar \;=\sqrt{3(3+1)}\,\hbar=\sqrt{12}\,\hbar$$

(b) For l = 3 the maximum value of the magnetic quantum number m_l is 3 :

$$L_z=m_l\hbar \;=3\hbar$$

PROBLEM 9

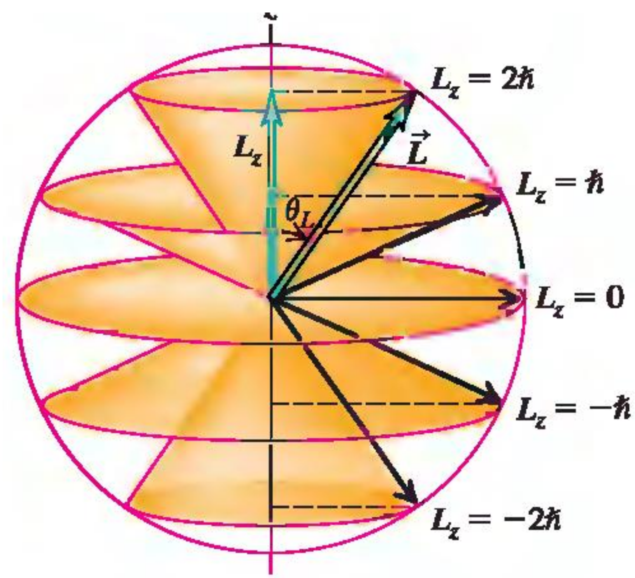
Consider the n = 4 states of hydrogen.
(a) What is the maximum magnitude L of the orbital angular momentum?
(b) What is the maximum value of L_z?
(c) What is the minimum angle between $\boldsymbol{L}$ and the z-axis?

SOLUTION

(c) The minimum allowed angle between $\boldsymbol{L}$ and the z-axis corresponds to the maximum allowed values of L_z and m_l

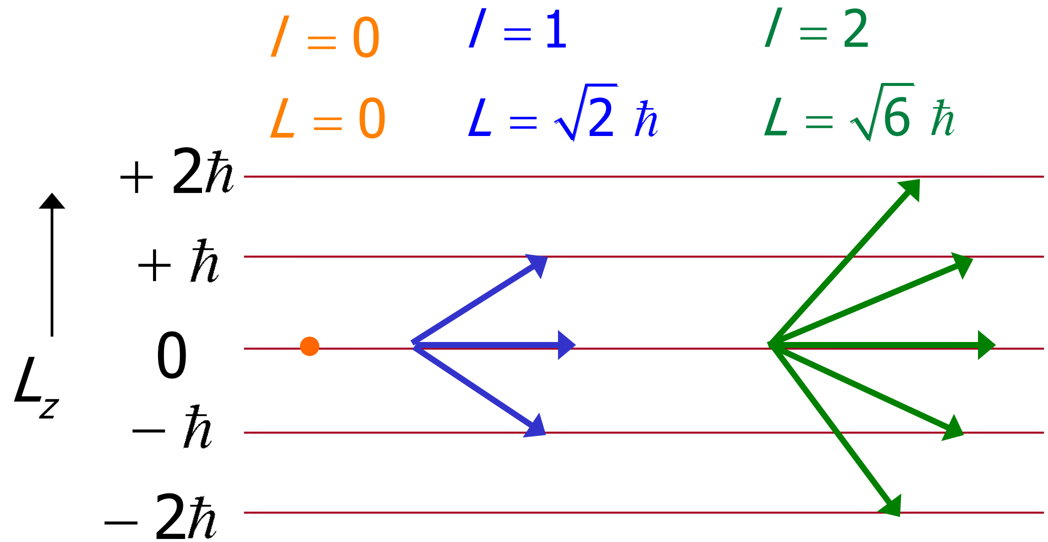
$$\cos\theta_{\text{min}} = \frac{(L_z)_{\text{max}}}{L} = \frac{3\hbar}{\sqrt{12}\,\hbar}$$

$$\theta_{\text{min}} = 30^0$$



PROBLEM 10 Represent all the possible orientations of the angular momentum with the value l = 0 ; 1 ; 2 ; 3

SOLUTION



- $\boldsymbol{l}$ = 0 : $\boldsymbol{L}$ = **0** ; $\boldsymbol{m_l}$ = **0**
- $\boldsymbol{l}$ = 1

$$L = \sqrt{l(l+1)}\,\hbar \quad = \sqrt{1(1+1)}\,\hbar = \sqrt{2}\,\hbar$$

$\boldsymbol{m_l}$ = **-1 ; 0 ; +1** $\longrightarrow L_z = m_l\hbar = 0 ; \pm 1\hbar$

- $\boldsymbol{l}$ = 2

$$L = \sqrt{l(l+1)}\,\hbar \quad = \sqrt{2(2+1)}\,\hbar = \sqrt{6}\,\hbar$$

$\boldsymbol{m_l}$ = **-2 ; -1 ; 0 ; +1 ; +2** $\longrightarrow L_z = m_l\hbar = 0 ; \pm 1\hbar ; \pm 2\hbar$

PROBLEM 11 **(a)** If the value of L_z is known, we cannot know either L_x or L_y precisely. But we can know the value of the quantity . Write an expression for this quantity in terms of l and m_l.

(b) What is the meaning of ?

(c) For a state of nonzero orbital angular momentum, find the maximum and minimum values of . Explain your results.

SOLUTION

(a) $\sqrt{L_x^2 + L_y^2} = \sqrt{L^2 + L_z^2} = \sqrt{l(l+1)\hbar^2 - m_l^2\hbar^2} = \hbar\sqrt{l(l+1) - m_l^2}$

(b) This is the magnitude of the component of angular momentum perpendicular to the z-axis

(c) The maximum value : $\left(\sqrt{L_x^2 + L_y^2}\right)_{MAX} = \hbar\sqrt{l(l+1)}$

when $m_l = 0$

The minimum value : $\left(\sqrt{L_x^2 + L_y^2}\right)_{MIN} = \hbar\sqrt{l}$ when $m_l = \pm l$

2.3 The spectroscopic notation and the shell notation

$l = 0$: s states
$l = 1$: p states
$l = 2$: d states
$l = 3$: f states
$l = 4$: g states
$l = 5$: h states

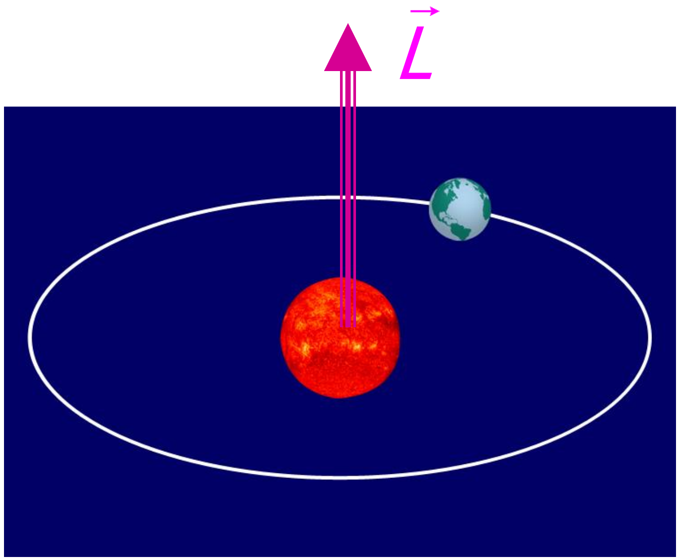
n	l	m_l	Spectroscopic Notation	Shell
1	0	0	1s	K
2	0	0	2s	L
2	1	−1, 0, 1	2p	
3	0	0	3s	
3	1	−1, 0, 1	3p	M
3	2	−2, −1, 0, 1, 2	3d	
4	0	0	4s	N
and so on				

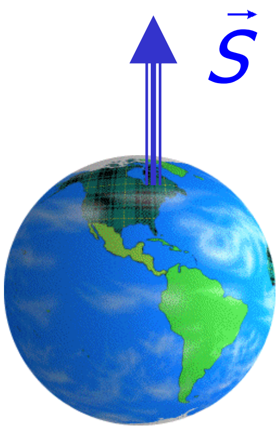
The existence of more than one distinct state with the same energy is called **degeneracy**

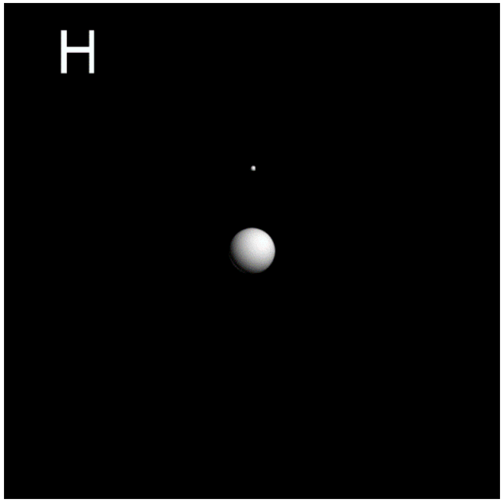
Example : n = 2 $\rightarrow$ 4 states : degeneracy ***g* = 4**

2.4 Electron Spin

Analogy : The earth travels in a nearly circular orbit around the sun, and at the same time it rotates on its axis. Each motion has its associated **angular momentum**. which we call the **orbital** and **spin angular momentum**, respectively.







Each electron possesses an intrinsic angular momentum called its **spin.**

Like orbital angular momentum. the **spin angular momentum** of an **electron** (denoted by ***S***) is found to be **quantized**.

$$\boxed{S = \sqrt{s(s+1)}\,\hbar\;;\; s = \frac{1}{2}} \longrightarrow S = \sqrt{\frac{1}{2}\left(\frac{1}{2}+1\right)}\,\hbar = \frac{\sqrt{3}}{2}\,\hbar$$

The projection of the spin on z-axis is called ***S*$_z$**

$$\boxed{S_z = m_s\hbar = \pm\frac{\hbar}{2}} \quad \left(\, m_s = \pm\frac{1}{2} : \textit{magnetic spin number}\right)$$

The spin angular momentum vector ***S*** can have only two orientations in space relative to the z-axis: "spin up" with a z-component of $+\dfrac{\hbar}{2}$ and "spin down" with a z-component of $-\dfrac{\hbar}{2}$

CONCLUSION :

State of an electron is defined by **5 quantum numbers** :

n **: the principal quantum number**

l**: the orbital quantum number**

m**$_l$: the orbital magnetic quantum number**

s : the spin number

m_s : the magnetic spin number

Wave function of an electron is denoted as :

$$\boxed{\psi_{n,l,m_l,s=1/2,m_s=\pm 1/2}}$$

PROBLEM 12

(a) Show that the total number of atomic states (including different spin states) in a shell of principal quantum number n is $2n^2$.

(b) Which shell has 50 states ?

SOLUTION

(a) $$N = 2\sum_{l=0}^{n-1}(2l+1) = 4\sum_{l=0}^{n-1} l + 2\sum_{l=0}^{n-1} 1 = 4\sum_{l=0}^{n-1} l + 2\sum_{l=0}^{n-1} 1$$

$$= 4\frac{(n-1)n}{2} + 2(n) = 2n^2 - 2n + 2n$$

$$\boxed{N = 2n^2}$$

(b) The n = 5 shell (O - shell) has 50 states

3. Many-Electron Atoms and the Exclusion Principle

3.1 The simplest approximation

To ignore all interactions between electrons and consider each electron as moving under the action only of the nucleus (considered to be a point charge).

The wave function for each electron is a function like those for the hydrogen atom, specified by four quantum numbers : (n , l , m_l , m_s) :

$$n \geq 1 \qquad 0 \leq l \leq n-1 \qquad |m_l| \leq l \qquad m_s = \pm\frac{1}{2}$$

(allowed values of quantum numbers)

The nuclear charge is *Ze* instead of *e*. The energy levels :

$$\boxed{E_n = -\frac{Z^2}{n^2}(13.6\ eV)}$$

3. Many-Electron Atoms and the Exclusion Principle

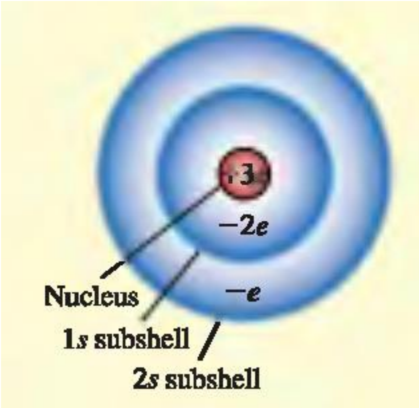
3.2 The Exclusion Principle

"No two electrons can occupy the same quantum-mechanical state in a given system"

$\Updownarrow$

"No two electrons in an atom can have the same values of all four quantum numbers (n , l , m_l , m_s)"

Therefore the principle also says, in effect, that no more than two electrons with opposite values of the quantum number m_s can occupy the same region of space



Quantum States of Electrons in the First Four Shells

n	l	m_l	Spectroscopic Notation	Number of States		Shell
1	0	0	1*s*	2		*K*
2	0	0	2*s*	2	8	*L*
2	1	−1, 0, 1	2*p*	6		
3	0	0	3*s*	2	18	*M*
3	1	−1, 0, 1	3*p*	6		
3	2	−2, −1, 0, 1, 2	3*d*	10		
4	0	0	4*s*	2	32	*N*
4	1	−1, 0, 1	4*p*	6		
4	2	−2, −1, 0, 1, 2	4*d*	10		
4	3	−3, −2, −1, 0, 1, 2, 3	4*f*	14		

3. Many-Electron Atoms and the Exclusion Principle

3.3 The Periodic Table

Electron configuration (or structure) of an atom **represents the manner in which the states are occupied**.

