

# Course

20/9/2022

$$h = 6,6 \cdot 10^{-34} \text{ J} \cdot \text{s}$$

energy  $\times$  time is called  
"action" in engineering

$\lambda \rightarrow$  wave

## Planck Hypothesis

① quanta  $\rightarrow E_n = h \nu = h \frac{c}{\lambda} = 1 \text{ single quantum}$

absolute freq.

integer

② 10 quanta  $\rightarrow E_{beam} = 10 \times h \nu$

energy is discrete quantization

e.m. radiation = made by quanta = photons

Quantization values: | momentum | angular momentum  
| energy | velocity ...

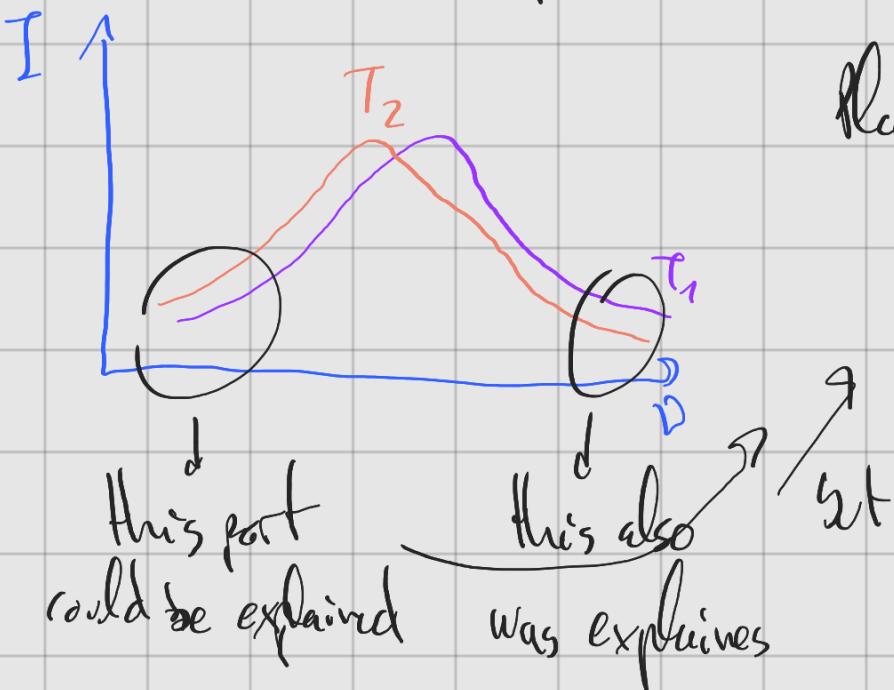
Planck's hypothesis leads to a 2 phenomena

① Photoelectric Effect

② Bohr Hydrogen Model

→ Black Body Radiation

from 1850 to 1900 there was no explanation  
for the shape of the plot



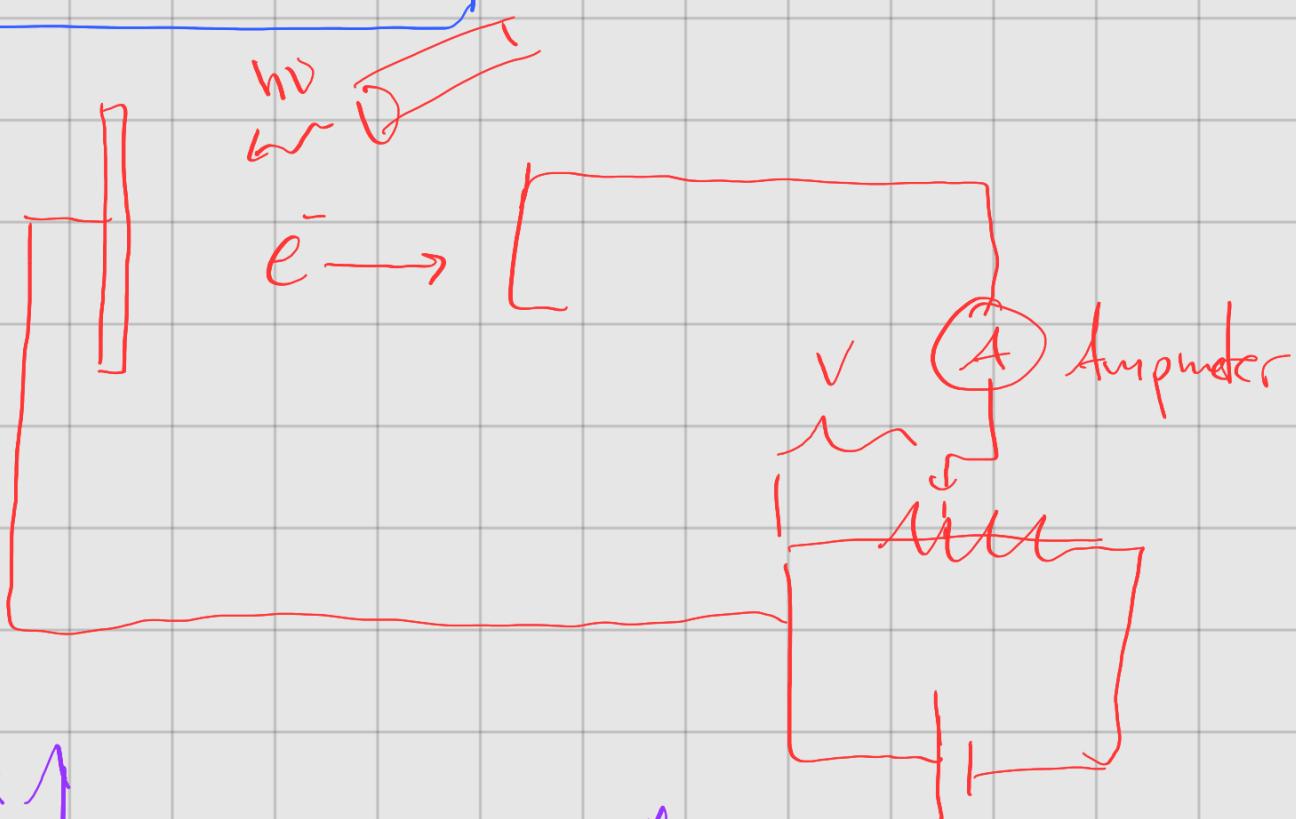
Planck's hypothesis  
gave the explanation  
for the full shape

