I| Introduction

- Element of quantum mechanics,
- energy Spectrum

1 Light

At the beginning of the 20^{th} century, light is known to be a wave.
(From the works of Huygens, Newton, Maxwell, Young, Fresnel)

The "wave theory" of light failed to explain the following experiments:

- Blackbody radiation
- the photoelectric effect.

a) Blackbody radiation [A.1.1]

Solid bodies emit a spectrum of radiation at all times. For a blackbody, the energy of this electromagnetic radiation (EM). depends directly on the temperature of the body.

- Classical mechanics fails to explain the energy spectrum of a blackbody.

* Planck explanation 1901 (Nobel 1918)

$\Rightarrow$ Electromagnetic energy can only be emitted in quantized form. (discrete energy values)

[A.1] $$\boxed{E_n = n h\nu \quad n = 0, 1, 2, \ldots}$$

ν is the frequency (Hz)

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

c = light velocity (m/s)

λ = wavelength (m)

$$\boxed{h = 6.62618 \times 10^{-34}\ \text{J.s} \quad \text{Planck constant}}$$

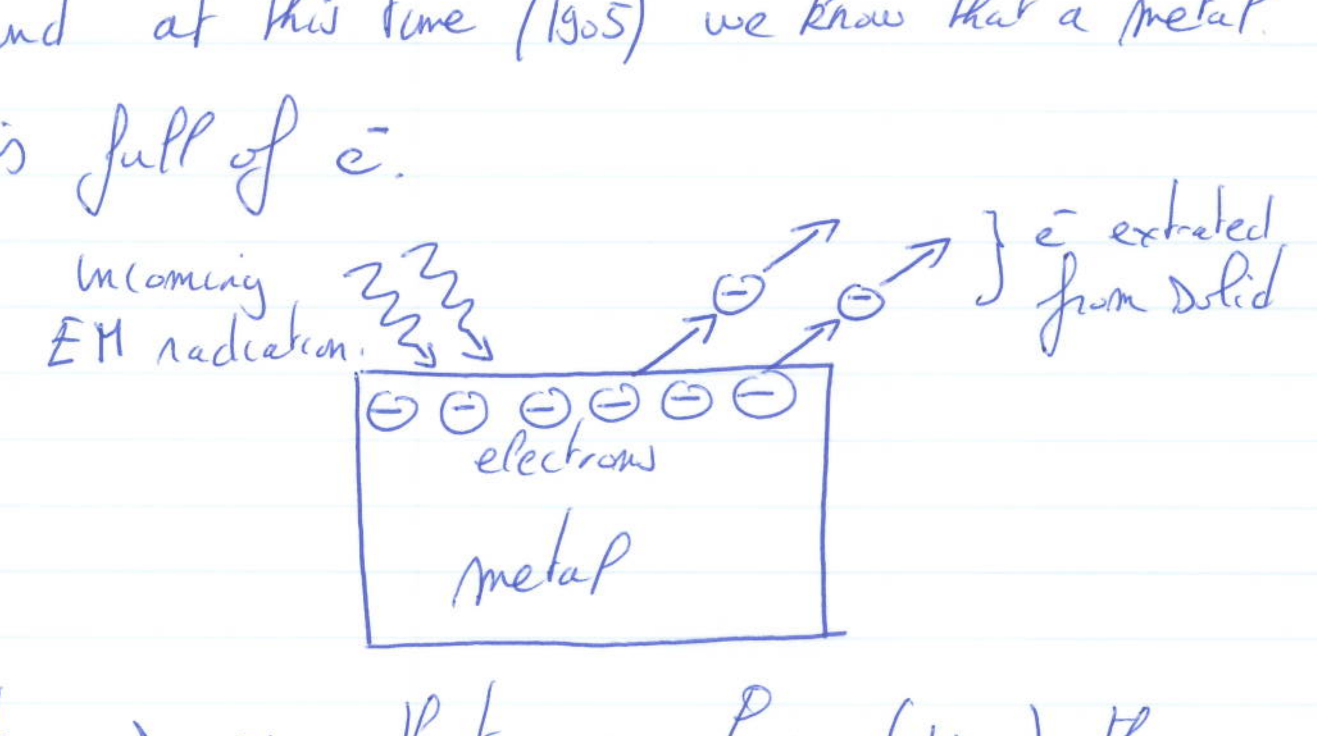
Energy is in Joules.

Important: Planck introduced the quantization of energy as a mathematical trick to explain (reproduce) the experiment.

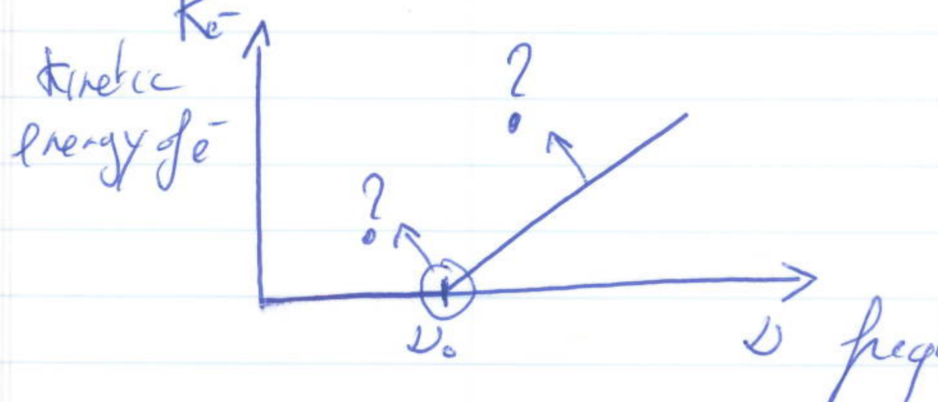
(b) Photoelectric effect

"hitting a metal with light to extract e^-"

e^- (electrons) are negatively charged particle, and at this time (1905) we know that a metal is full of e^-.