EXAMPLE: Electronic configuration

$$Hydrogen\,({}_1^1H):1s^1$$

$$Helium\,({}_2^4He):1s^2$$

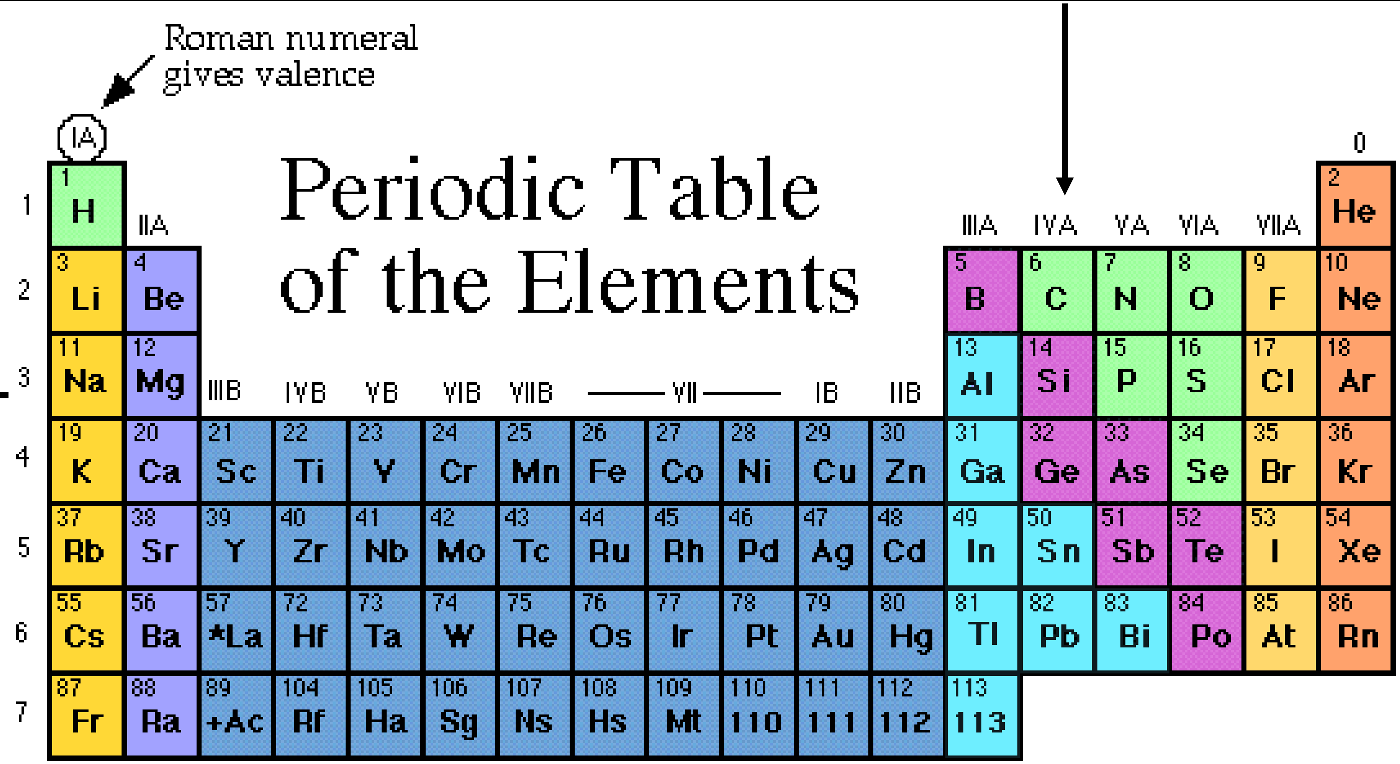
$$Sodium\,({}_{11}^{23}Na):1s^2\,2s^2\,2p^6\,3s^1$$

<u>PERIODIC TABLE</u>: All the elements have been classified according to the **electrons configurations**

In **the periodic table**, the elements are situated, with increasing atomic number, in **seven horizontal rows** called **periods**.

The arrangement is such that all the elements arrayed in a given column (or **group**) have similar valence electron structure, as well as chemical and physical properties.

7 periods



4. Quantum Computing
(Joseph Stelmach, Wolfgang Bauer,…)

4.1 What is a quantum computer?

- **Quantum computer: Type of computer that uses QUANTUM MECHANICS so that it can perform certain kinds of computation more efficiently than a regular computer can.**
- **Quantum mechanical phenomena: SUPERPOSITION and ENTANGLEMENT,…**

- **Classical physics: SUPERPOSITION**

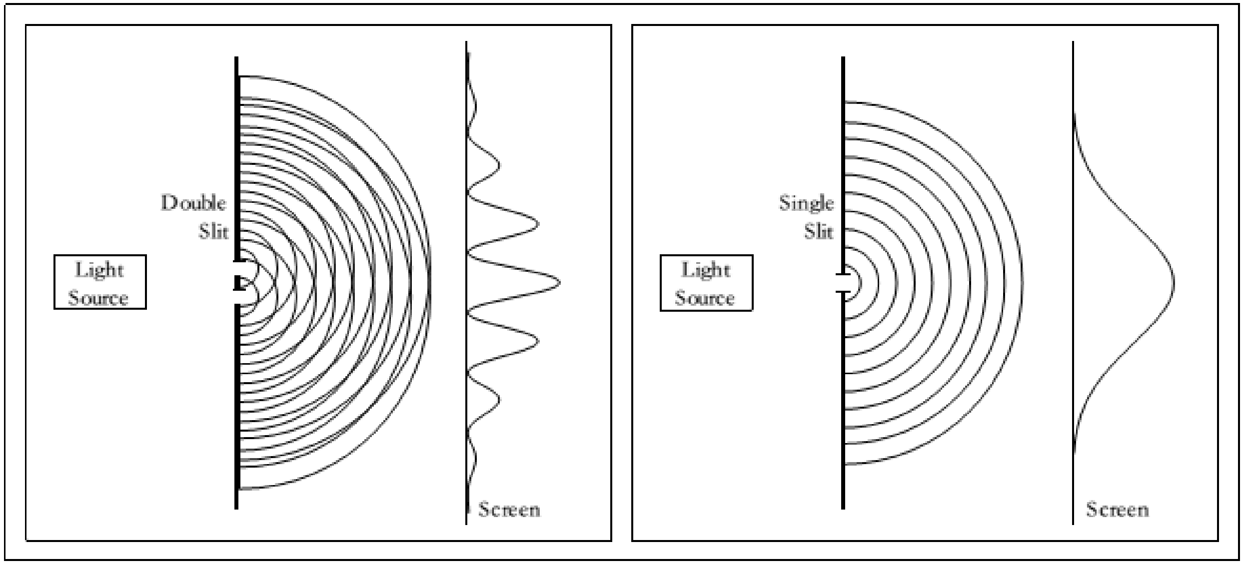
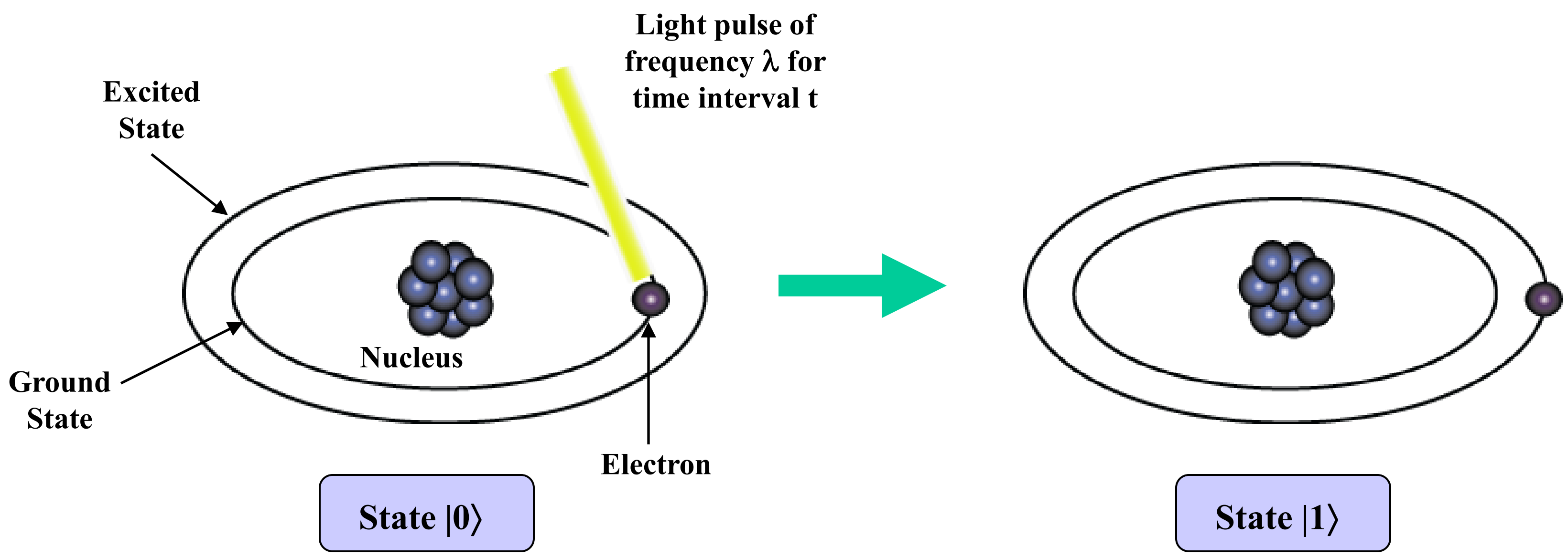


Figure 1.1: Double- and single-slit diffraction. Notice that in the double-slit experiment the two paths interfere with one another. This experiment gives evidence that light propagates as a wave.

• Quantum mechanical phenomena: SUPERPOSITION

An excited state |1⟩ and a ground state |0⟩



• Quantum mechanical phenomena: SUPERPOSITION

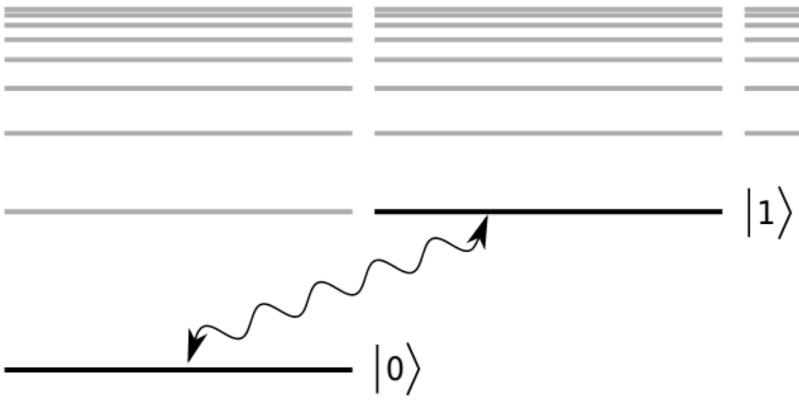


Figure 1.3: Energy level diagram of an atom. Ground state and first excited state correspond to qubit levels, $|0\rangle$ and $|1\rangle$, respectively.

***Superposition* of the two states: Addition of the state vectors:**

$$|\psi\rangle = a_1\,|0\rangle + a_2\,|1\rangle$$

$|a_1|^2$: : Probability of the superposition collapsing to $|0\rangle$

(a_1 and a_2 : complex numbers and $|a_1|^2 + |a_2|^2 = 1$)

- **Quantum mechanical phenomena: ENTANGLEMENT**

Entanglement $\rightarrow$ **Relationships among data:**

The ability of quantum systems to exhibit CORRELATIONS between states within a superposition.

In the state $|0\rangle + |1\rangle$ (a superposition of $|0\rangle$ and $|1\rangle$), we can *entangle* the two states such that the measurement of one state is always correlated to the measurement of the other state.

4.2 Quantum Bit (Qubit) vs Classical Bit

Classical computer stores information in a series of 0’s and 1’s.

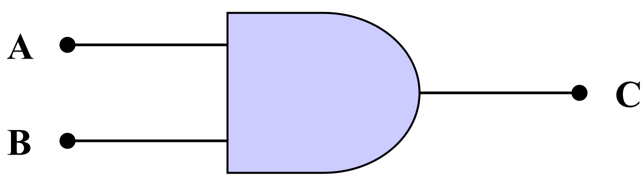
Each unit in this series of 0’s and 1’s : a bit.

A bit can be set to either 0 or 1.

2 basic states – off or on: 0, 1 (Mutually exclusive: Nothing appears between 0 and 1: it’s **all or nothing**)

Electricity: high voltage:1, low voltage: 0.

EXAMPLE: The AND Gate



Input		Output
A	B	C
0	0	0
0	1	0
1	0	0
1	1	1

In these 3 cases, information is being destroyed

- **This type of gate cannot be used. We must use *Quantum Gates*.**

Classical Bit

A “**byte**” is a collection of 8 bits.

EXAMPLE:

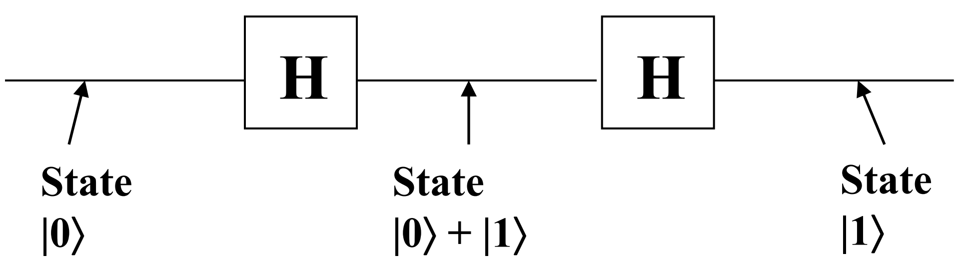
A possible representation for one particular value of a byte could be 01100010

(the 8 bits that make up this byte are in their respective on or off positions as indicated by the numbers, one digit for each bit)

Quantum computing: ***Qubits* (*Quantum bits*)** **are the basic unit and their value can be 1, 0, or 1 and 0 *simultaneously* (laws of quantum physics)**
→ *qubits* (as opposed to bits) can take on various values *at one time* and can perform calculations that a conventional computer cannot.

Quantum Gates - Hadamard

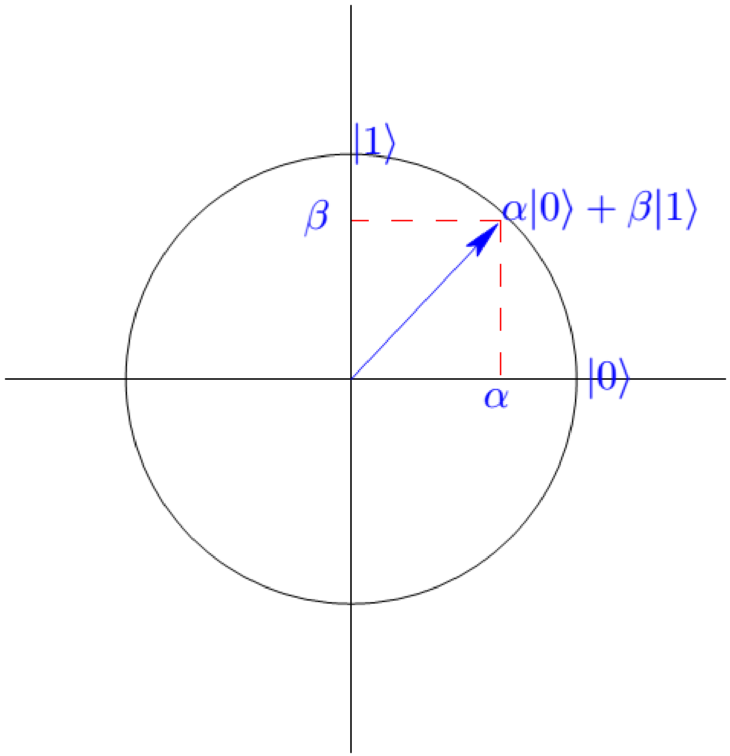
- **Simplest gate involves one qubit and is called a *Hadamard Gate (*also known as a square-root of NOT gate.) Used to put qubits into superposition.**



Quantum Bit (Qubit):

System od 1 qubits $\rightarrow$ $c_1 |1\rangle + c_2 |0\rangle$

Qubits



A qubit may be visualised as a unit vector on the plane.