→ Duality of light

Dual  $\rightarrow$  Wave: Maxwell  $\{\lambda, \nu\}$

$\rightarrow$  Particle: Planck  $\{ \text{photons} \}$

## Photoelectric Effect



$$I = \frac{q}{t}$$

1905 A. Einstein

1 quantum  $\rightarrow 1 e^-$   
approximation

Before of the impact of the light on the metal we only have the light ( $E = h\nu$ )

Energy balance:

$$h\nu = E_k + \Phi$$

a single photon energy ↗  
a single  $e^-$  kinetic energy of  
a single  $e^-$

↳ the potential energy we need to extract the  $e^-$  from the metal (work function) → material dependent parameter.

$$E_k = h\nu - \Phi$$

Since kinetic energy can't be negative:

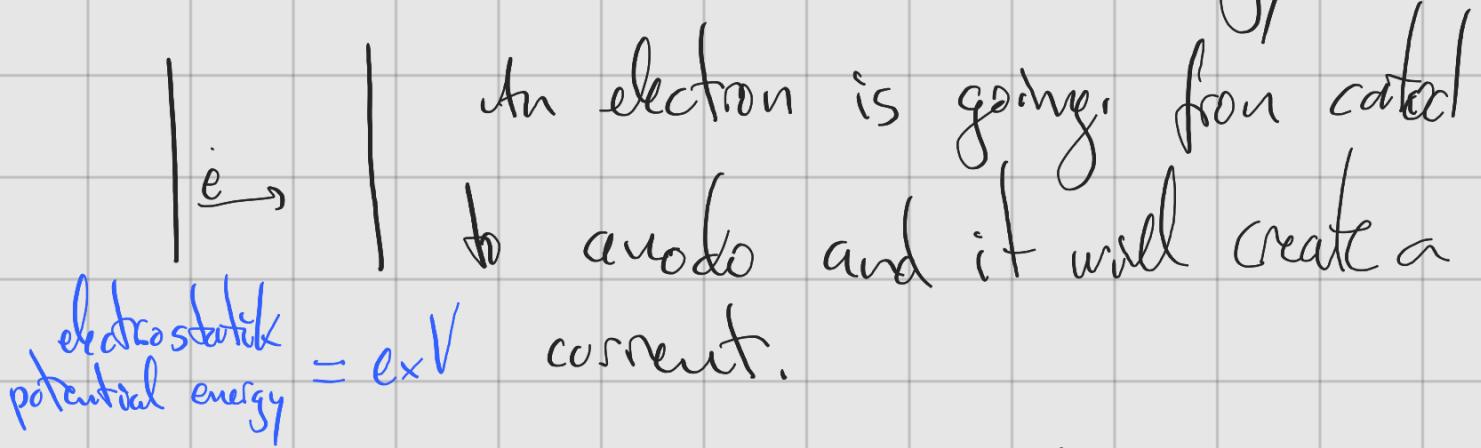
$$h\nu - \Phi \geq 0$$

$$h\nu \geq \Phi$$

$$\nu \geq \frac{\Phi}{h} = \nu_{th}$$

There is a threshold freq

To measure the kinetic energy



If we charge negatively the right side it will make the  $e^-$  stop eventually.

When there is an energy that makes  $e^-$  stop there will be no more current. At that point  $eV_{stop} = E_k$

That's how we calculate kinetic energy

→ Now:

We have

$$J = 2 \text{ A/m}^2 \rightarrow 2 \cdot \frac{S}{S} \cdot \frac{1}{\text{m}^2}$$

$$\lambda = 250 \text{ nm}$$

If I want to know the flux

$$\text{flux} = \frac{\text{n}^{\circ} \text{ part}}{A \cdot t} \Rightarrow \frac{I}{h\nu}$$

→ If  $\lambda = 250 \text{ nm}$

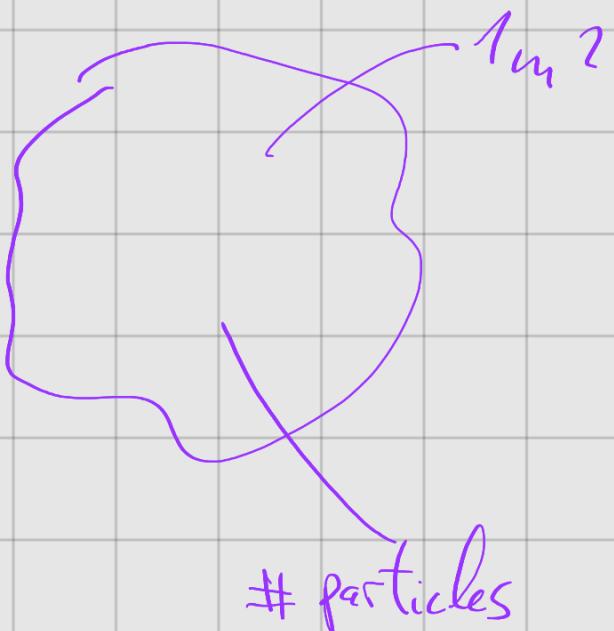
$$E = h\nu = \frac{hc}{\lambda} = \frac{12,4 \cdot 10^3 \text{ eV A}^0}{250 \text{ nm}} \approx 5 \text{ eV}$$

$$\frac{2J}{m^2 s} \cdot \frac{1}{E} = \frac{2J}{m^2 s} \cdot \frac{1}{h\nu} = \frac{\# \text{ part.}}{m^2 s} =$$

$$= \frac{2J}{5 \text{ eV}} \frac{1}{m^2 s} = \frac{2J}{5 \times 1,6 \cdot 10^{-19} \text{ J m}^2 \text{ s}} \approx 10^{18}$$