Experiment: Let us suppose that we change (vary) the frequency of the light, and we look at the kinetic energy of the e^- (extracted).



2 problems with classical mechanics

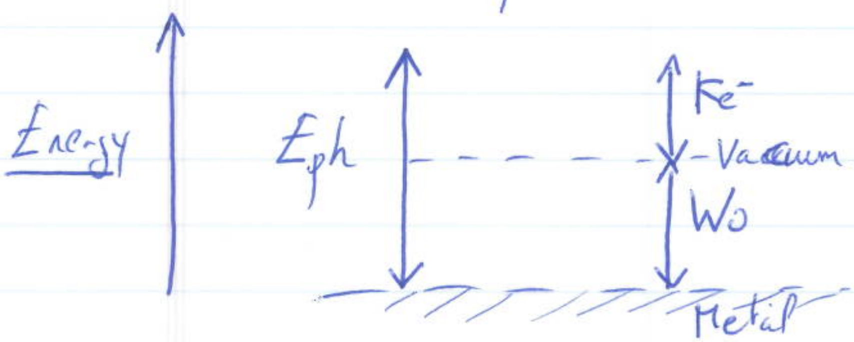
(i) in EM theory, the kinetic energy of e^- should be proportional to the intensity of the light and it should not depend on the frequency.

(ii) Nothing happens below a certain threshold ν_0.

* Einstein explanation (1905) (Nobel 1921)

$\Rightarrow$ $E = h\nu$ has a physical meaning, it is the energy of a 'light quanta', a particle that is called (later on) a "photon" $(E = E_{ph})$

$\Rightarrow$ photoelectric effect can then be explained using a <u>collision between 2 particles</u>: <u>photons and $\bar{e}$</u>.
we also consider a loss in energy $\Rightarrow$ inelastic collision process.



$$\boxed{E_{ph} = W_0 + K_{e^-}}$$

<u>Before collision.</u> | <u>After collision</u>

W_0 is called the work function, it is the energy that is required by $1\bar{e}$ to leave the metal (it is also a potential barrier).

we then obtain

$$E_{ph} = h\nu = W_0 + K_{e^-}$$

for $K_{e^-} = 0$ (no extraction) $\Rightarrow h\nu_0 = W_0$

$$\Rightarrow h\nu = h\nu_0 + K_{e^-}$$

$$\Rightarrow \boxed{K_{e^-} = h(\nu - \nu_0)}$$

that confirms the experimental data!

Conclusion $\Rightarrow$ light is both a wave and a particle!

(2) Electrons

e^- is known to be a particle.

Classical mechanics failed to explain the energy spectrum of EM radiation of an excited Hydrogen gas; which is discrete (?).

a) The Bohr Atom [A.1.2]

Let us ~~suppose~~ consider the Hydrogen atom and the "planetary model of the atom" by Rutherford.

$\Rightarrow$ $\bar{e}$ rotates around a positive charge center (nucleus) == 1 proton.

electrostatics potential between $1\bar{e}$, 1 proton is

$$\boxed{V(\vec{r}) = \frac{q}{4\pi\epsilon_0 r}}$$

- q = charge of the electron (absolute value) $1.602 \cdot 10^{-19}$ Coulomb.
- ϵ_0 vacuum permittivity.
- r distance from center to e^-

Energy potential is defined by:

$$\boxed{U(\vec{r}) = -qV(r)}$$

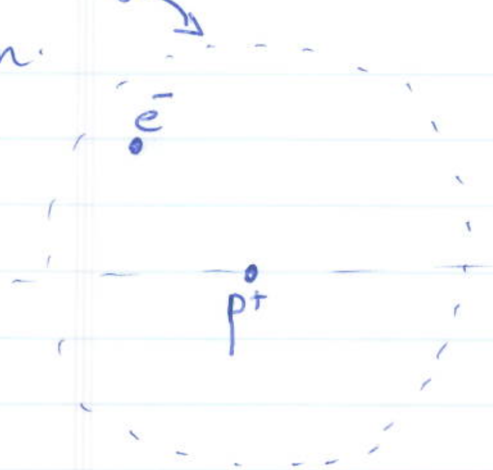
V is in Volt.
U is in Joule (International system)

In the class, we will express $U(r)$ in eV (electron Volt)

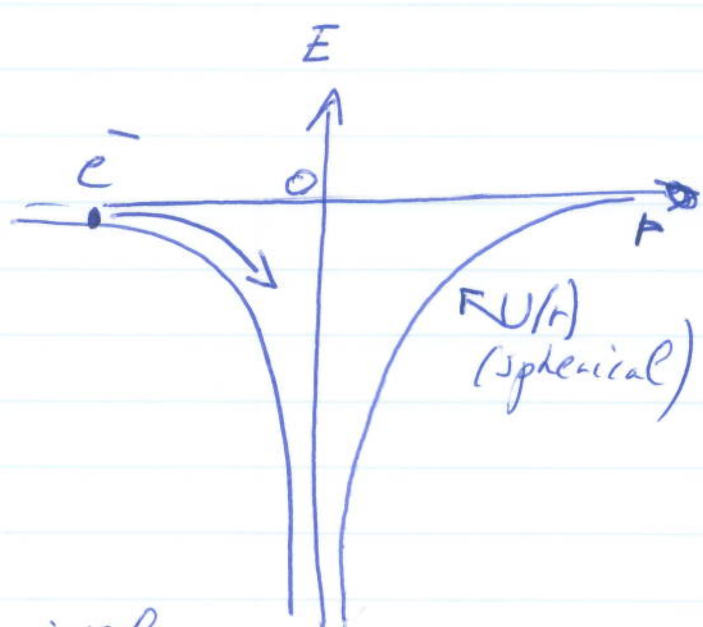
$$\boxed{1\,eV \Leftrightarrow q \text{ Joules}}$$

<u>Advice</u>: once you get the result in Joule, just divide by q to get in eV

outer shell of the atom.