In general, however, α and β are *complex* numbers.

Quantum Bit (Qubit):

Qubits represent *atoms* (spin of the electron in which the two levels can be taken as spin up and spin down), *ions*, *photons* and their respective control devices that are working together.

Because a quantum computer can contain these multiple states simultaneously, it has the potential to be millions of times more powerful than today's most powerful supercomputers.

Quantum Bit (Qubit):

System of 1 qubits $\rightarrow \; c_1 \, |1\rangle + c_2 \, |0\rangle$

System of 2 qubits

$\rightarrow \; c_{11} \, |11\rangle + c_{10} \, |10\rangle + c_{01} \, |01\rangle + c_{00} \, |00\rangle$

System of 3 qubits

$\rightarrow \; c_{111} \, |111\rangle + c_{110} \, |110\rangle + c_{101} \, |101\rangle + c_{100} \, |100\rangle$

$c_{011} \, |011\rangle + c_{010} \, |010\rangle + c_{001} \, |001\rangle + c_{000} \, |000\rangle$

…

Classical computer operates on a register of *n* bits

$\rightarrow$ *n* operations simultaneously.

Quantum computer operates on a register of *n* qubits

$\rightarrow$ 2^n operations simultaneously.

PROBLEM 13

Consider the quantum state: $|\psi\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{e^{i\theta}}{\sqrt{2}}|1\rangle$

(a) Compute the probability to find the system in state $\langle 0|$ and in state $\langle 1|$?

(b) Compute the probability of measuring $|+\rangle$ and $|-\rangle$ in the new basis: $|+\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$ and $|-\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right)$

SOLUTION

(a) $|0\rangle : \left(\frac{1}{\sqrt{2}}\right)^2 = \frac{1}{2}$ $\quad |1\rangle : \left(\frac{e^{i\theta}}{\sqrt{2}}\right)^2 = \frac{1}{2}$

PROBLEM 13

Consider the quantum state: $|\psi\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{e^{i\theta}}{\sqrt{2}}|1\rangle$

(b) Compute the probability of measuring $|+\rangle$ and $|-\rangle$ in the new basis: $|+\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$ and $|-\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right)$

SOLUTION

(b) $|0\rangle = \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)$ and $|1\rangle = \frac{1}{\sqrt{2}}(|+\rangle - |-\rangle)$

$$\begin{aligned}
|\psi\rangle &= \frac{1}{\sqrt{2}}\,|0\rangle + \frac{e^{i\theta}}{\sqrt{2}}\,|1\rangle) \\
&= \frac{1}{2}\,(|+\rangle + |-\rangle) + \frac{e^{i\theta}}{2}\,(|+\rangle - |-\rangle) \\
&= \frac{1+e^{i\theta}}{2}\,|+\rangle + \frac{1-e^{i\theta}}{2}\,|-\rangle \quad .
\end{aligned}$$

the Euler relation, $e^{i\theta} = \cos\theta + i\sin\theta$

Probability of measuring $|+\rangle$: $\cos^2(\theta/2)$, of $|-\rangle$: $\sin^2(\theta/2)$

Quantum Bit (Qubit):

INFORMATION CONTENT IN MULTIPLE QUBITS

- 2^n complex coefficients describe the state of a composite quantum system with n qubits.
- Imagine to have 500 qubits $\rightarrow$ 2^{500} complex coefficients describe their state.

2^{500} is larger than the number of atoms in the universe!

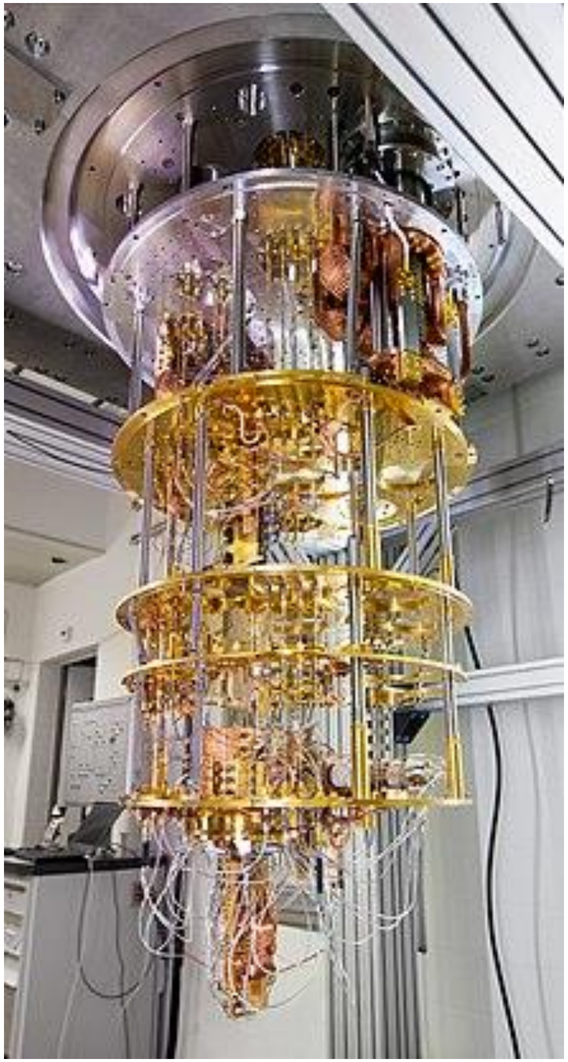
Impossible in classical bits!

4.3 DIFFERENCES BETWEEN QUANTUM AND TRADITIONAL COMPUTING

Programming language Quantum computing does not have its own programming code and requires the development and implementation of very specific algorithms.

Functionality Quantum computers: not intended for widespread, everyday use, unlike personal computers (PC). These supercomputers are so complex that they can only be used in the corporate, scientific and technological fields.

Architecture Quantum computers have a simpler architecture than conventional computers and they have no memory or processor. The equipment consists solely of a set of qubits that makes it run.



Quantum computer based on superconducting qubits developed by IBM Research in Zurich, Switzerland. The qubits in the device shown here will be cooled to under 1 kelvin.

4.4 MAIN USES OF QUANTUM COMPUTING

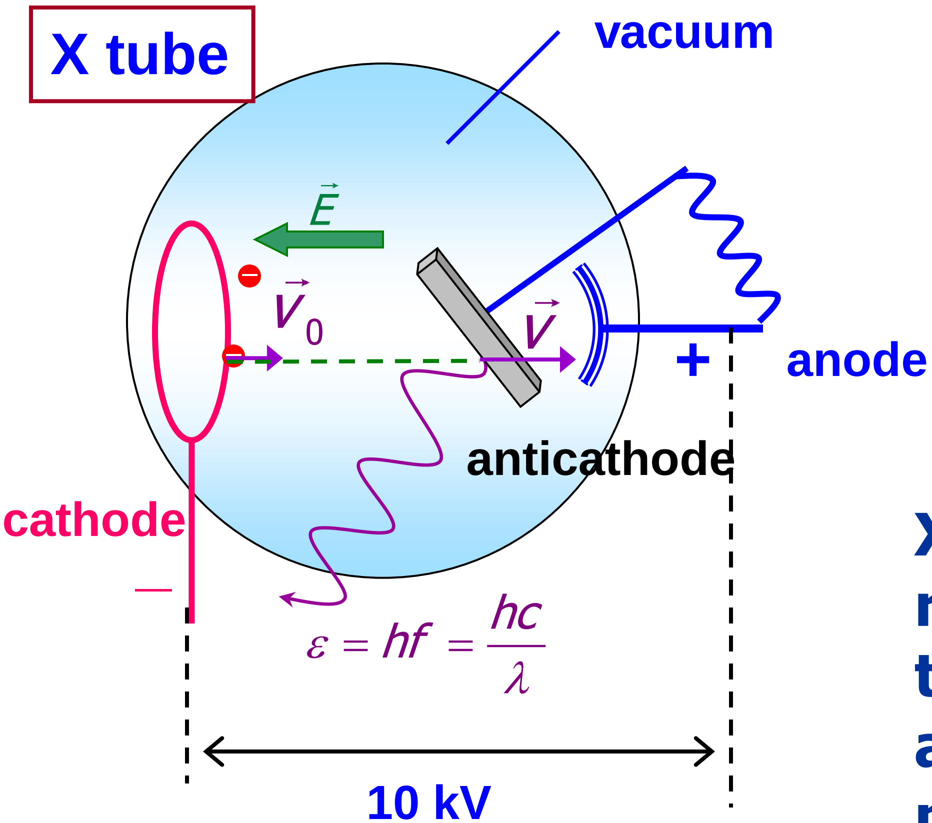
Finance Optimize their investment portfolios and improve fraud detection and simulation systems.

Healthcare Development of new drugs and genetically customized treatments, as well as DNA research.

Cybersecurity Advances in data encryption. This is a new technique for sending sensitive information that uses light signals to detect intruders in the system.

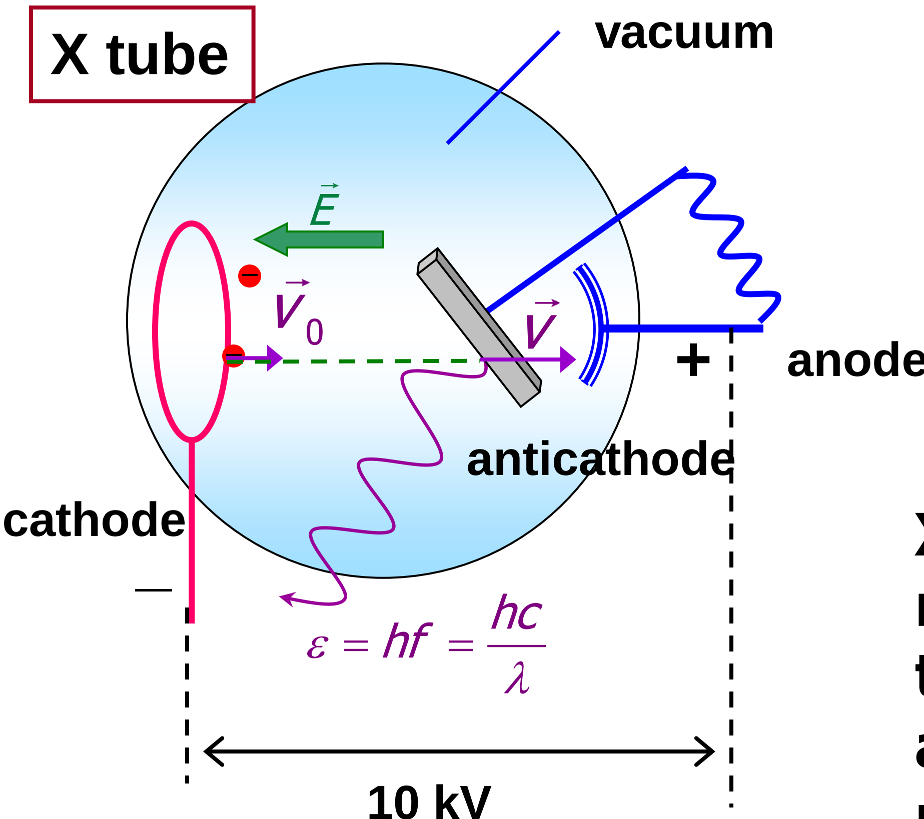
Mobility and transport Design more efficient aircraft. Qubits will also enable significant progress in traffic planning systems and route optimization.

5. X-Ray Production and Scattering

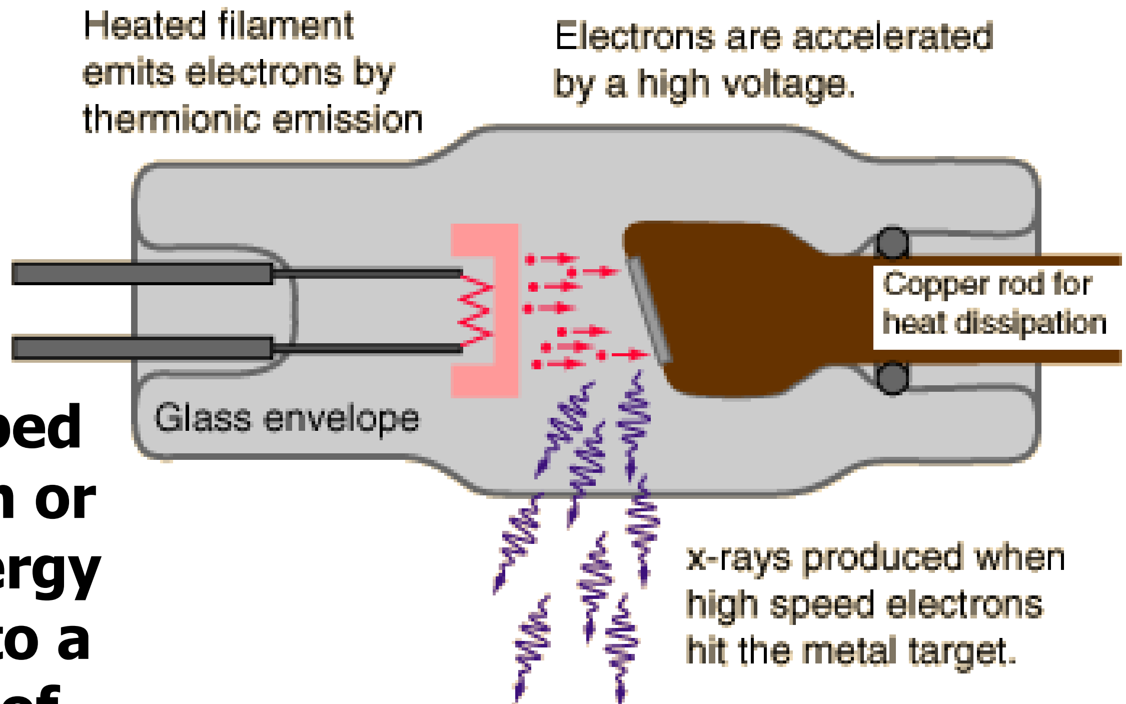


X rays are produced when rapidly moving electrons that have been accelerated through a potential difference of the order of 10^3 to 10^6 V strike a metal target.