How many photons?  
 $1 \text{ m}^2$     $1 \text{ sec}$

total energy  
energy of a single quantum



## Review

\* Fotoelectric effect equation:

$$E_k = h\nu - \Phi$$

\* Threshold frequency:  $h\nu = \Phi \Rightarrow \nu_{th} = \frac{\Phi}{h}$

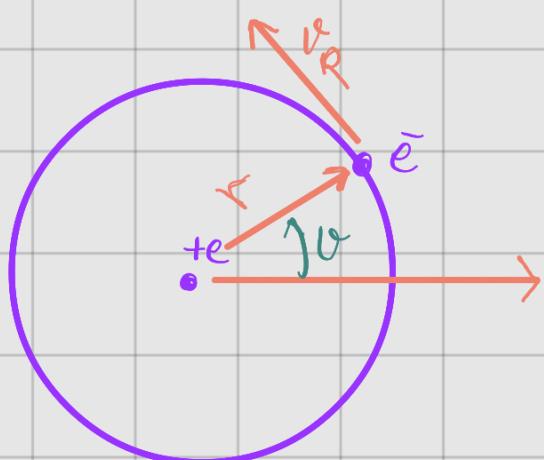


\* Measure the kinetic energy:

$$E_k = eV_{stop}$$

21/9/2022

# Bohr's Model A



Angular momentum:  $\vec{L} = \vec{r} \times \vec{p}$

In model A:

$$\vec{L} = rmv_r \hat{\theta} \quad \begin{matrix} \text{pointing out} \\ \text{of circle:} \end{matrix}$$

$$\vec{L} = L_0 \hat{\theta}$$



Bohr's hypothesis

$$\int_G L_0 d\theta = h n$$

line integral

$$L_0 = \frac{h n}{2\pi} = h n$$

$$\int_G L_0 d\theta = L_0 \int_G d\theta = L_0 2\pi$$

$$\Rightarrow L_0 = nh$$

The angular momentum is quantized

# 1

## Force Balance

$$m \frac{V_R^2}{r} = \frac{e^2}{r^2} \Rightarrow \frac{L_0^2}{mr^3} = \frac{e^2}{r^2} \Rightarrow r = \frac{L_0^2}{me^2} = \frac{\hbar^2 n^2}{me^2}$$

centrifugal  
Coulomb

fundamental  
constants  
 $\approx 0.51^\circ$

$$\Rightarrow r = \zeta n^2$$



The radius of the orbits are quantized. Discrete orbits

$$\begin{aligned} r_1 &= r_0 \\ r_2 &= 4r_0 \\ r_3 &= 9r_0 \end{aligned}$$

## 2 Velocity

$$V_R = \frac{L_0}{mr} = \frac{1}{mr} \cdot \frac{\hbar n}{\frac{\hbar^2}{me^2} n^2} = \frac{e^2}{\hbar} \cdot \frac{1}{n} \quad V_R = \alpha c \frac{1}{n}$$

$$n=1 \rightarrow V_{R,1} = \frac{e^2}{\hbar c} \cdot c = \alpha c$$

$$\text{fine structure constant} = \frac{1}{137}$$

Velocity is quantized

(3)

## Energy

$$E = \frac{1}{2}mv_R^2 - \frac{e^2}{r} = \frac{1}{2}m \left[ \frac{e^2}{\hbar} \frac{1}{n} \right]^2 - \frac{e^2}{\hbar^2 n^2} me^2 =$$

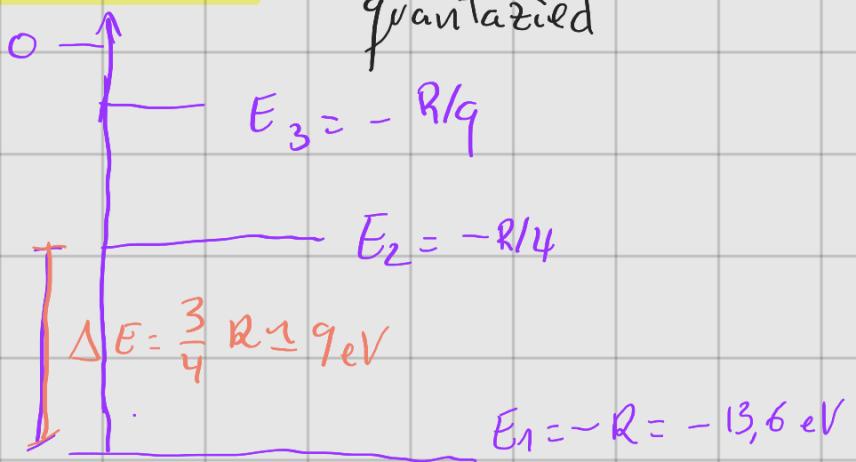
$$= \frac{1}{2}m \frac{e^4}{\hbar^2} \frac{1}{n^2} - \frac{me^4}{\hbar^2} \frac{1}{n^2} = \frac{1}{n^2} \left[ -\frac{1}{2}m \frac{e^4}{\hbar^2} \right] = -\frac{R}{n^2}$$

$E_n = -\frac{R}{n^2}$

Energy is quantized

$$R = \frac{me^4}{2\hbar^2} = R_{\text{Rydberg constant}}$$

$$R = 13,6 \text{ eV}$$



Doing the difference between  $E_1$  and  $E_2$ :

$$\Delta E = E_2 - E_1 = h\nu_{21} \rightarrow \nu_{21} = \frac{E_2 - E_1}{h} = \frac{9 \cdot 1.9 \cdot 10^{-19}}{6.6 \cdot 10^{-34} \text{ J} \cdot \text{s}}$$