Energy Spectrum

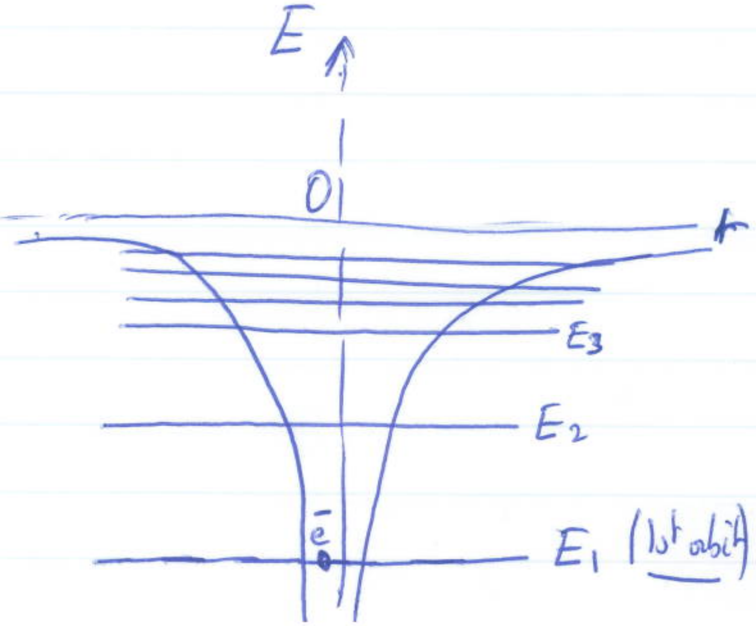


in classical mechanics, the e^- will fall into the nucleus. ⇒ Principle of minimization of the Energy.

* Bohr Solution (1913) (Nobel 1922).

orbits of the Hydrogen atom are quantized.

different quantized orbits.



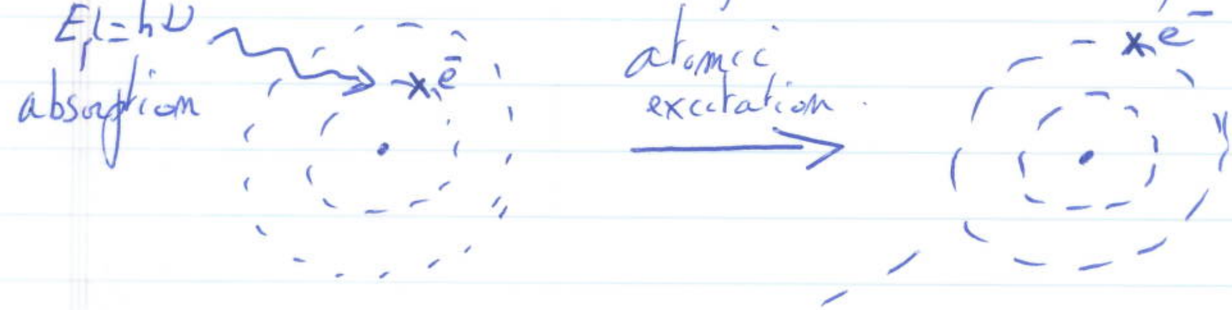
At equilibrium the e^- is at the first orbit we have $\boxed{E_n = -\dfrac{m q^4}{2(4\pi\epsilon_0 n \hbar)^2} = -\dfrac{13.6}{n^2}\ eV}$ [A.7] [2.1]

$\boxed{\hbar = \dfrac{h}{2\pi}}$

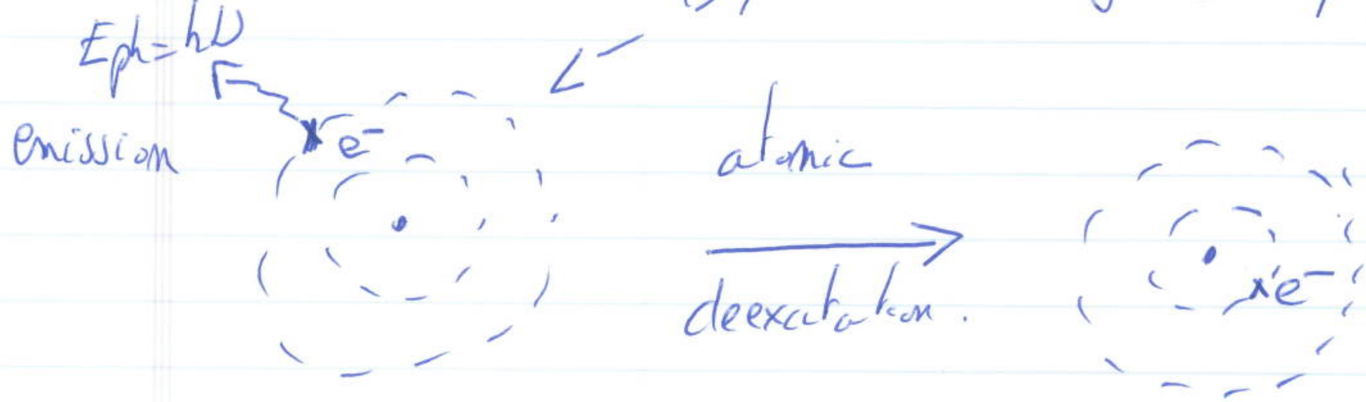
So the energy of the $\bar{e}$ in the 1^{st} orbit is $\underline{-13.6 eV}$.

* In order to explain the discrete energy spectrum of the Hydrogen gas, Bohr supposes that $\bar{e}$ can make transition between the orbits via

(i) excitation (by absorption of light-photon).



(ii) or deexcitation (by emission of light-photon)



All The transition between the energy levels are described in Figure [A.2]

The Bohr model has some problems:

- it works perfectly well for the Hydrogen atom but it does not provide a general framework for solving problem of this type.
- it leaves many unanswered questions, what happens to the fundamental electrostatic interaction between $\bar{e}$ and protons (2 particles) ?