5. X-Ray Production and Scattering



X rays are produced when rapidly moving electrons that have been accelerated through a potential difference of the order of 10^3 to 10^6 V strike a metal target.



Some electrons are slowed down or stopped by the target, and pan or all of their kinetic energy is converted directly to a continuous spectrum of photons, including x rays. This process is called bremsstrahlung (German for "braking radiation").

The maximum frequency and minimum wavelength of the x ray is given by :

$$\boxed{eV_{AC} = hf_{\max} = \frac{hc}{\lambda_{\min}}}$$

PROBLEM 14 Electrons in an x-ray tube are accelerated by a potential difference of 10.0 kV. If an electron produces one photon on impact with the target, what is the minimum wavelength of the resulting x rays? Answer using both SI units and electron volts.

SOLUTION

$$\lambda_{\min} = \frac{hc}{eV_{AC}} = \frac{(6.626 \times 10^{-34}\ \mathrm{J \cdot s})(3.00 \times 10^{8}\ \mathrm{m/s})}{(1.602 \times 10^{-19}\ \mathrm{C})(10.0 \times 10^{3}\ \mathrm{V})}$$

$$= 1.24 \times 10^{-10}\ \mathrm{m} = 0.124\ \mathrm{nm}$$

$$\lambda_{\min} = \frac{hc}{eV_{AC}} = \frac{(4.136 \times 10^{-15}\ \mathrm{eV \cdot s})(3.00 \times 10^{8}\ \mathrm{m/s})}{e(10.0 \times 10^{3}\ \mathrm{V})}$$

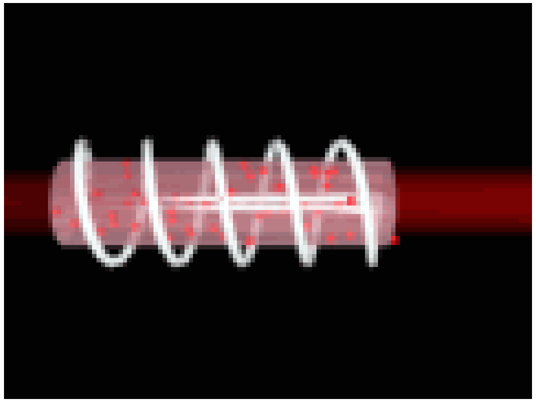
$$= 1.24 \times 10^{-10}\ \mathrm{m} = 0.124\ \mathrm{nm}$$

6. The laser

• **Ordinary light source**: radiative electron transitions **spontaneous** (occur independently of one another and at random times) producing radiation that is **incoherent**

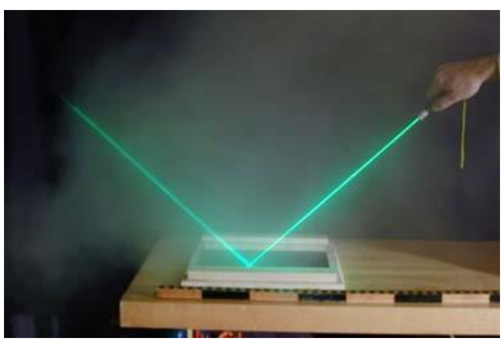
• **Laser light**: **coherent light** is generated by electron transition initiated by **external stimulus**

• **Laser** : acronym for **L**ight **A**mplification by **S**timulated **E**mission of **R**adiation



6.1 Characteristics of laser light

- **Highly monochromatic** (light from an ordinary incandescent light-bulb is spread over a continuous range of wavelengths: not monochromatic)
- **Highly coherent** (Individual long waves: hundred kilometers long. Light-bulb: less than a meter)
- **Highly directional** (A laser beam spreads very little)
- **Sharply focused** (A focus spot can have an intensity of $10^7 W/cm^2$)



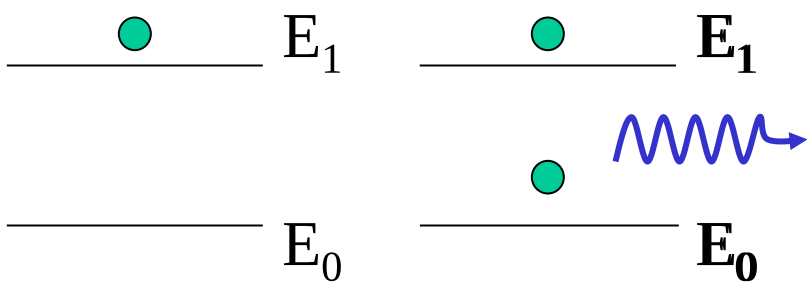
6.2 Lasing

- **Three possible processes** by which an atom can move from one state to another:

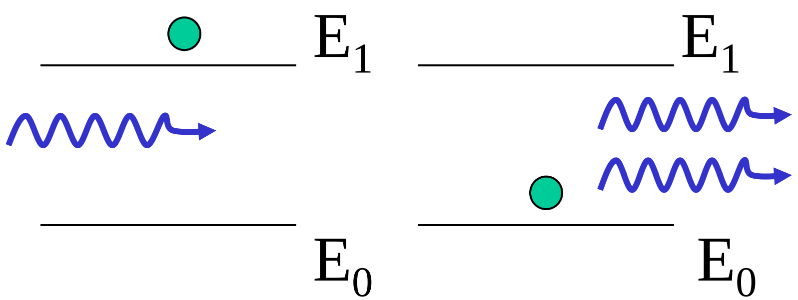
Absorption (when the atom is placed in an electromagnetic field of frequency *f*, it can absorb an amount *hf* and move to higher energy state)

Spontaneous emission (the emission is not triggered by any outside influence)

Stimulated emission (An incoming photon with the correct energy Induces an electron to change energy levels)



spontaneous emission



stimulated emission

• When a sample is in **thermal equilibrium**, the number of atoms in the state of energy E is:

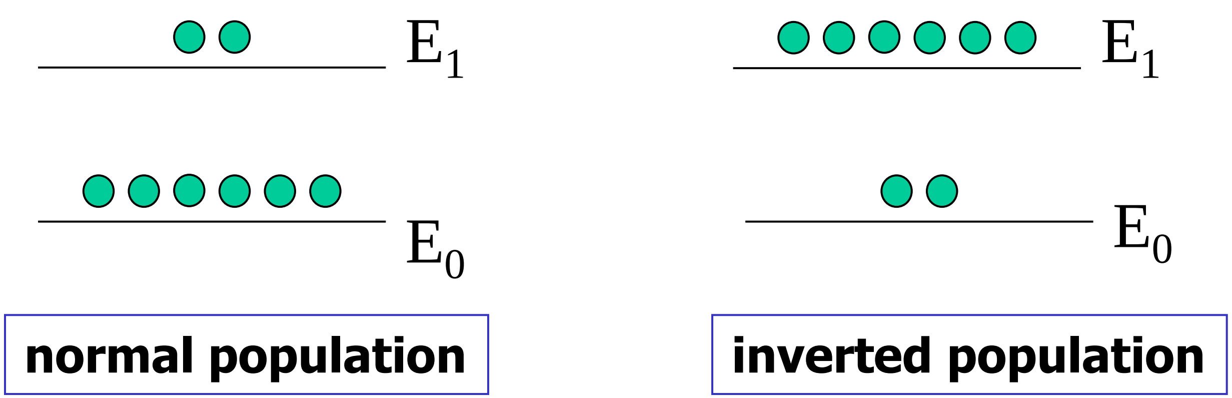
$$\boxed{N = N_0 e^{-(E-E_0)/kT}}$$

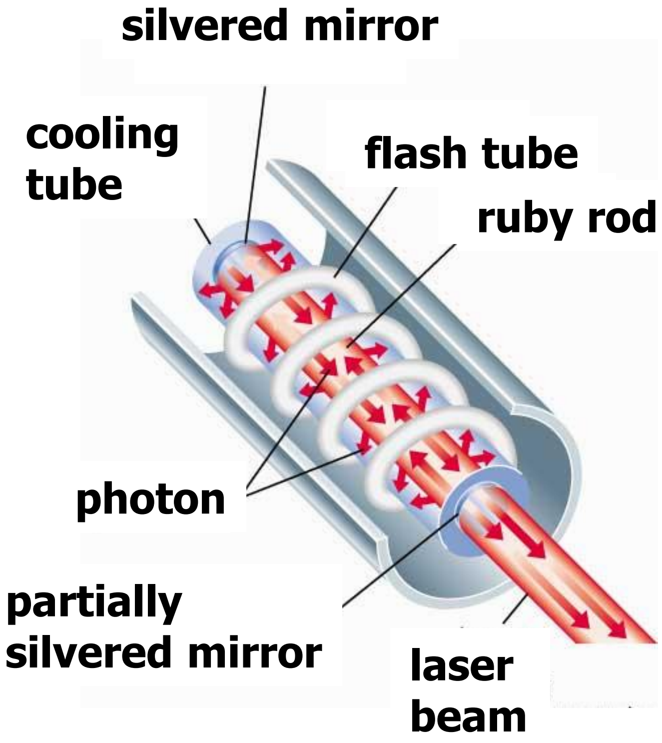
where N_0 is the number of atoms in the ground state of energy E_0

$$\longrightarrow \quad N \leq N_0$$

• **Produce laser**: we must have a situation in which **stimulated emission dominates**: more atoms in the excited state than in the ground state

$\longrightarrow$ **Population inversion**





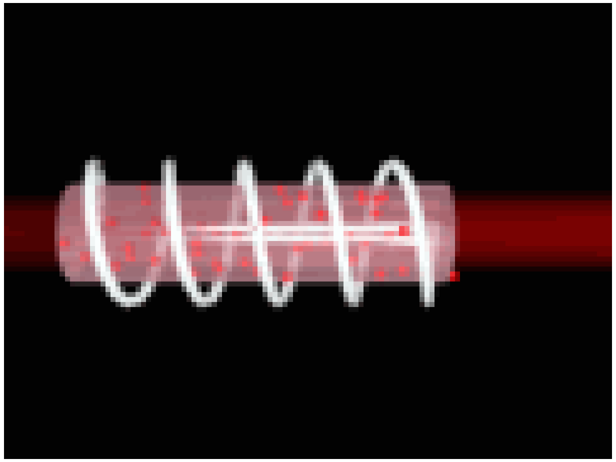
6.3 Solid laser

Ruby laser:

Ruby is a crystal of sapphire (Al_2O_3) contains about 0.005% Cr^{3+} ions

The xenon flash lamp excite the Cr^{3+} ions to a higher energy level

Photons from the spontaneous decay cause other excited Cr^{3+} ions to radiate



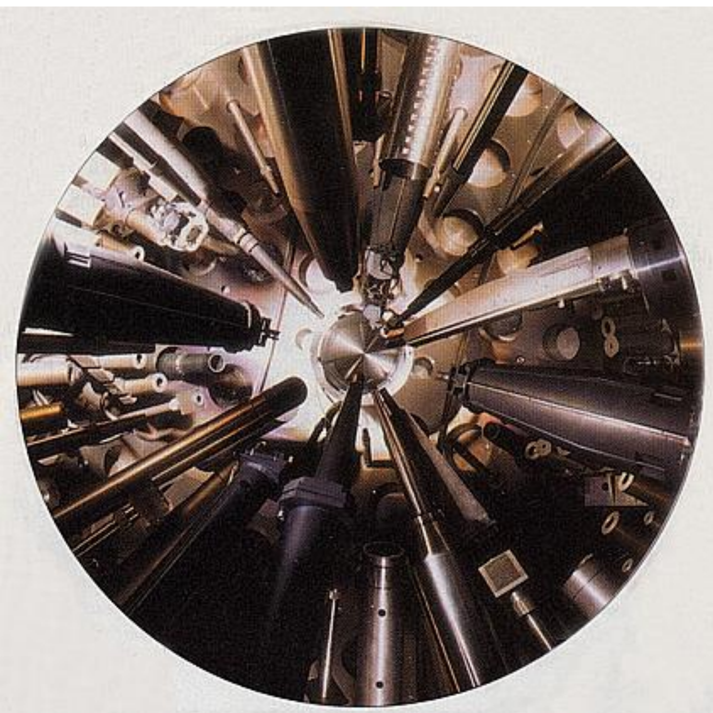
Result: A large pulse of **single-frequency coherent red light** from the partly silvered end of the rod

6.4 Semiconductor laser:

The **stimulated recombination** of excited electrons in the conduction band with holes in the valence band gives rise to a laser beam

6.5 Applications of laser:

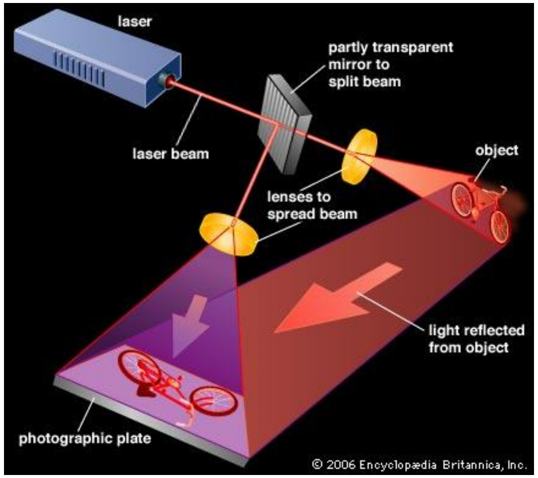
Medical applications (in ophthalmology to correct for myopia, photodynamic therapy to treat cancer), **holography**, voice and data transmission over **optical fibers**, **nuclear fusion** research, **industry** (infra-red lasers can cut through metal), military applications,…

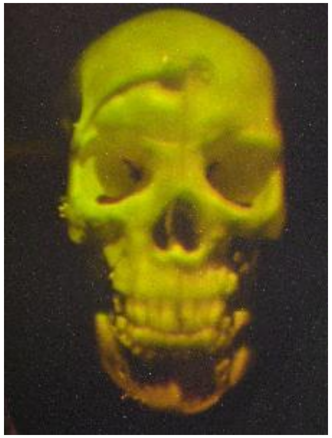


Laser fusion:
Use of **inertial confinement** approach to cause deuterium-tritium **thermonuclear reaction** with **intense lasers**

Holography

(from the Greek, *όλος-hòlòs* whole + *γραφή-grafè* writing, drawing) is the science of producing **holograms**. It is a technique that allows the light scattered from an object to be recorded and later reconstructed so that it appears as if the object is in the same position relative to the recording medium as it was when recorded. The image produced changes as the position and orientation of the viewing system changes in exactly the same way is if the object were still present





PROBLEM 15 In the helium-neon laser, laser action occurs between two excited states of the neon atom. However, in many lasers, lasing occurs between the ground state and the excited state.