and it's the exact freq. of the photon after extracting it

## •) Planck

$$E = h\nu = \hbar\omega$$

## •) Photoelectric effect

$$V_{th} = \Phi/h$$

$$h\nu = E_k + \Phi$$

$$\hookrightarrow E_k = eV_{stop}$$

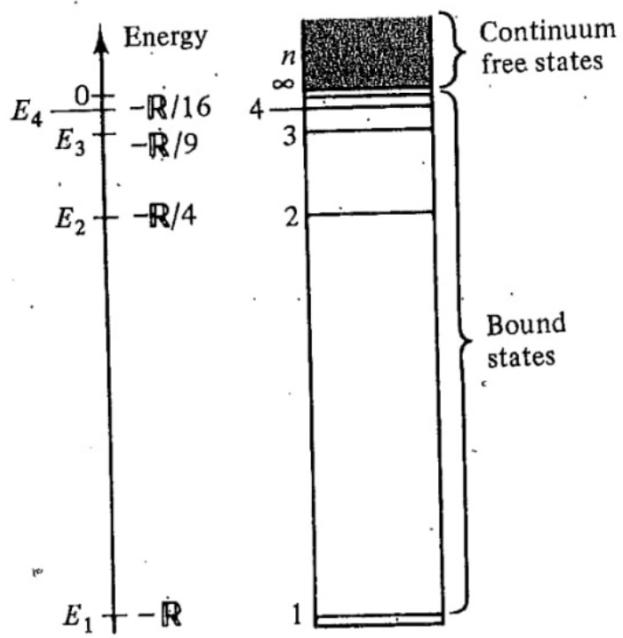
## •) Bohr's Atom

$$f_n = f_0 n^2, n = 1, 2, 3, \dots$$

$$V_{An} = \alpha c \frac{1}{n}, \alpha = \frac{1}{137}$$

$$E_n = -\frac{R}{n^2}, R = 13.6 \text{ eV}$$

\* We use these results for the Hydrogen



If we are not at  $E_1$  (i.e.  $E_2$ ), we cannot stay there forever. There is a limited time we can stay at that other level.

The time we can stay:  $\tau$ : lifetime

$$\begin{aligned} n=2 & \xrightarrow{\text{emit } h\nu_{21}} \lambda_{21} = E_2 - E_1 = h\nu_{21} = \frac{hc}{\lambda_{21}} \\ n=1 & \\ \rightarrow \lambda_{21} &= \frac{hc}{-\frac{1}{4} + R} = \frac{12.41 \cdot 10^3 \text{ eV} \cdot \text{\AA}}{3/4 \cdot 13.6 \text{ eV}} \\ \Rightarrow \lambda_{21} &= 0.12 \mu\text{m} \end{aligned}$$

Each decay level corresponds to a series for  $\lambda_{32}, \lambda_{41}$  and so on....

Balmer formula:  $\frac{1}{\lambda} = R \left( \frac{1}{n^2} - \frac{1}{m^2} \right)$ ,  $R$ : Rydberg constant =  $1,097 \cdot 10^7 \text{ m}^{-1}$

$n=1 \rightarrow$  Lyman,  $n=2 \rightarrow$  Balmer,  $n=3 \rightarrow$  Paschen

We can see that the potential is negative, therefore the  $e^-$  is attracted to the nucleus

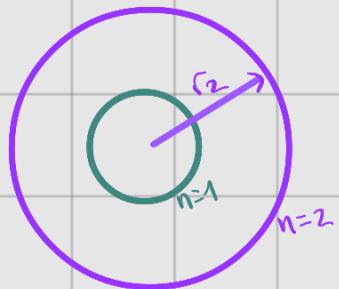
As the energy level increases the energy required is less until the  $e^-$  is free and is

not longer bounded to the proton.

The energy required to release the  $e^-$  from the atom is: 13.6 eV

Now we are going to calculate how long it will take to the  $e^-$  to fall from  $E_2$  to  $E_1$  (fund. state).

$$T_{21} = 10^{-8} \text{ sec}$$



$$\left. \begin{aligned} v_2 &= \alpha c \frac{1}{n=2} = \alpha c \frac{1}{2} \\ r_2 &= r_0 (n=2)^2 = 4r_0 \end{aligned} \right\} \quad \begin{aligned} \omega_2 &= \frac{v_2}{r_2} \\ \text{angular velocity: } v &= \omega r \end{aligned}$$

$\omega_2$  or better to call  $\omega_{21}$  will be related to the period we spend in  $E_2$

$$\omega_{21} \cdot T_{21} = 2\pi \rightarrow T_{21} = \frac{2\pi}{\omega_{21}} = \frac{r_2 \cdot 2\pi}{v_2} = \frac{4r_0 \cdot 2\pi \cdot 2}{\alpha c} = 1.15 \cdot 10^{-15} \text{ sec}$$

$T_{21}$  is the time an  $e^-$  expend doing a rotation. Thus, to decay it

will need:  $N = \frac{T_{21}}{T_{21}} = \frac{10^{-8} \text{ sec}}{1.15 \cdot 10^{-15} \text{ sec/rotation}} \approx 10^7 \text{ sec}$  to decay

# Wave Nature of Matter

Planck stated that the energy of one photon is:  $E = h\nu$

The kinetic energy is:  $E = \frac{1}{2}mv^2 = \frac{p^2}{2m}$

Now, we want to find the momentum of a single photon. According to Newton the momentum would be zero because photon has no matter. But, according to Einstein and relativity we know that:

$$E^2 = E_0^2 + (pc)^2$$

$E \rightarrow$  total energy,  $E_0 \rightarrow$  rest energy

$E_0 = m_0 c^2 \rightarrow$  In the case of photon:  $m_0 = 0 \Rightarrow E_0 = 0$

Therefore,  $E^2 = (pc)^2 \Rightarrow p = \frac{E}{c} = \frac{h\nu}{c} = \frac{h}{\lambda}$

Momentum of a single photon:

$$p = \frac{h}{\lambda} \quad p = \hbar k \quad k = \frac{2\pi}{\lambda} \text{ wavenumber}$$

We saw the corpuscular nature of light, is there a wave nature of particles?

$\Rightarrow$  De Broglie.