[A.1.3] b) De-Broglie hypothesis (1924) Nobel 1929

	wave	particle.
light	Yes	Yes.
electron.	So why not?	Yes.

De-Broglie : Generalization of duality wave - particle for all form of matter (beyond light, ... not only electron).

"It was an assumption not based on experiments."

particle $\Longleftrightarrow$ wave.

momentum $\vec{p}$ $(\equiv m\vec{v})$ — wave vector $\vec{k}$ $\left(\equiv \frac{2\pi}{\lambda}\right)$

$$\boxed{\vec{p} = \hbar \vec{k}}$$

or $\boxed{p = \frac{h}{\lambda}}$ [A.8]

Ⓒ Consequences of duality wave $\Leftrightarrow$ particle

(i) All form of matter is a wave.

if λ is of the order of ($\sim$) the dimension of the displacement of the object, the wave nature of the object needs to be considered.

Classical mechanics (particle)	Quantum mechanics (wave)
$(\vec{r}, t)$	$\Psi(\vec{r}, t)$
$\vec{r}$: position, t: time	wave function (state)

Ψ has no physical meaning, only $|\Psi|^2 = \Psi\Psi^*$ has one. It is the probability to find the e^- in position $\vec{r}$ at time t.

(ii) we know that the total energy of a particle "object" is

$$\boxed{E = \underset{\text{kinetic}}{K} + \underset{\text{potential}}{U}}$$

Let us consider e^-. if $\underline{U = 0}$ the e^- is then a free e^-. (no potential energy, only kinetic energy).

$$E = \frac{p^2}{2m} \Longrightarrow \boxed{E = \frac{\hbar^2 k^2}{2m}}$$

classical mechanics — quantum physics.

General solution for Ψ

$$\boxed{\Psi(\vec{r},t) = e^{i\vec{k}.\vec{r}} e^{-i\omega t}}$$

the free $\bar{e}$ is a plane wave.

(iii) Let us suppose $U \neq 0$ and known.
For an arbitrary energy potential, the wave function and energy of the $\bar{e}$ are solution of the Schrödinger equation (1926 - Nobel 1933)

time dependent $\left\{ -\frac{\hbar^2}{2m}\Delta_{\vec{r}}\Psi + U\Psi = i\hbar\frac{\partial\Psi}{\partial t} \right.$ [A.9)

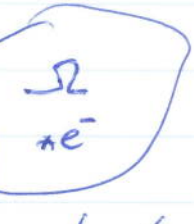
time independent $\left\{ \begin{array}{l} \Psi_{(\vec{r},t)} = \psi_{(\vec{r})}\, e^{-i\omega t} \\ \boxed{-\frac{\hbar^2}{2m}\Delta_{\vec{r}}\psi + U\psi = E\psi} \; * \end{array} \right.$

Solving (*) we get $\psi_{(\vec{r})}$ and E for any $U_{(\vec{r})}$.

(d) quantum effects

* confinement effects ("quantization")

Let us suppose that the $\bar{e}$ is confined in a region of the space Ω.

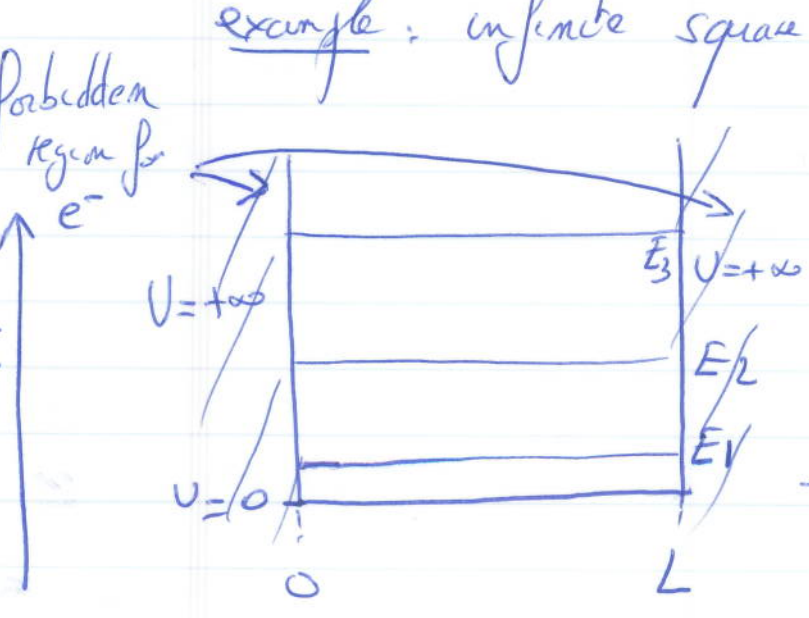


This means that one cannot find $\bar{e}$ outside Ω ($\Psi = 0$ outside Ω) where the potential energy is too big.

confinement effect

→ quantum mechanics (i.e. solving the Schrödinger equation) tell us that the $\bar{e}$ cannot take ~~only~~ any energy levels; only ~~a certain~~ some discrete energy are allowed.

example: infinite square well.



$$\boxed{E_n = \frac{n^2 \hbar^2 \pi^2}{2 m L^2}}$$

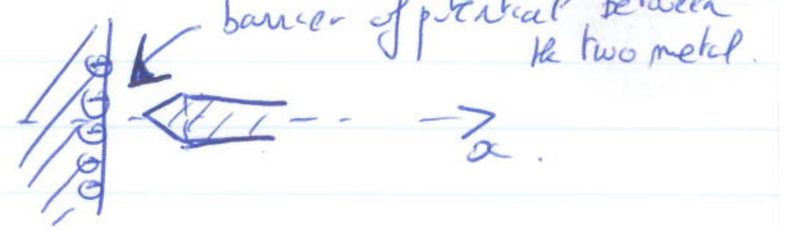
$$\boxed{\Psi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n \pi x}{L}\right)}$$