1/ Consider such a laser that emits at wavelength 550nm. What is the ratio of the population of atoms in state E_1 to the population in the ground state E_0 at room temperature?

2/ For the condition of 1/, at what temperature would this ratio to be 1/2?

SOLUTION

1/ We use the expression: $\boxed{N = N_0 e^{-(E-E_0)/kT}}$

The energy separation between two states for the lasing:

$$\Delta E = h\nu = \frac{hc}{\lambda} = \frac{6.63\times10^{-34}\times3\times10^{8}}{550\times10^{-9}\times1.6\times10^{-19}} = 2.26\ eV$$

$$kT = \frac{1.38\times10^{-23}\times300}{1.6\times10^{-19}} = 0.0259\ eV \quad \Rightarrow \frac{N}{N_0} = e^{-2.26/0.0259} = 1.3\times10^{-38}$$

Comment: N/N_0 is extremely small; its thermal energy is too small

$$2/ \quad \frac{N}{N_0} = \frac{1}{2} = e^{-(E-E_0)/kT} \quad \Rightarrow \quad T = \frac{E-E_0}{k(\ln 2)}$$

$$T = \frac{2.26\ eV}{(8.62\times10^{-5} eV/K)\ln 2}$$

$$T = 38\,000\ K$$

Comment: We need specific techniques to invert the population

7 Semiconductivity

7.1 *Electrical conductivity*

• ***Electrical conductivity*** $\boldsymbol{\sigma}$ is used to specify the electrical character of a material. It is **the reciprocal of the resistivity**

$$(\Omega - m)^{-1} \longleftarrow \boxed{\sigma = \frac{1}{\rho}}$$

$\boldsymbol{\sigma}$ is indicative of the ease with which a material is capable of conducting an electric current.

• Ohm's law may be written as: $\boxed{J = \sigma \mathscr{E}}$ (2)

in which J is the **current density** (the current per unit of specimen area I/A), and $\mathscr{E}$ is the **electric field intensity** (the voltage difference between two points divided by the distance separating them):

$$Vm^{-1} \longleftarrow \boxed{\mathscr{E} = \frac{V}{l}}$$

CLASSIFICATION OF MATERIALS:

One way of classifying solid materials is according to the ease with which they conduct an electric current: **conductors**, **semiconductors**, and **insulators**

- Metals are good **conductors**, having conductivities on the order of:

$$10^{7}(\Omega - m)^{-1}$$

- At the other extreme are **electrical insulators**, with very low conductivities, ranging between

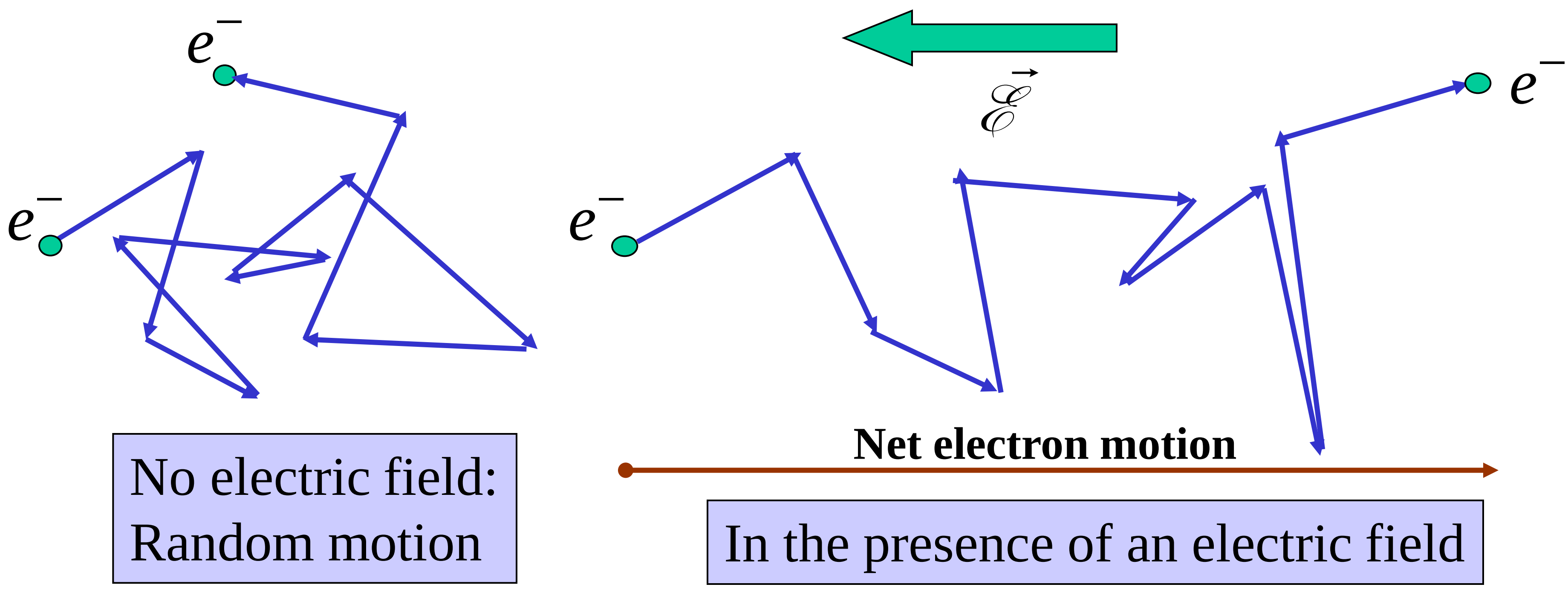
$$10^{-10}(\Omega - m)^{-1} \text{ and } 10^{-20}(\Omega - m)^{-1}$$

- Materials termed **semiconductors** with intermediate conductivities, generally

$$\text{from } 10^{-6}(\Omega - m)^{-1} \text{ to } 10^{4}(\Omega - m)^{-1}$$

Within most solid materials a current arises from the **flow of electrons** (termed **electric conduction**).

For ionic materials, a net **motion of charged ions** possible of producing a current is termed **ionic conduction** (Faraday' law)



- The **conductivity σ** of most materials may be expressed as

$$\boxed{\sigma = ne\mu_e}$$

where n is the number of free or conducting electrons per unit volume (e.g. per cubic meter) and e is absolute magnitude of electrical charge of an electron, and μ_e is **the electron mobility**

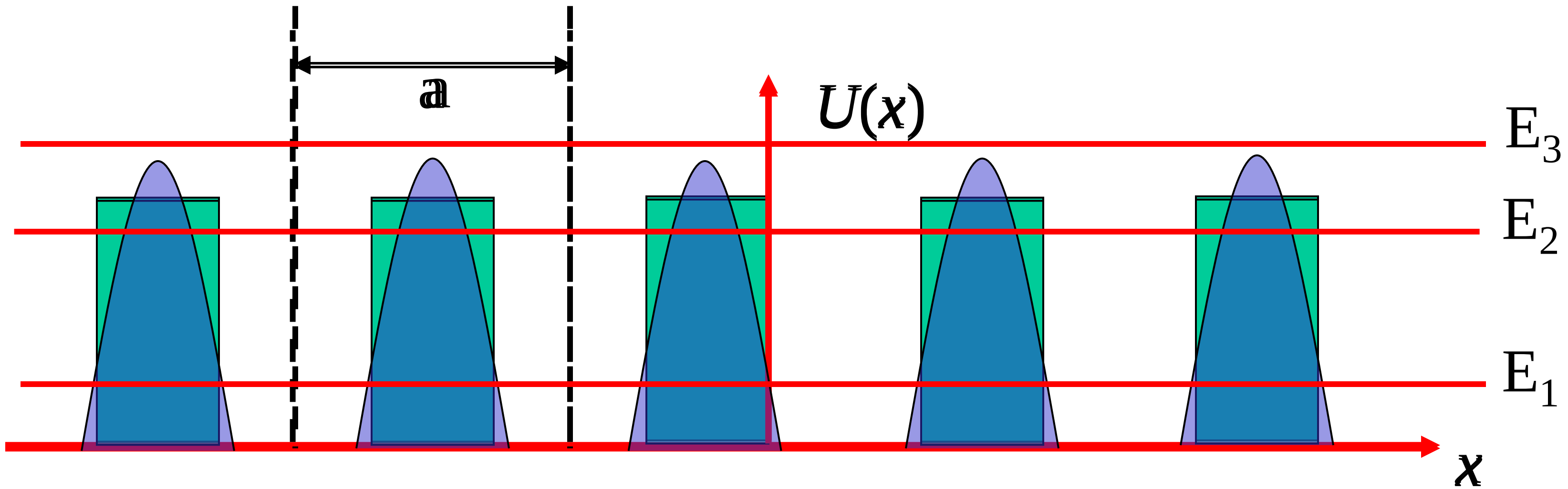
Thus, the electrical conductivity is proportional to both the number of free electrons and the electron mobility μ_e

7.2 *Kronig-Penney Model*

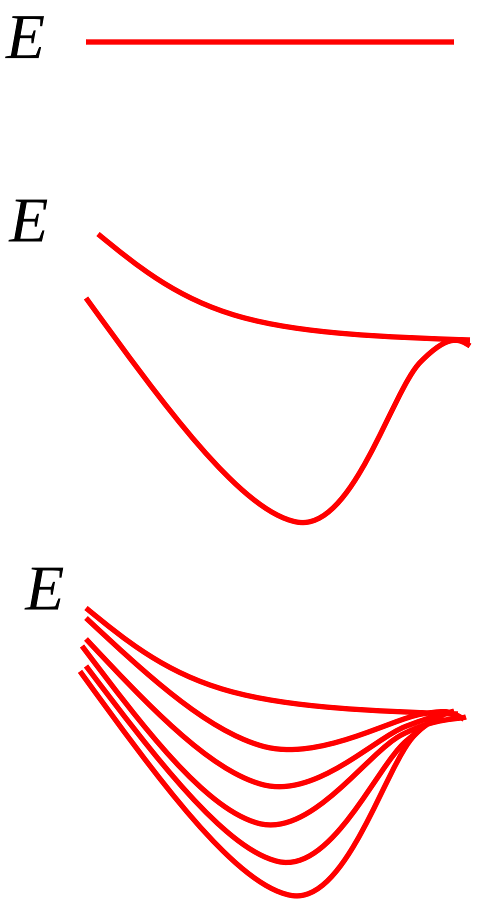
A solid may be thought of as consisting of a large number *N* of atoms **initially separated** from one another, which are subsequently **brought together and bonded** to form the ordered atomic arrangement found in the crystalline materials: **Lattice**

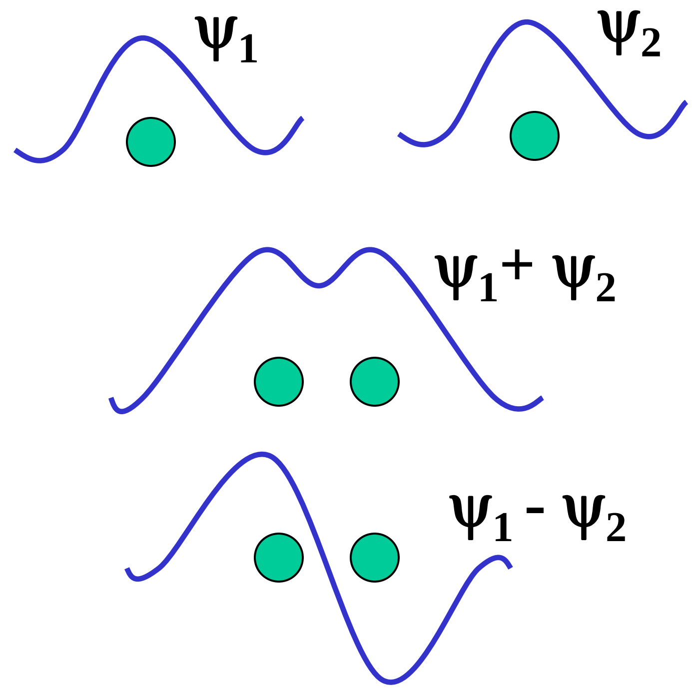
At relatively large separation distances, each atom is independent of all the others

Because the atoms are arranged periodically, the potential $U(x)$ is periodic: Square well periodic potential (**Kronig-Penney** model)