EM radiation has a dual particle-wave nature. De Broglie stated that matter has a dual particle-wave nature also.

$$\lambda_{DB} = \frac{h}{p} = \frac{h}{m \cdot v}$$

a) Wavelength of a ball

$$m = 0,01 \text{ kg} > \lambda_{DB} = \frac{h}{m \cdot v} \approx 6,6 \cdot 10^{-33} \text{ m}$$
$$v = 10 \text{ m/s}$$

$$\Rightarrow \lambda_{DB, \text{Ball}} \approx 0$$

b) Wavelength of a neutron

$$E = 0,05 \text{ eV/neutron} \rightarrow \lambda_{DB} = \frac{h}{p} = \frac{h}{\frac{1}{2m} E} \approx 1,28 \cdot 10^{-10} \text{ m}$$

$$\lambda_{DB, \text{Neutron}} \approx 1,28 \cdot 10^{-10} \text{ m}$$

Conclusions: Massive objects have no wavelength or it is so small we can never measure it. But particles have a measurable wavelength

We use this for electronical microscopes. For instance, if the object is  $d = 2.5 \text{ \AA}$

$$E = h\nu \approx \frac{hc}{\lambda} = \frac{12.4 \cdot 10^3 \text{ eV \AA}^{-1}}{2.5 \text{ \AA}} \approx 5 \text{ keV}$$

?

$$\text{Used wavelength: } \lambda_{DB} = \frac{h}{\sqrt{2mE_k}} \Rightarrow E_k = \frac{h^2}{\lambda_{DB}^2 \cdot 2m_e} = 24.2 \text{ eV}$$

$\hookrightarrow 2.5 \text{ \AA}$

We need to use way way less energy and if we want to see objects with different sizes we just need to change the energy

a) Example: We want to create an  $e^-$  with de Broglie wavelength  $\lambda_{DB} = 1 \text{ \AA}$   
how fast should we accelerate it.

$$E_k = \frac{1}{2} m v^2 = \frac{1}{2} \frac{p^2}{m} = \frac{1}{2m} \left( \frac{h}{\lambda_{DB}} \right)^2 \approx 150 \text{ eV}$$

How do we give such an energy to an  $e^-$ ? We know that a given electrostatic energy is required to cause this, a plate such that it imparts this energy

$$e \cdot V = E_k \Rightarrow \text{Voltage} = \frac{E_k}{e \text{ charge}} , \quad eV = 1.6 \cdot 10^{-19} \text{ Coulomb}$$

$$V = \frac{E_k}{[e^-]} = \frac{150 \text{ eV} \cdot 1.6 \cdot 10^{-19} \text{ J/eV}}{1.6} = 150 \text{ J/C} = 150 \text{ volt}$$

This shows that is very easy to have a de Broglie wavelength very small with particles with a very low energy

For free particles:

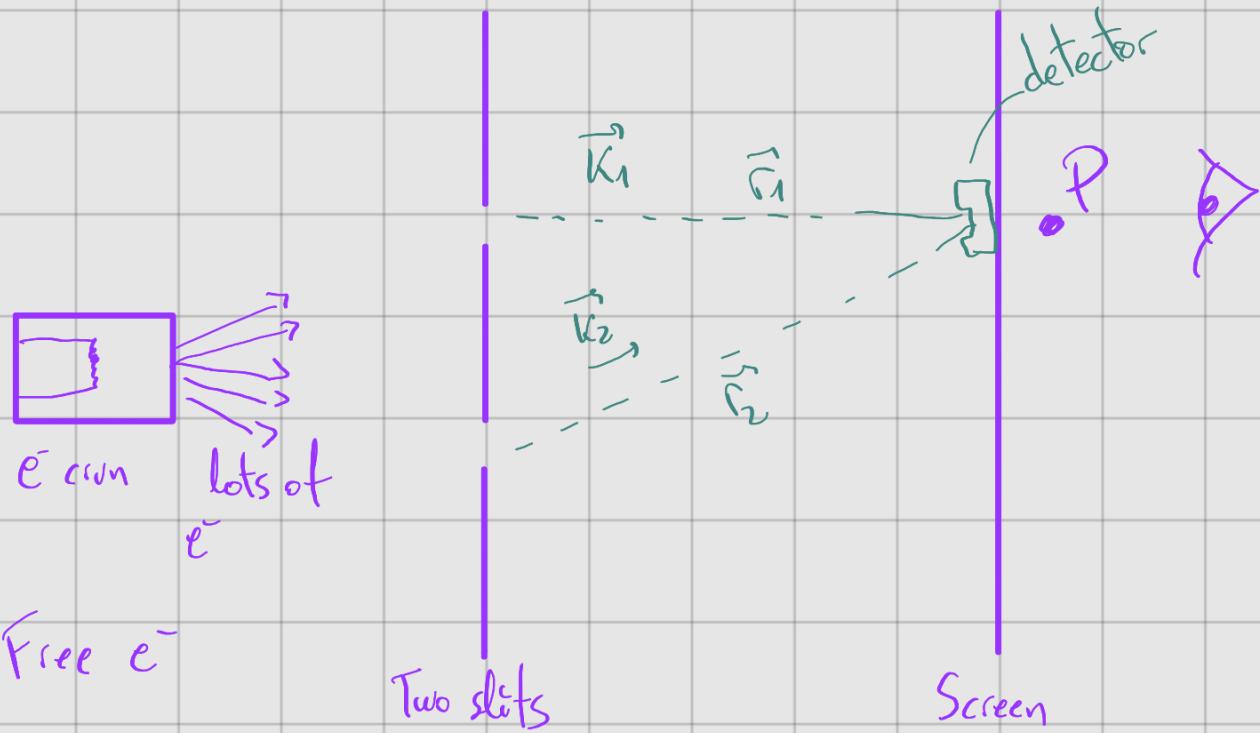
$$E_k = \frac{p^2}{2m}$$

$$\lambda_{DB} = \frac{h}{p}$$

$$\boxed{\lambda_{DB} = \frac{h}{\sqrt{2m E_k}}}$$

# Particle Interference

Let's see what happens with the double slit experiment using  $e^-$ .