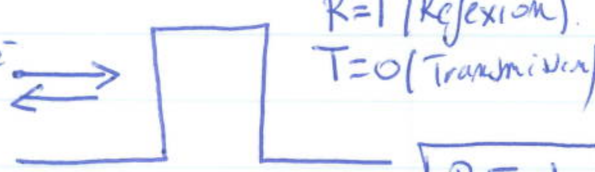
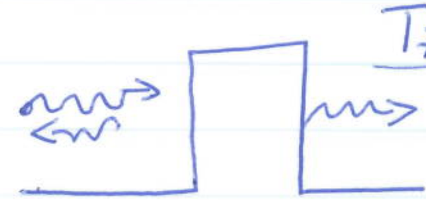
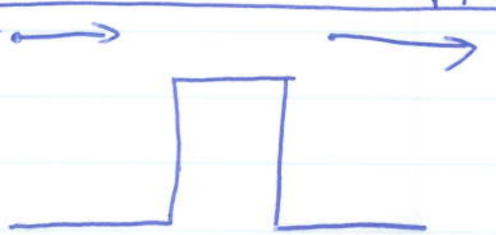
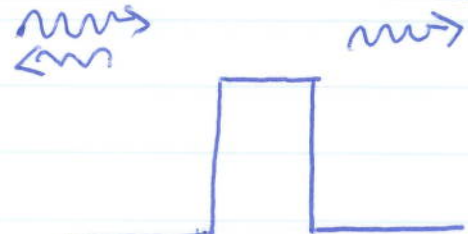
* tunneling and Interference effects

Let us suppose a barrier of potential

and e^- coming from the left.

For example, this barrier of potential can be created by having a metal tip very close to a metal surface full of e^-.



incoming $\bar{e}$ energy	Classical mechanics	Quantum mechanics
$E < U_0$	 R=1 (Reflexion). T=0 (Transmision) $\boxed{R+T=1}$	 $T \neq 0$! tunneling effect.
$E > U_0$	 R=0 T=1	 $R \neq 0$! interference effects.

II Semiconductors : Definitions

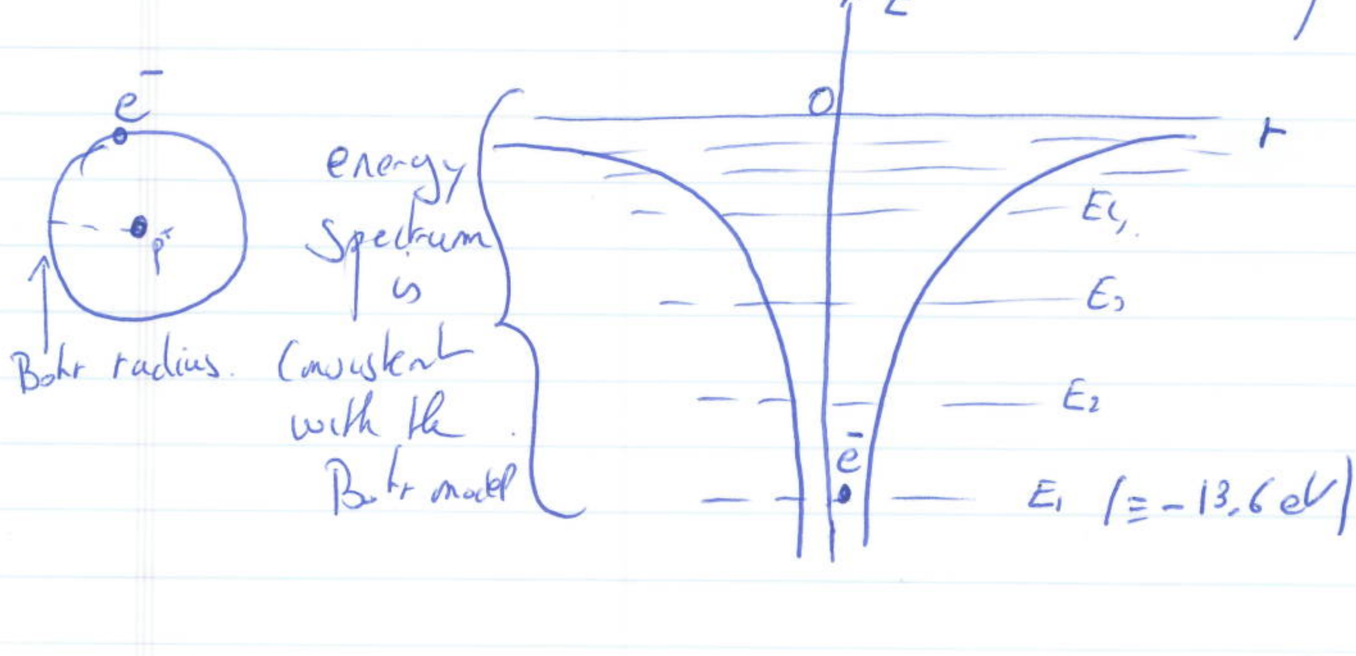
1 From one to many atoms

a) The Hydrogen atom ($1 e^-$) [Fig 2.1]

$$V(r) = \frac{q}{4\pi \epsilon_0 r} \qquad U(r) = -qV(r)$$

$U(r)$: energy potential "seen" by the e^-.