7.3 *Band structure in Solids*





Two atoms at large separation

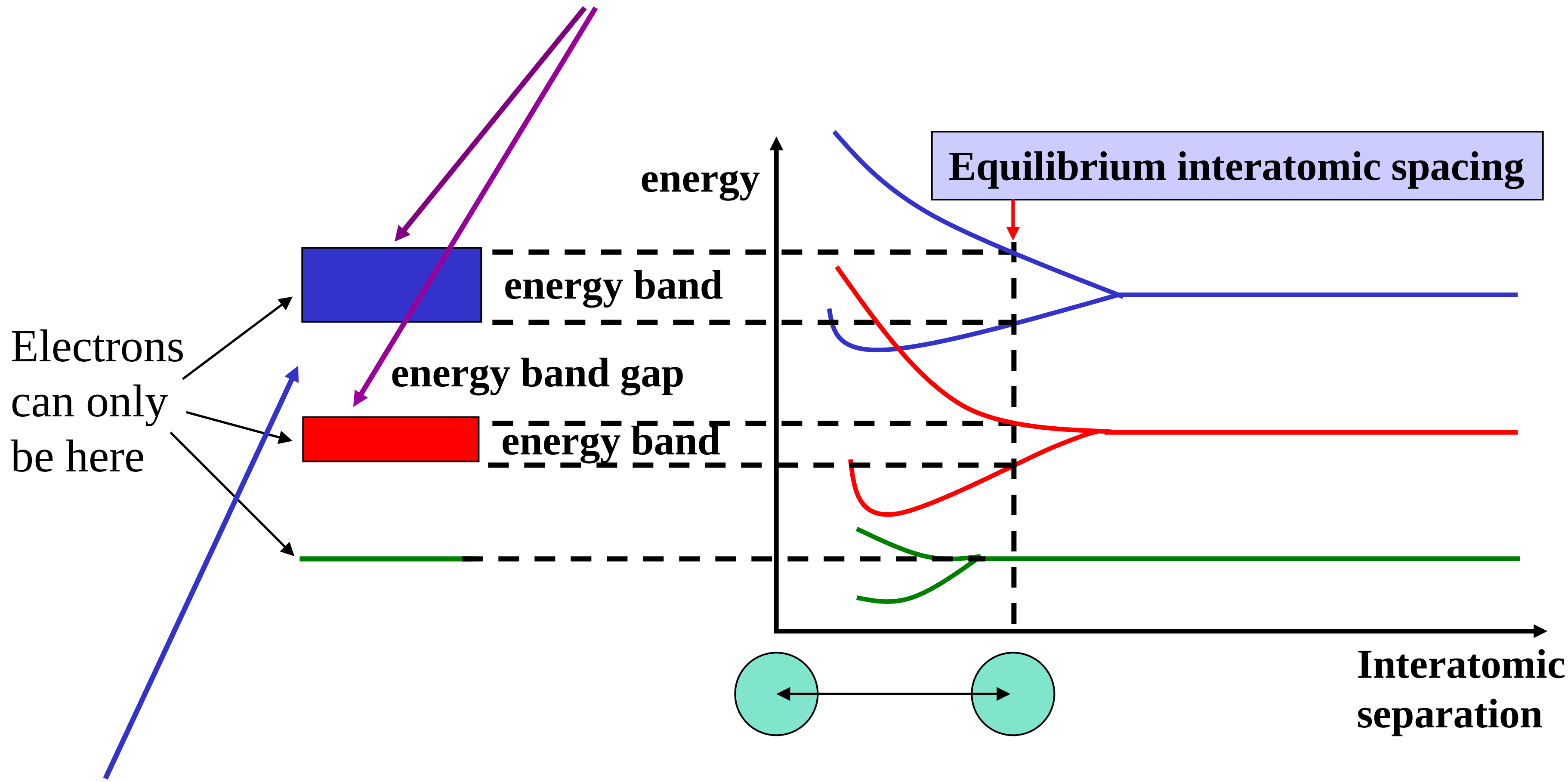
Two atoms at small separation

Many atoms at small separation

When many atoms are brought close together, energy is **split into many levels very close together** $\rightarrow$ **continuous** – **band energy**

• Energy band gap

Each distinct atomic state may split into a series of closely spaced electron states in solid, to form an ***electron energy band***



Gaps may exist between adjacent bands; normally, energies lying within these band gaps are **not available** for electron occupancy

7.4 *Conduction in Metals, Insulators, and Semiconductors*

• **Electron band structure:** the arrangement of the outermost electron bands and the way in which they are filled with electrons

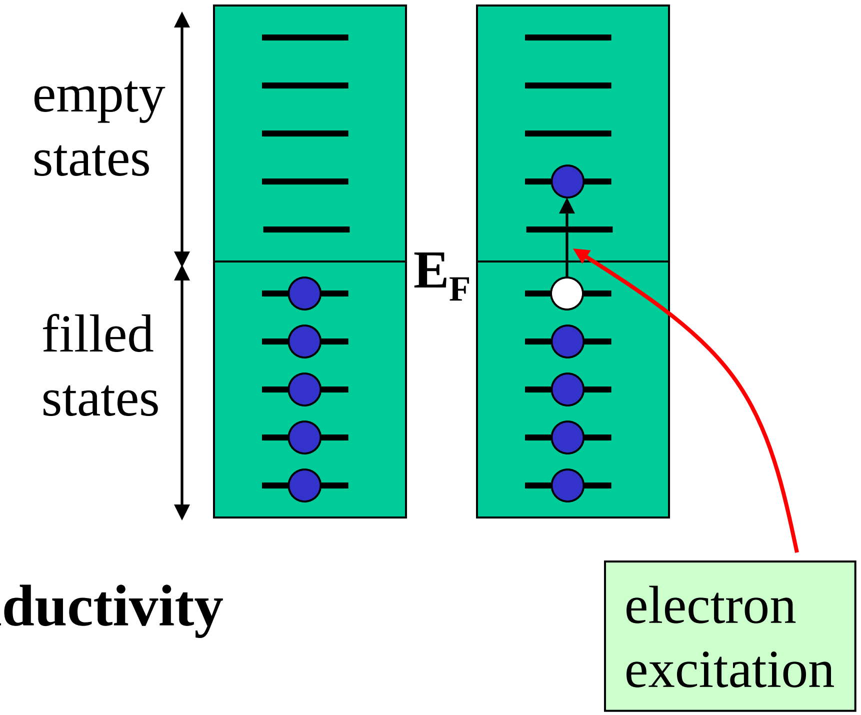
• The electrical properties of a solid are the **consequence of its electron band structure**

• Materials are classified according to their **electrical conductivity**: Metals, insulators, and semiconductors

a/ Metals:

There are many vacant energy states adjacent to the highest filled states at the temperature of 0 K (**Fermi energy** E_F)

Little energy is required to promote electrons into the low lying empty states



→ Metals have **high electrical conductivity**

b/ Insulators:

There are: the **valence band** (completely filled with electrons), the **conduction band** (completely empty at 0 K), and an **energy band gap *Eg*** lying between the two first bands

***Eg* ≈ 10eV :** too large, there are so few electrons occupying conduction band

→ **High resistivity of insulators**

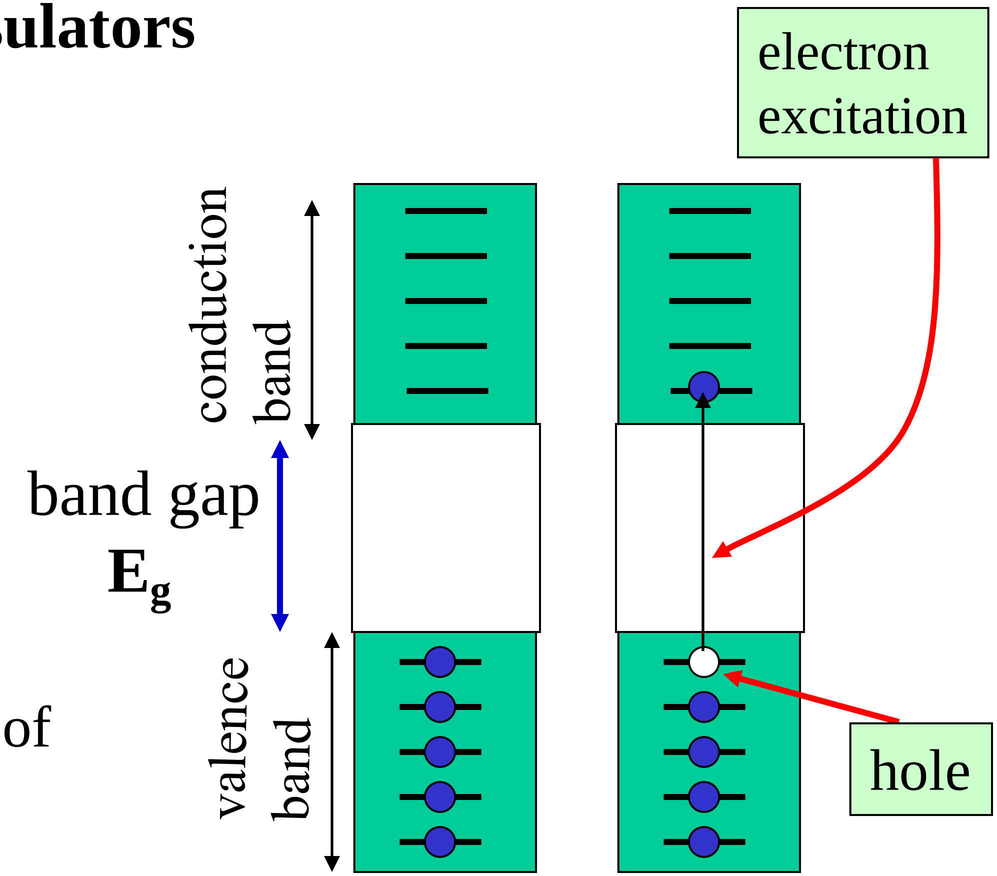
c/ Semiconductors:

Semiconductors are materials that have small energy gap E_g

Example: At 0 K

Si → 1.17 eV

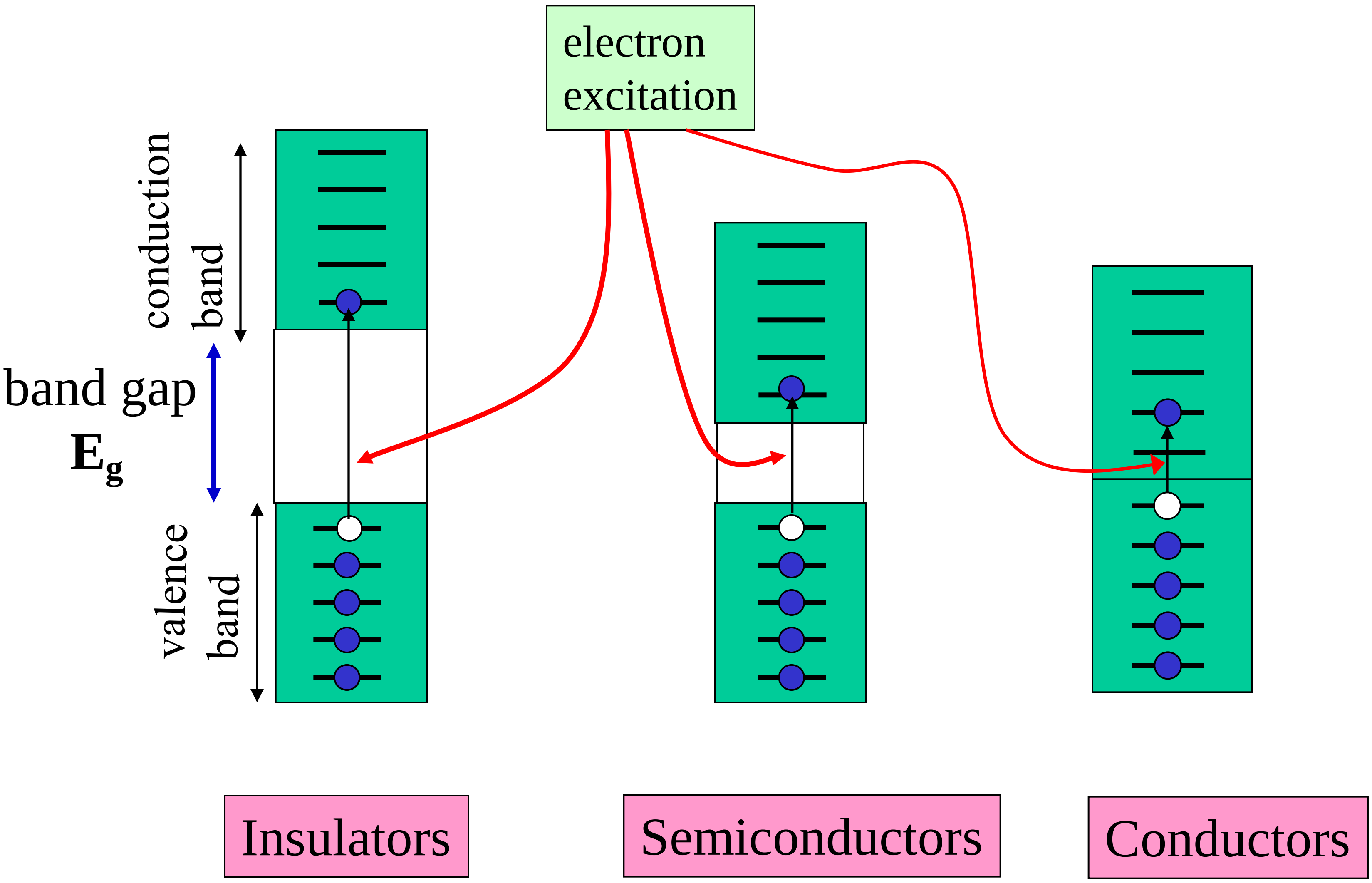
Ge → 0.74 eV



- **At low temperature**: no electrons in conduction band: **poor conductor**
- **At ordinary temperature**: numbers of electrons are thermally excited to the conduction band

→ **The conductivity of semiconductors increases rapidly with temperature**

• Comparison : Insulators, Semiconductors, and Conductors



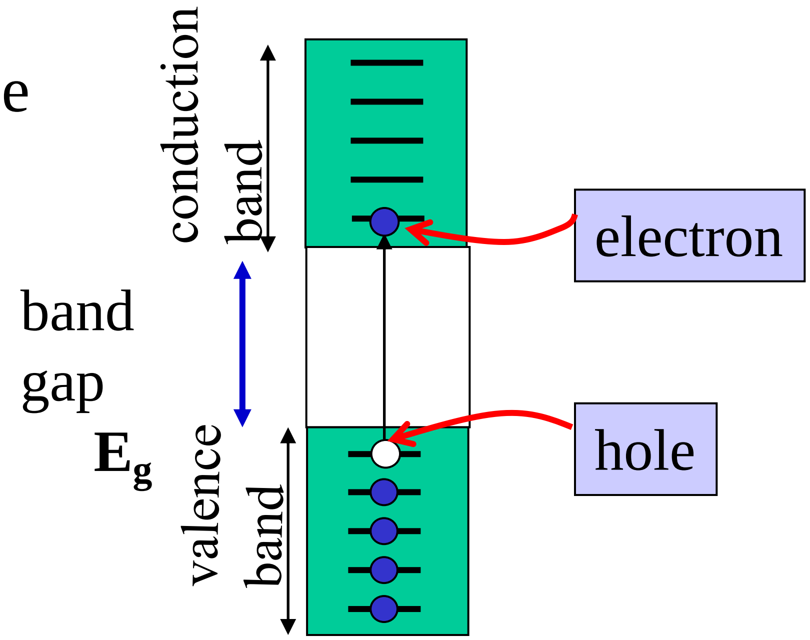
7.5 *Semiconductors*

• The main difference between the insulator and the semiconductor:

The semiconductor has a much smaller **energy band gap** E_g between the top of the highest filled band (**valence band**) and the bottom of the vacant band (**conduction band**)