The  $e^-$  being fixed are free  $e^-$  described by plane waves:

$$A \cdot e^{i\vec{k} \cdot \vec{r}}, \quad \vec{R} = \vec{k}_{DB} = k_{DB} \hat{\vec{k}} = \frac{2\pi}{\lambda_{DB}} \hat{\vec{k}}, \quad \vec{k}_{DB} \text{ is } \perp \text{ to the screen and slits}$$

L vector (unit vector)

At point P we observe any  $e^-$  that hit the screen. As the  $e^-$  travel, they will eventually hit the slits and on the other side will be described by two equations:  $A_1 e^{i\vec{k}_1 \cdot \vec{r}_1}$ ,  $A_2 e^{i\vec{k}_2 \cdot \vec{r}_2}$

The result we will observe at the screen will be the superposition of these two equations:  $A_1 e^{i\vec{k}_1 \cdot \vec{r}_1} + A_2 e^{i\vec{k}_2 \cdot \vec{r}_2}$

We can measure the intensity:  $|A_1 e^{i\vec{k}_1 \cdot \vec{r}_1} + A_2 e^{i\vec{k}_2 \cdot \vec{r}_2}|^2 = \text{Intensity at P}$

If the slits are exactly the same  $\rightarrow A_1 = A_2$

$$I_p = |A|^2 \left| e^{i\vec{k}_1 \cdot \vec{r}_1} + e^{i\vec{k}_2 \cdot \vec{r}_2} \right|^2$$

Another approx. the screen is far enough from the slits and the two slits are close enough to each other  $\Rightarrow \vec{k}_1 \approx \vec{k}_2 \approx \vec{k}$

$$I_p = |A|^2 \left| e^{i\vec{k} \cdot \vec{r}_1} + e^{i\vec{k} \cdot \vec{r}_2} \right|^2 = 2|A|^2 \left[ 1 + \cos[\vec{k} \cdot (\vec{r}_1 - \vec{r}_2)] \right]$$

We can get max. and mins.

$$\hookrightarrow I_p \text{ max} = 4|A|^2 \text{ when } \vec{k} \cdot (\vec{r}_1 - \vec{r}_2) = 2n\pi, n = 0, 1, 2, \dots \text{ (even)}$$

$$\hookrightarrow I_p \text{ min} = 0 \text{ when } \vec{k} \cdot (\vec{r}_1 - \vec{r}_2) = (2n+1)\pi, n = 0, 1, 2, \dots \text{ (odd)}$$

what we have to see is the phase difference

$$\vec{k} \cdot (\vec{r}_1 - \vec{r}_2) = \vec{k} \cdot \vec{d} = k \cdot d \cdot \cos\left[\frac{\pi}{2} - \theta\right] = kd \sin\theta$$

$$\hookrightarrow \text{max: } 2n\pi, k = \frac{2\pi}{\lambda_{DB}} \Rightarrow \frac{2\pi}{\lambda_{DB}} d \sin\theta = 2n\pi \Rightarrow n\lambda_{DB} = d \sin\theta_n$$

$$\hookrightarrow \text{min: } (2n+1)\pi, k = \frac{2\pi}{\lambda_{DB}} \Rightarrow \left(n + \frac{1}{2}\right)\lambda_{DB} = d \sin\theta_n$$

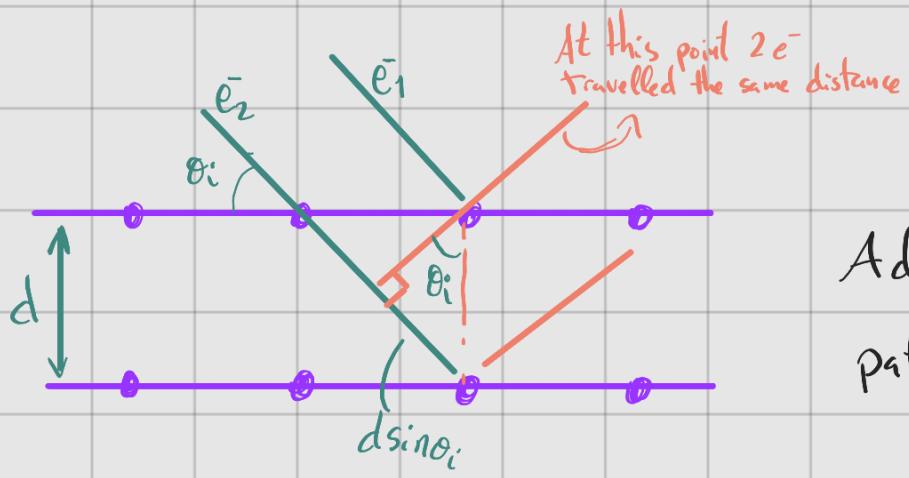
Finally we obtain:

$$\text{Constructive interference} \xrightarrow{\text{Max}} d \sin\theta_n = n \lambda_{DB}$$

$$\text{Destructive interference} \xrightarrow{\text{Min}} d \sin\theta_n = \left(n + \frac{1}{2}\right) \lambda_{DB}$$

# Diffraction

The diffraction of light can be described by a reflective grating



Adding both sides of the extra path (optical path difference)  
 $2 d \sin \theta$

To see the maximum of interference at the output we can use previous results.

$$k \cdot 2d \sin \theta_i = 2\pi n \rightarrow \frac{2\pi}{\lambda} 2d \sin \theta_i = 2\pi n$$

$$2d \sin \theta_i = n \lambda_{DB}$$

$d \rightarrow$  separation of planes known as bragg planes

$n \rightarrow$  diffraction order

There is a relationship between diffraction order  $n$  and angle of incidence  $\theta_i$ .

If we fix  $d$  and  $\theta$  there will instead have a relation between  $n$  and  $\lambda_{DB}$ . Thus, we only need to fix  $\lambda_{DB}$  to see different diffraction orders

# Schrödinger Equation

$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}, t) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}, t) \right] \Psi(\vec{r}, t)$$

$\Psi(\vec{r}, t)$ : wavefunction  $\rightarrow$  quantum state

$V(\vec{r}, t)$ : potential

$\hookrightarrow$  If it doesn't depend on time

$$V(\vec{r}, t) = V(\vec{r}) \rightarrow \text{conservative}$$

When the potential is non time dependent we can split:

$$\Psi(\vec{r}, t) = \underbrace{\Psi(\vec{r})}_{\substack{\text{wavefunc.} \\ \hookrightarrow \text{eigenfunc.}}} e^{-i\frac{E}{\hbar}t}$$

$$\boxed{\nabla^2 \Psi(\vec{r}) + \frac{2m}{\hbar^2} (E - V(\vec{r})) \Psi(\vec{r}) = 0}$$