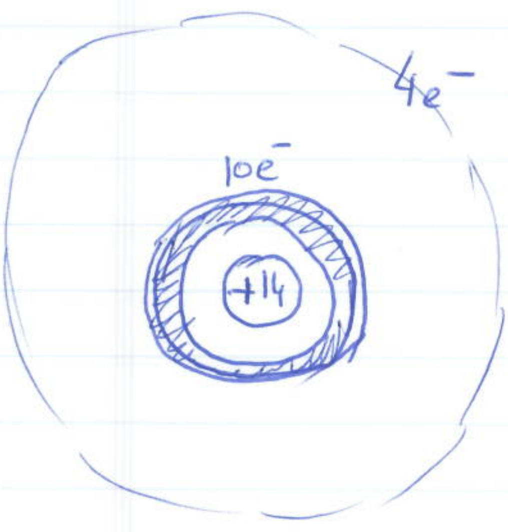
Since Ψ vanishes if $r \nearrow$ (increases), the e^- is confined and we get discrete energy levels (solving the Schrödinger equation)

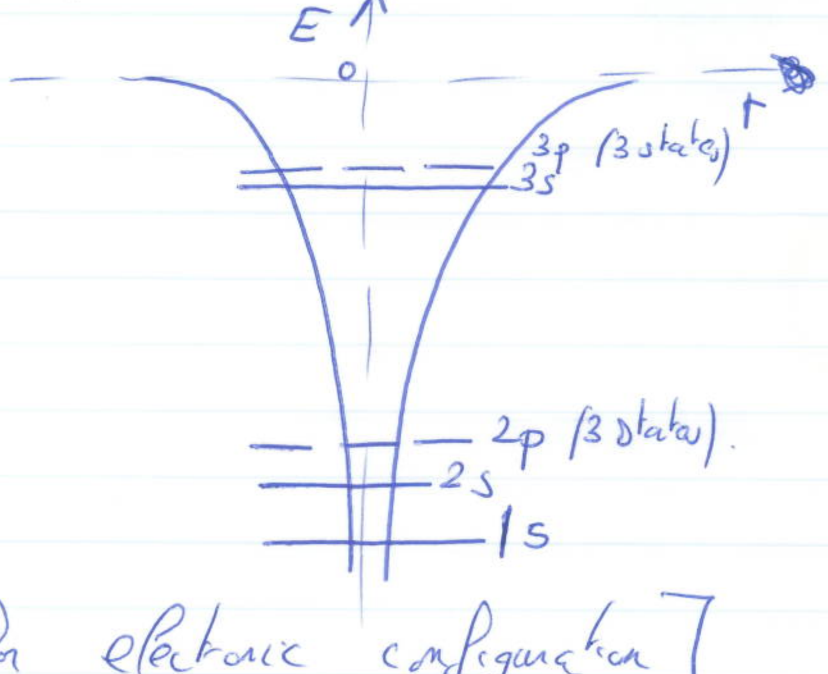


5 <u>The Silicon atom</u> (many e^-) [Fig 2.2] [A.3.2]

A Silicon atom Si is composed by $14e^-$ and then the charge of the nucleus is $+14q$.
(i.e. "14 times deeper" than the Hydrogen atom).

[we also get a discrete energy spectrum, ~~but~~ some energy levels can be degenerated, (i.e. many states for 1 energy).

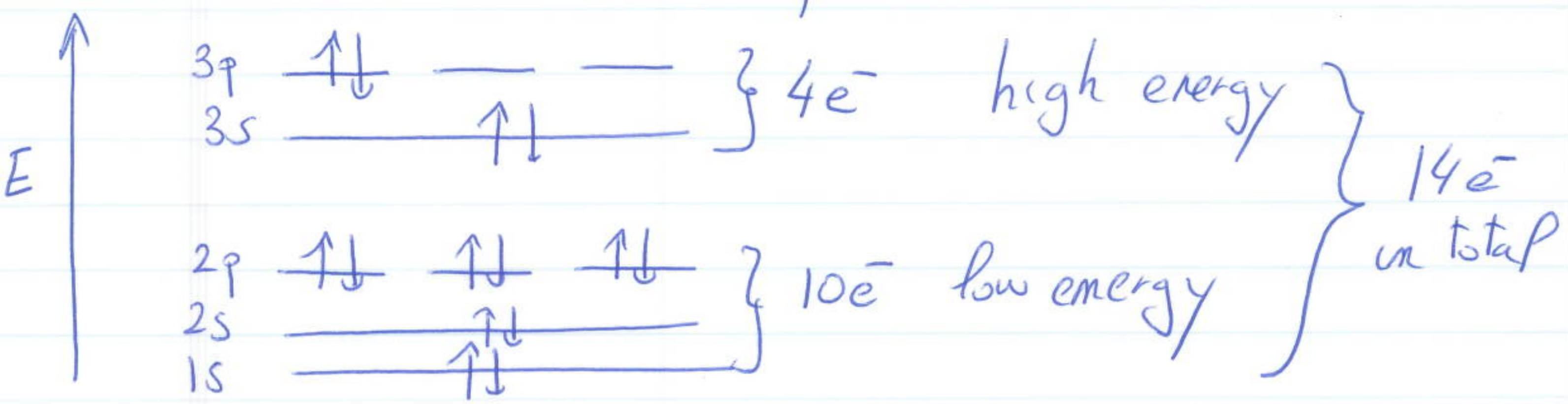




[See Table [A.3] for electronic configuration]

To fill up the energy state with e^-, we use the <u>Pauli exclusion principle</u> $\Rightarrow$ $2e^-$ with the same energy and spin cannot occupied the same state.