• At room temperature, thermal agitation will cause the electron jump from valence band to the conduction band, leaving an equal number of **unoccupied energy states** called **holes**

• If an electric field $\mathscr{E}$ is set up, the **electrons tend to drift in the direction opposite** $\mathscr{E}$, the position of the holes tend to **drift in the direction** of $\mathscr{E}$

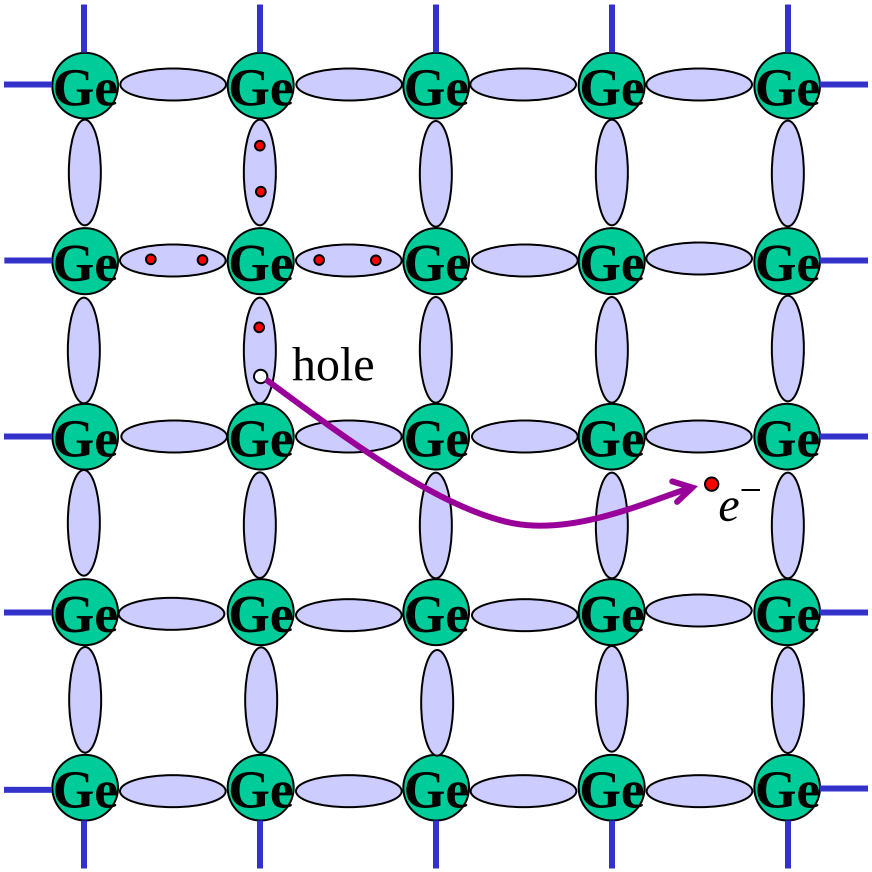


→ The holes behave like moving particles of charge +*e*

→ With an electric field, both electrons and holes are charge carriers

1/ *Intrinsic Semiconductors*

• This conductivity, based on the inherent property of the material, not by impurities, is called **intrinsic semiconductivity**



• Because there are two types of carriers (electrons and holes), the **conductivity** is:

$$\boxed{\sigma = ne\mu_e + pe\mu_h}$$

n is the electrons density

μ_e is the electron mobility

p is the holes density

μ_h is the hole mobility

Because $n = p$, we put:

$\boxed{n = p = n_i} \rightarrow$ intrinsic carrier concentration

The total **conductivity**: $\boxed{\sigma = ne(\mu_e + \mu_h) = n_i e(\mu_e + \mu_h)}$

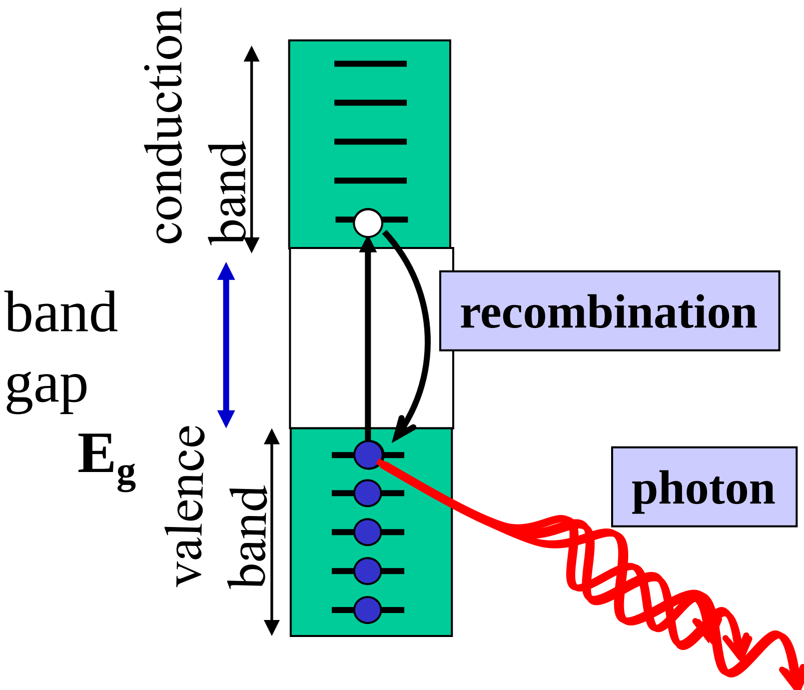
• Two elemental intrinsic semiconductors: **silicon** (*Si*, E_G = 1.1eV) and **germanium** (*Ge*, E_G = 0.7eV), both are <u>covalently bonded</u>. Compound semiconducting materials: **gallium arsenide** (*GaAs*), and **indium antimonide** (*InSb*)

• **Recombination:** Since all materials are more stable when they reduc their energies, electron-hole pairs recombine sooner or later and **energy is released**

E**nergy released** may appears as heat, **or light (luminescence)**

If the electrons have been activated to the conduction band by a **stream of electrons** (cathode rays) that is: **electroluminescence**

(**Example**: in a television tube, when the electrons and the holes recombine, visible light is emitted)



PROBLEM 16

In germanium, the electron density in conduction band (and the hole density in valence band) is a function of energy gap E_g =0.7eV according to:

$$n_i \propto e^{-E_g/2kT}$$

Because the conductivity is proportional to the number of carriers:

$$\sigma = \sigma_0 \, e^{-E_g/2kT}$$

The resistivity of germanium at 20°C is 0.5Ω.m. What is its resistivity at 40°C?

SOLUTION

$$\frac{\rho_1}{\rho_2} = \frac{\sigma_2}{\sigma_1} = \frac{\sigma_0 \, e^{-E_g/2kT_2}}{\sigma_0 \, e^{-E_g/2kT_1}} \longrightarrow \ln\frac{\rho_1}{\rho_2} = \frac{E_g}{2k}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)$$

$$\ln\frac{\rho_1}{\rho_2} = \frac{0.7\times1.6\times10^{-19}}{2\times13.8\times10^{-24}}\left(\frac{1}{293} - \frac{1}{313}\right) = 0.9 \longrightarrow \frac{\rho_1}{\rho_2} = 2.5$$

$$\rho_2 = \frac{\rho_1}{2.5} = \frac{0.5}{2.5} = 0.2\Omega.m$$

2/ *Extrinsic Semiconductors*

- When the electrical behavior of the material is determined by **impurities**: **Extrinsic Semiconductors**
- **Impurities,** when present in even minute concentration, introduce **excess electrons or holes** ⟶ **Doping** semiconducting materials

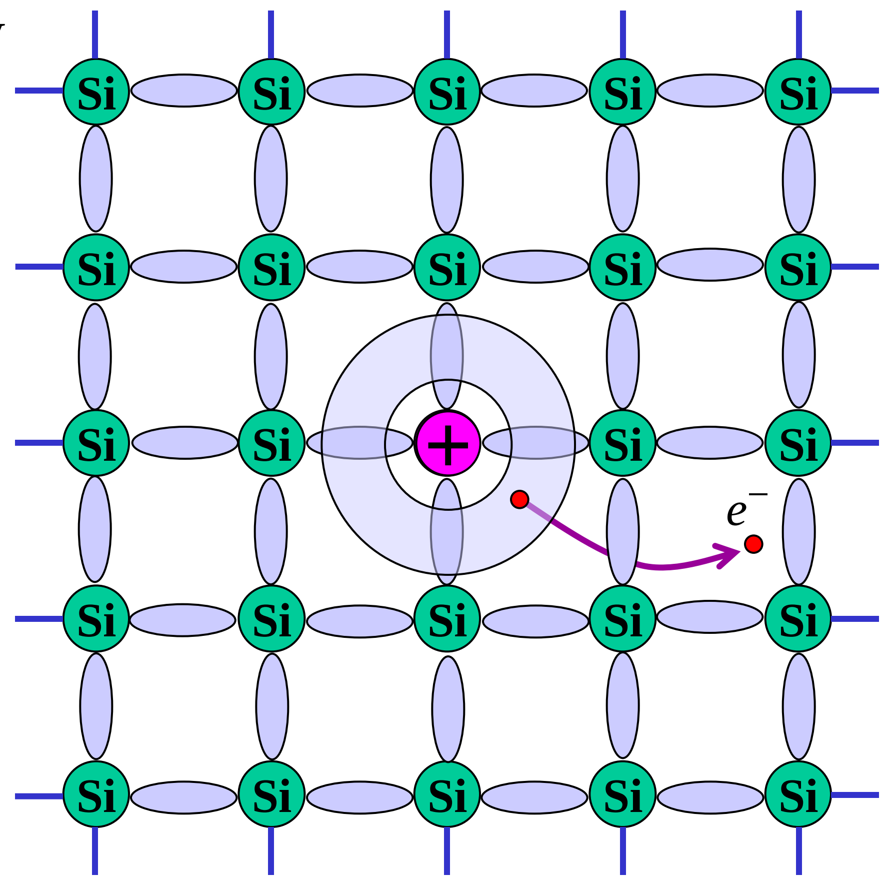
a/ *n-type Extrinsic Semiconductors*

An *Si* atom has 4 electrons covalently bonded to four adjacent *Si* atoms

If an phosphorus atom *P* with the valence of 5 is added to a silicon:

The extra nonbonding electron is loosely bound to the region around the impurity atom

⟶ It is easily removed from impurity atom *P*, and **becomes a free (or conducting) electron**



Each excitation event **supplies or donates** a single electron to the conduction band; this impurity is termed **donors**

In **n-type extrinsic semiconductors (n: negative)**, the number of electrons in the conduction band far exceeds the number of holes in the valence band: **The electrons are majority carriers**

→ The conductivity: $\boxed{\sigma \approx ne\mu_e}$

b/ *p-type Extrinsic Semiconductors*

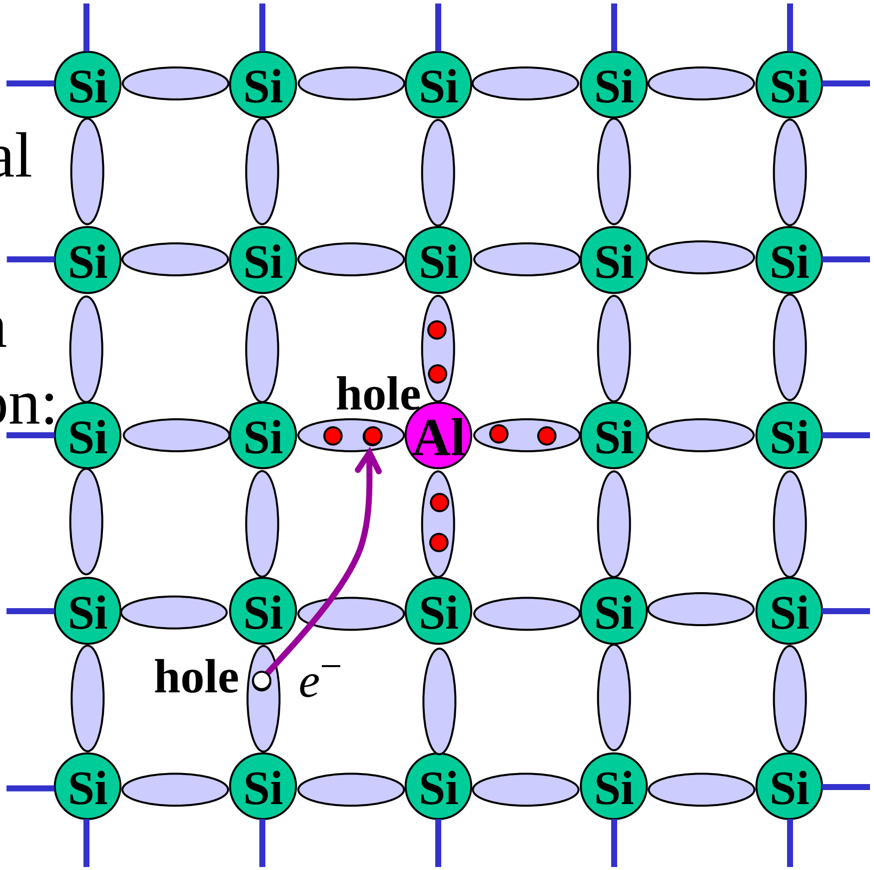
Add to silicon a **trivalent** substitutional impurities (aluminium, boron)

One of the covalent bonds around each of these atoms is deficient in an electron: a hole weakly bound to the *Al* atom

→ A moving hole participates in the conduction process.

This impurity is called **acceptor**

→ The conductivity: $\boxed{\sigma \approx pe\mu_h}$



PROBLEM 17

For intrinsic gallium arsenide, the room temperature conductivity is 10^{-6} $(\Omega\text{-m})^{-1}$; the electron and hole mobilities are, respectively, 0.85 and 0.04 m^2/V-s .
Compute the intrinsic carrier concentration n_i at room temperature.

SOLUTION

The material is intrinsic $\longrightarrow$ the intrinsic carrier concentration n_i is computed by:

$$\boxed{\sigma = ne(\mu_e + \mu_h) = n_i e(\mu_e + \mu_h)}$$

$$\longrightarrow \quad n_i = \frac{\sigma}{e(\mu_e + \mu_h)} = \frac{10^{-6}}{1.6\times10^{-19}\times(0.85+0.04)} = 7.0\times10^{12}\,m^{-3}$$

PROBLEM 18

The number density n_0 of conduction electrons in pure silicon at room temperature is about 10^{16} m^{-3}. Assume that, by doping the silicon lattice with phosphorus, we want to increase this number by a factor of a million.