S.E.  
stationary  
states

$$\underbrace{\left\{ E, \Psi_E(\vec{r}) \right\}}_{\substack{\text{Energy} \\ \Psi_E(\vec{r}) \rightarrow E}}$$

$$\sum_{E \in S} C_E \Psi_E(\vec{r}) e^{-i\frac{E}{\hbar}t} = \Psi(\vec{r}, t)$$

Most general solution

$$\text{If we have two solutions } \begin{cases} E_1, \Psi_{E_1}(\vec{r}) \\ E_2, \Psi_{E_2}(\vec{r}) \end{cases} \Rightarrow \Psi(\vec{r}, t) = C_1 \Psi_{E_1}(\vec{r}) e^{-i\frac{E_1}{\hbar}t} + C_2 \Psi_{E_2}(\vec{r}) e^{-i\frac{E_2}{\hbar}t}$$

superposition

## eigenfunction Properties

①  $\Psi_E(\vec{r})$  must be: Continuous, Differentiable, Finite  $\rightarrow |\vec{r}| \rightarrow \infty$

$$\text{② } \int \Psi_{E_1}^*(\vec{r}) \Psi_{E_2}(\vec{r}) d\vec{r} = \delta_{E_1, E_2} \quad (\text{Kronecker: } \delta_{\alpha\beta} = \begin{cases} 1 & \alpha = \beta \\ 0 & \alpha \neq \beta \end{cases})$$

$\delta(E_1 - E_2)$  (Dirac when  $E_1, E_2$  continuous)

Orthogonality condition

## Wavefunction Properties

① Probability of finding a particle:  $|\Psi(\vec{r}, t)|^2 d\vec{r}$  prob. to find a part. in:  $\vec{r} \rightarrow \vec{r} + d\vec{r}$

$$\int |\Psi(\vec{r}, t)|^2 d\vec{r} = 1 \rightarrow \text{Normalization condition}$$

From all the results we obtain we care about whos  $\Psi(\vec{r}, t) \rightarrow \text{square}$ :  $\int$

②  $\int \Psi^*(\vec{r}, t) \hat{O} \Psi(\vec{r}, t) d\vec{r} = \langle \hat{O}(t) \rangle$

$\hat{O}$ : observable

↳  $\hat{p}$  = momentum  $\rightarrow -i\hbar \frac{d}{dx}$

↳  $\hat{x}$  = position  $\rightarrow x$

example:  $E_1 \rightarrow \Psi_1 e^{-i\frac{E_1 t}{\hbar}}$

$$\int \Psi_1^*(x) e^{+i\frac{E_1 t}{\hbar}} \left[ -i\hbar \frac{d}{dx} \right] \Psi_1(x) e^{-i\frac{E_1 t}{\hbar}} dx = \langle p(t) \rangle$$

value of the momentum  
at a given time

## Free particle "m"

$\nabla^2 \Psi(\vec{r}) + \frac{2m}{\hbar^2} E \Psi(\vec{r}) = 0$   $\rightarrow$  S.E. stationary states of a free p.r.e. (M)

$\frac{d^2}{dx^2} \Psi(x) + \frac{2m}{\hbar^2} E \Psi(x) = 0$  sol:  $\Psi(x) = A e^{\pm i\eta x}$

Demos. for ④:  $-A\eta^2 e^{\pm i\eta x} + \frac{2m}{\hbar^2} E A e^{\pm i\eta x} = 0$

If:  $\eta^2 = \frac{2m}{\hbar^2} E \rightarrow E = \frac{\hbar^2}{2m} \eta^2$   
 $\left\{ \frac{\hbar^2}{2m} k^2, A e^{\pm ikx} \right\} \quad \eta \rightarrow k = \frac{2\pi}{\lambda_{DB}}$

e.f.  $\rightarrow$  free p.r.e.

e.v.  $\rightarrow E = \frac{\hbar^2}{2m} k^2$

$\therefore k = \frac{\sqrt{2mE}}{\hbar}$

De Broglie

$$E = \frac{p^2}{2m} = \frac{(\hbar k)^2}{2m} = \frac{\hbar^2}{2m} k^2$$

$$k = \frac{2\pi}{\lambda_{DB}}$$

$$p = \frac{\hbar}{\lambda_{DB}} = \hbar k$$

Demos for  $\oplus$   $A$   $|A|^2 \int dx e^{-ikx} e^{+ikx} = \delta(k-k')$  Dirac  $(k, k')$  continuous

$$|A|^2 \int_{-\infty}^{+\infty} dx e^{i(k-k')x} = \delta(x-x')$$

$$\hookrightarrow \frac{1}{2\pi} \int_{-\infty}^{+\infty} dx e^{i(k-k')x}$$

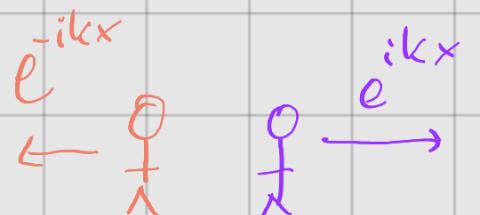
$$\Rightarrow |A|^2 = \frac{1}{2\pi} \rightarrow A = \sqrt{\frac{1}{2\pi}}$$

Solution of Sch eq. for stationary state for free part.

$\hookrightarrow$  2 sets of sols.

$$\left\{ \frac{\hbar^2}{2m} k^2, \frac{1}{\sqrt{2\pi}} e^{+ikx} \right\}$$

$$\left\{ \frac{\hbar^2}{2m} k^2, \frac{1}{\sqrt{2\pi}} e^{-ikx} \right\}$$



General sol. of Schö for a free particle:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} e^{ikx} e^{-i\frac{\hbar^2 k^2 t}{2m}} + \frac{1}{\sqrt{2\pi}} e^{-ikx} e^{-i\frac{\hbar^2 k^2 t}{2m}}$$

Superposition

Calculation of the momentum:

$$\langle p \rangle = \int dx \frac{1}{\sqrt{2\pi}} e^{-ikx} e^{+i\frac{\hbar^2 k^2 t}{2m}} \left[ -i\hbar \frac{d}{dx} \right] \frac{1}{\sqrt{2\pi}} e^{+ikx - i\frac{\hbar^2 k^2 t}{2m}} = -i\hbar (ik) \frac{1}{2\pi} \int dx e^{i(k-k)x} =$$