So maximum of $2\bar{e}$ per State ($\uparrow\downarrow$)

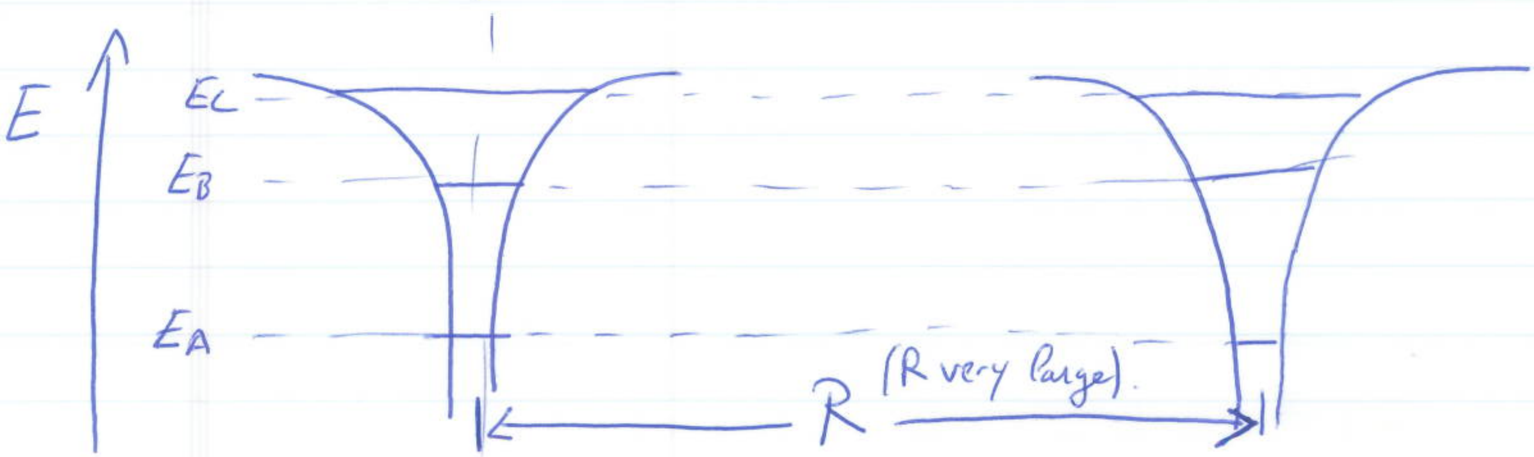


we say that Silicon has 10 core $\bar{e}$, 4 valence $\bar{e}$

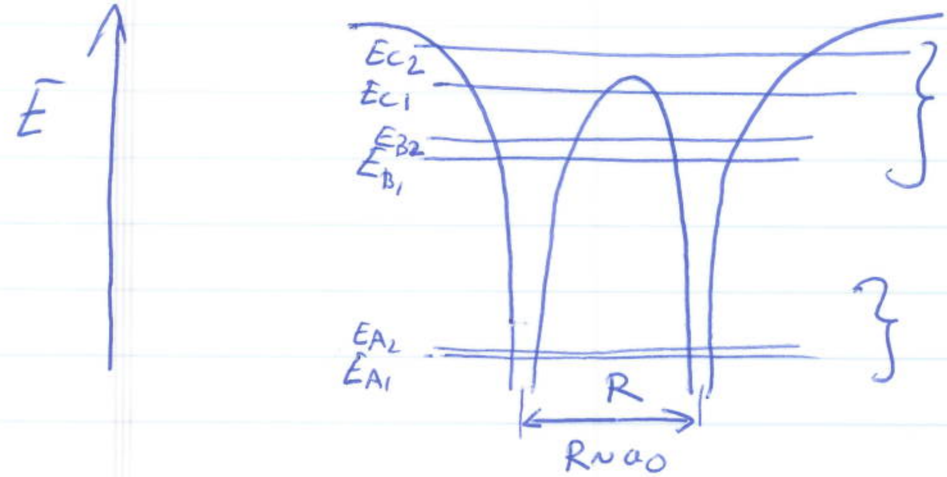
[$\bar{e}$ of valence : It is an $\bar{e}$ in an outer-shell of an atom that can participate in forming chemical bonds with other atoms

3 2 atoms system

Let us suppose 2 isolated atoms (hypothetical atoms).

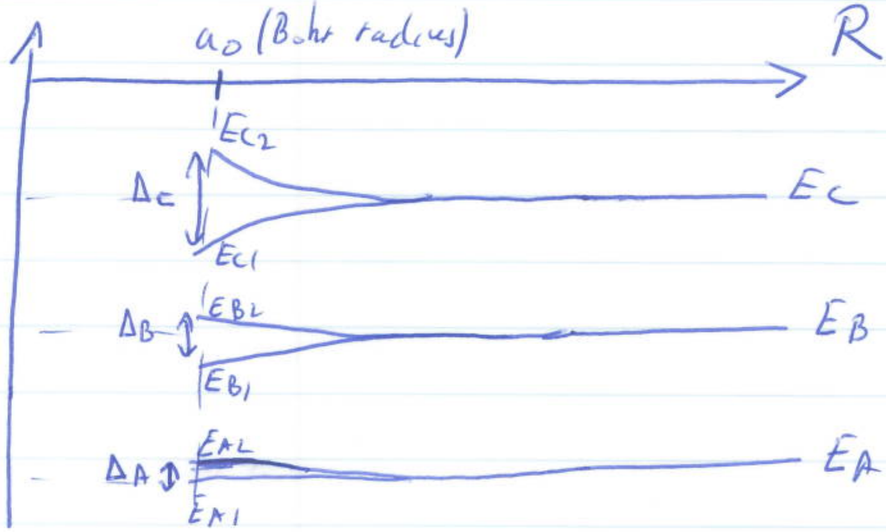


we bring these 2 atoms closer.



Because of tunneling and interference effects, the states are coupled.