What fraction of silicon atoms must we replace with phosphorus atoms? The density mass of silicon is 2.33g/cm^3, and the molar mass of silicon is 28.1g/mol

SOLUTION

Each phosphorus atom contributes only one conduction electron

The total number density of conduction electrons must be $10^6 n_0$

$\longrightarrow$ The number density n_p of phosphorus atoms is given by:

$$10^6 n_0 = n_0 + n_p \longrightarrow n_p = 10^6 n_0 - n_0 \approx 10^6 n_0$$

$$n_p = 10^{16} \times 10^6 = 10^{22} m^{-3}$$

(We must add 10^{22} atoms of phosphorus per cubic meter of silicon)

PROBLEM 19

To high-purity silicon is added 10^{23} m^{-3} arsenic atoms.

1/ Is this material *n*-type or *p*-type?

2/ Calculate the room-temperature electrical conductivity of this material

We have: $\mu_e = 0.07 m^2 / V - s$

3/ Compute the conductivity at 100° C (373 K), we have:

$$\mu_e = 0.04 m^2 / V - s$$

SOLUTION

1/ Arsenic (*As*) is a group VA element $\longrightarrow$ *As* act as donor in silicon: *n*-type

2/ At room temperature (298 K), **all** arsenic have donated electrons

$$\longrightarrow \quad n = 10^{23} m^{-3}$$

Because: $\boxed{\sigma \approx ne\mu_e}$, with: $\mu_e = 0.07 m^2 / V - s$

$$\sigma \approx 10^{23} \times 1.6 \times 10^{-19} \times 0.07 = 1120 (\Omega - m)^{-1}$$

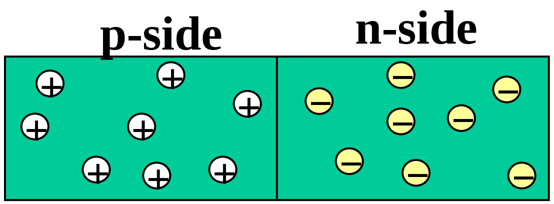
3/ At 273 K: $\mu_e = 0.04 m^2 / V - s$

$$\sigma \approx 10^{23} \times 1.6 \times 10^{-19} \times 0.04 = 640 (\Omega - m)^{-1}$$

3/ Semiconductor devices

***a/ The p-n rectifyer (diode)*:** Electronic device that allows the current to flow **in one direction only**

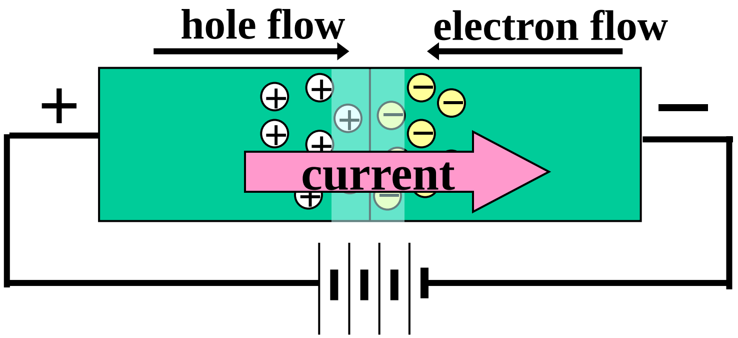
- **The p-n rectifying junction** is constructed from from a single piece of semiconductor that is doped so as to be **<u>n-type on one side</u>** (dominant carriers: electrons) and **<u>p-type on the other</u>**.(dominant carriers: holes)



- When a battery is used with the positive terminal connected to p-side (**forward bias**)

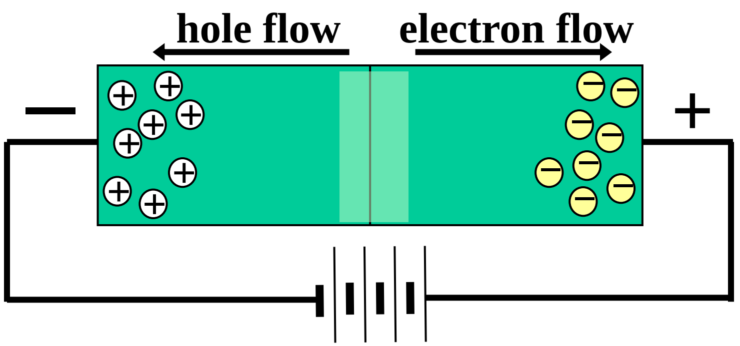
→ the holes and the electrons are attracted to the junction, recombine and annihilate each other

→ large numbers of charge carriers flow across the device: **<u>appreciable current</u>**

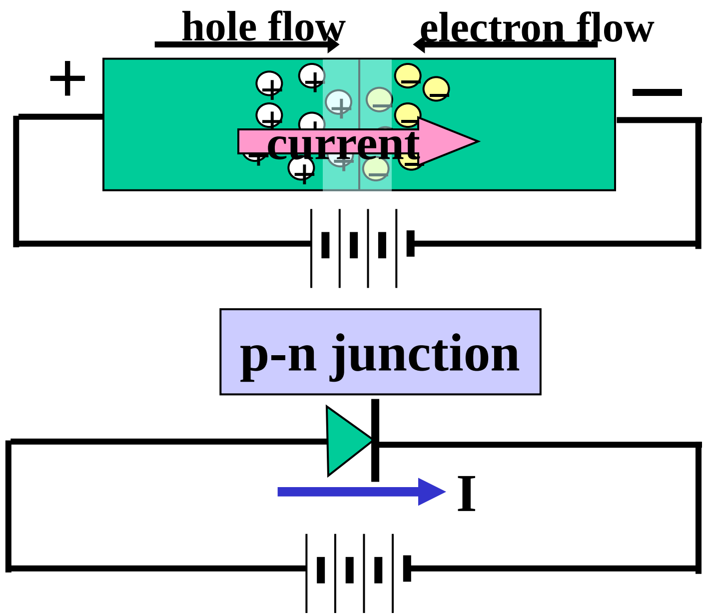


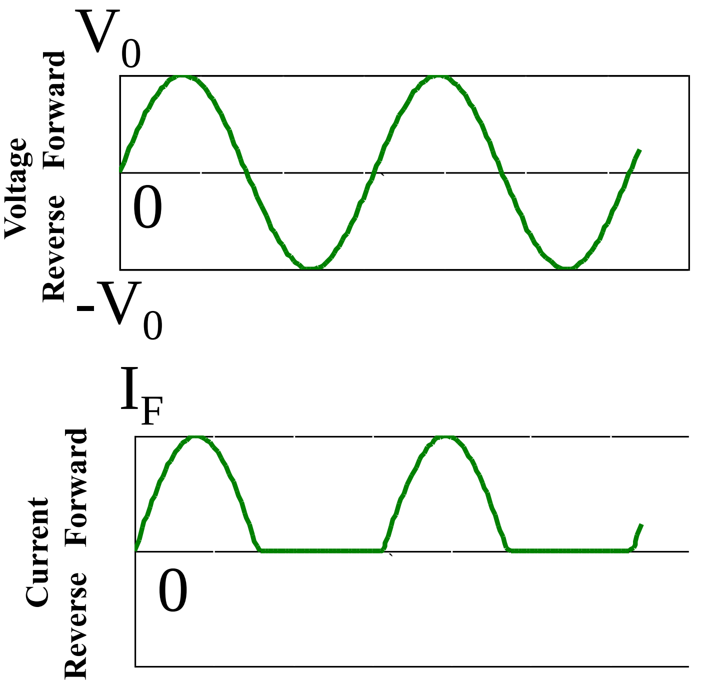
- When the polarity is **reverse bias**: both holes and electrons are rapidly drawn away from the junction, leaves this region free of mobiles charge carriers:

→ The junction is **<u>highly insulative</u>**



The junction rectifyer





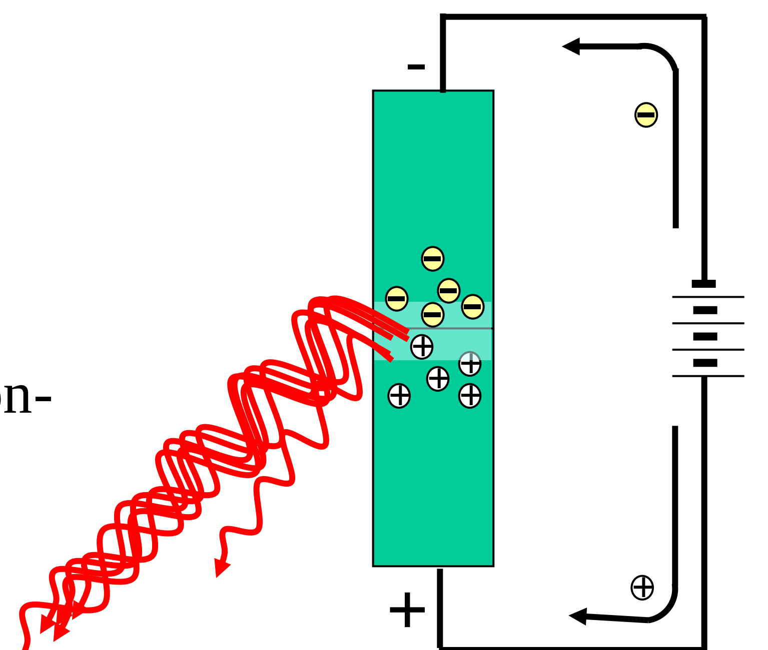
• The Light-Emitting Diode (LED)

(remote control, calculator, clock, …)

The current *I* through the device serves to inject electrons into the *n*-type material and to inject holes into the *p*-type material

If the doping is heavy enough, many electron-hole combination occur $\rightarrow$ light emitted:

$$\lambda = hc/E_g$$



PROBLEM 20

An LED is constructed from a p-n junction on a certain Ga-As-P semiconducting material whose energy gap is 1.9 eV.
What is the wavelength of the emitted light?

SOLUTION

Assume that the transitions are from the bottom of the conduction band to the top of the valence band

$$\longrightarrow \quad \boxed{\lambda = hc/E_g}$$

$$\lambda = \frac{6.63\times10^{-34}\times3\times10^{8}}{1.9\times1.6\times10^{-19}}$$

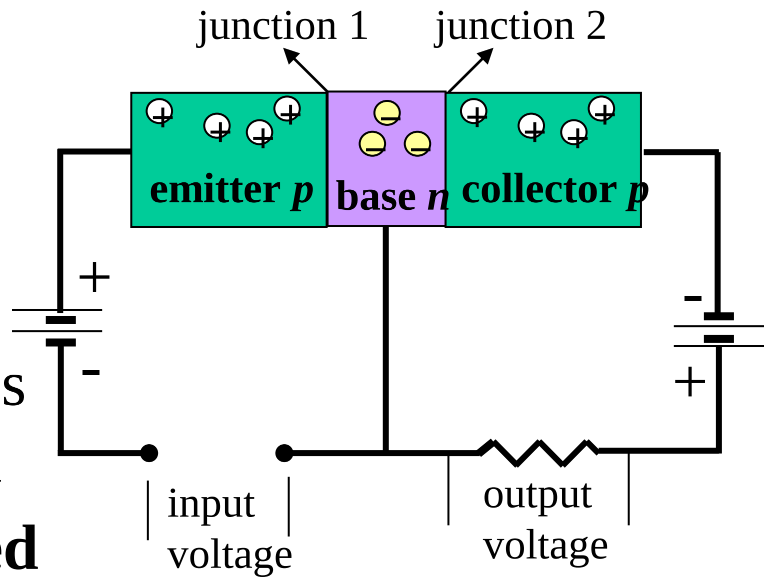
$\lambda = 0.65\times10^{-6}\,\mu m$: **<u>Light is red</u>**

b/ The transistor

- **The junction transistor:** either *n-p-n* or *p-n-p* configuration
- For *p-n-p* configuration: A very thin *n-type* ***base*** is sandwinched in between *p-type* ***emitter*** and ***collector*** regions

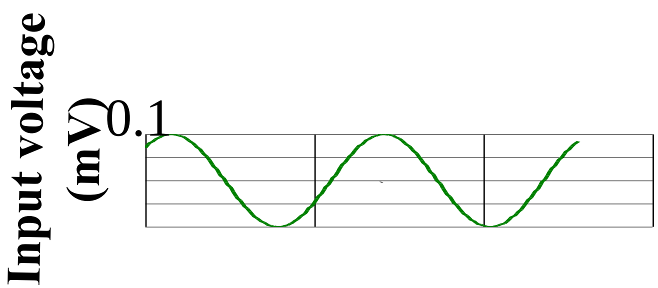
The emitter-base junction 1 is forward biased, the base-collector 2 is reverse biased

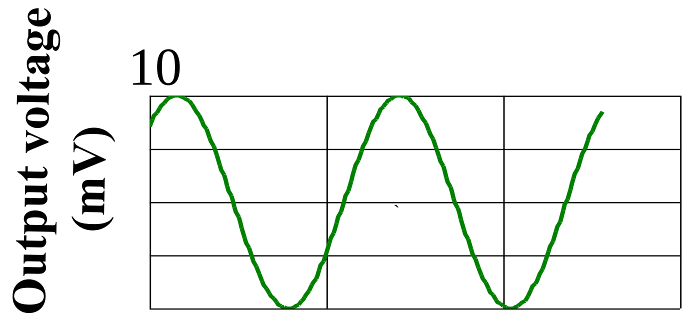
Most of the holes in the Emitter will be swept through the base without recombination, then across the junction 2 and into the collector



A small increase in input voltage produces a large increase in voltage across the load resistor $\rightarrow$ **a voltage signal is amplified**

The total current is controlled by the Emitter voltage





PROBLEM 21

In a transistor, the collector current I_C changes exponentially in function of the emitter voltage V_S according to:

$$I_C = I_0 e^{V_S / B}$$

where I_0 and B are constant for any given temperature.
A transistor has a collector current of 4.7 milliamperes when the emitter voltage is 17 mV. At 28 mV, the current is 27.5 milliamperes. Given that the emitter voltage is 39 mV, estimate the current

SOLUTION

$$\ln I_C = \ln I_0 + V_S / B \longrightarrow \ln 4.7 = \ln I_0 + 17 / B$$

$$\ln 27.5 = \ln I_0 + 28 / B$$

$$\longrightarrow \ln I_0 = -1.17, \;\; B = 6.25\, mV$$

At 39 mV: $\ln I_C = -1.17 + 39 / 6.25 = 5.07$

$$\longrightarrow I_C = 160\ milliamp$$