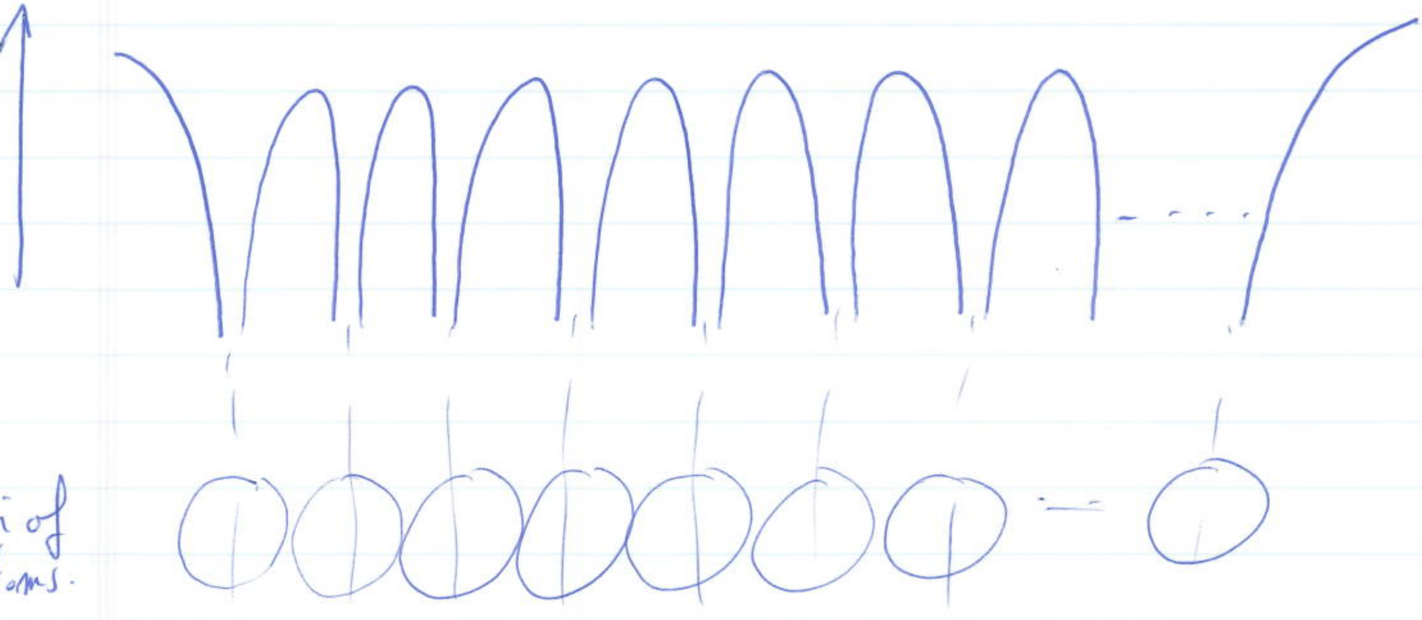
$\Rightarrow \begin{cases} \text{the energy } E_A \text{ is split between } E_A^1, E_A^2 \\ \quad '' \quad '' \quad E_B \quad '' \quad '' \quad E_B^1, E_B^2 \\ \quad '' \quad '' \quad E_C \quad '' \quad '' \quad E_C^1, E_C^2 \end{cases}$



[Distance Δ depends on the strength of the coupling.
[If Energy increases the coupling is stronger.

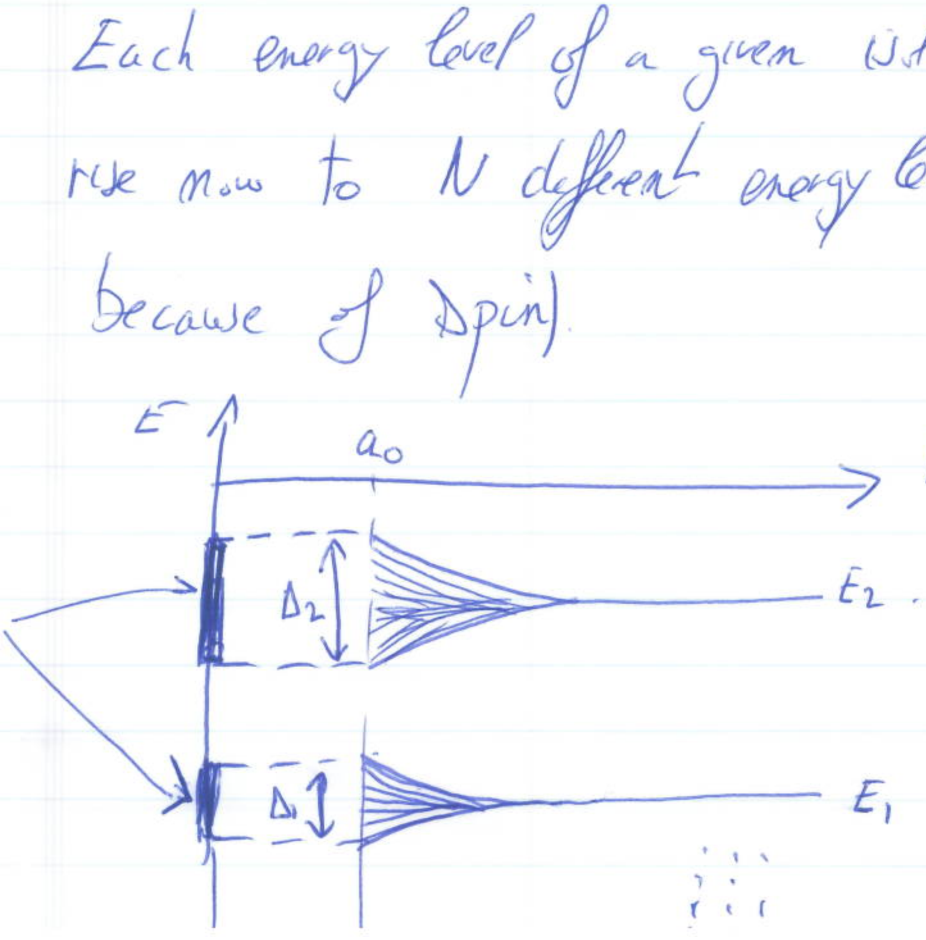
d) Many atoms system

Let us consider N atoms (chain of atoms).



Chain of atoms.

Each energy level of a given isolated atom gives rise now to N different energy levels (actually 2N because of spin).



if N is large, the energy levels are so close one another that they form a continuum $\Rightarrow$ band of energy

It appears some forbidden energy band between permitted energy band $\Rightarrow$ energy gap.

the $\bar{e}$ are still filling up the energy levels from the bottom (lowest energies) to the top (highest energies)