$= +\hbar k \delta(x)$   $\rightarrow$  To solve this singularity of the delta we take 2 very close states  $k, k'$  and do the limit  $\lim_{k \rightarrow k'}$

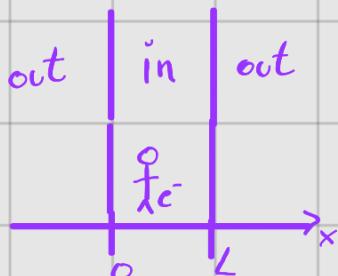
What is happening is that a plane wave with a single  $k$  doesn't exist. We have a wave packet that is just weighted with an exact plane wave



$$\int_{-\infty}^{+\infty} e^{iK_0 x} f(K) dK = \text{wave packet}$$

## Particle confined

Potential Well :  $V = \begin{cases} \infty & x < 0 \quad x > L \\ 0 & 0 \leq x \leq L \end{cases}$



$$\text{"OUT"} \rightarrow \Psi(x,t) = \Psi(x)e^{-i\frac{E}{\hbar}t} \equiv 0$$

$$\text{"IN"} \rightarrow \Psi(x,t) \xrightarrow{\text{for free } \epsilon} e^{+ikx} e^{-i\frac{E}{\hbar}t}$$

$e^{+ikx}, e^{-ikx}, \sin kx, \cos kx$   
 eigenfunctions  
 obtained by a linear comb. of eigenfunc.  
 A linear comb. of solution is a solution.

Remember:

$$i\hbar \frac{\partial}{\partial t} \Psi(x,t) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(x,t) \right] \Psi(x,t)$$

Prob. of finding  $\epsilon$  in  $x \rightarrow x+dx$ :  $|\Psi(x,t)|^2 dx$

$$|\Psi(x,t)|^2 dx = |\Psi(x)|^2 dx \rightarrow 0$$

$$\text{free part.} \rightarrow \left\{ \frac{1}{\hbar m} e^{\pm ikx}, \frac{\hbar^2}{2m} k^2 \right\}$$

There are 4 math. valid solutions but there is only one physical valid solution  $\rightarrow \sin kx$

$$\sin kL = 0 \Rightarrow kL = n \cdot \pi \Rightarrow k_n = \frac{n\pi}{L}$$

$$\text{The energy: } E_n = \frac{\hbar^2}{2m} k_n^2 = \frac{\hbar^2}{2m} \left( \frac{n\pi}{L} \right)^2 n^2$$

Confined particle

$$\left\{ A \sin \left( \frac{n\pi}{L} x \right), E_n = \frac{\hbar^2}{2m} \left( \frac{n\pi}{L} \right)^2 n^2 \right\}$$

In order to calculate the constant  $\rightarrow$  Orthogonality

$$\int_0^L A^* \sin \left( \frac{n\pi}{L} nx \right) A \sin \left( \frac{n'\pi}{L} n'x \right) dx = \delta_{nn'} \quad \text{discrete (Kronecker)}$$

$$\hookrightarrow \text{Case ① } n=n' : |A|^2 \int_0^L \sin^2 \left( \frac{n\pi}{L} nx \right) dx = |A|^2 \int_0^L \frac{1 - \cos(2 \cdot \frac{n\pi}{L} nx)}{2} dx =$$

$$= \frac{|A|^2}{2} \int_0^L dx + \frac{|A|^2}{2} \int_0^L \cos \left( \frac{2n\pi}{L} x \right) dx = |A|^2 \frac{L}{2} + \frac{|A|^2}{2} \cdot \frac{L}{4n\pi} \int_0^L \sin \left( \frac{2n\pi}{L} x \right) dx$$

$$= |A|^2 \frac{L}{2} \Rightarrow |A|^2 \frac{L}{2} = 1 \Rightarrow A = \sqrt{\frac{2}{L}}$$

The result for confined particle:

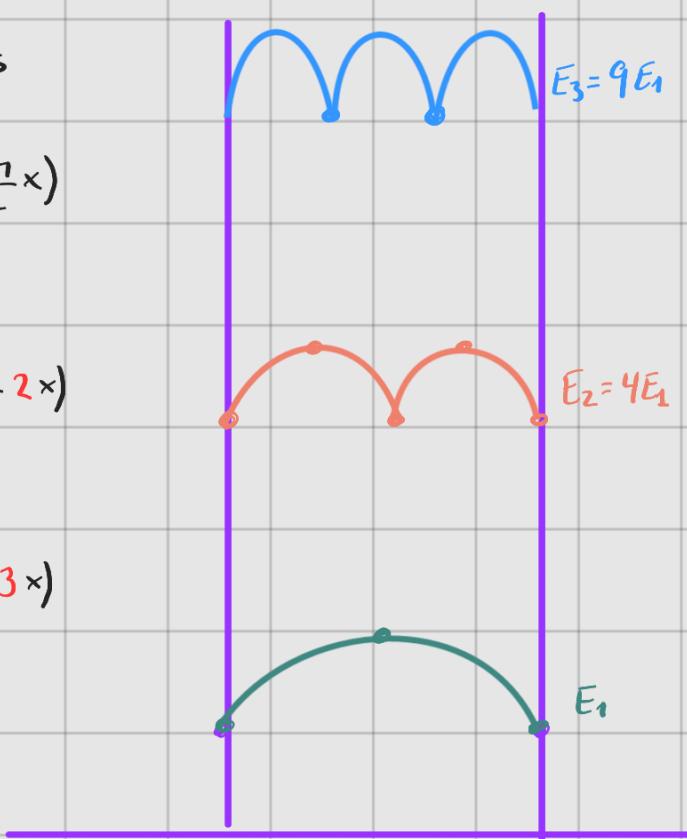
$$\left\{ \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right), E_n = \frac{\hbar^2}{2m} \left(\frac{n\pi}{L}\right)^2 \right\}$$

Prob. to find the prob. for different energies

$$n=1 \rightarrow \Psi_1(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi}{L}x\right) \rightarrow |\Psi_1(x)|^2 = \frac{2}{L} \cdot \sin^2\left(\frac{\pi}{L}x\right)$$

$$n=2 \rightarrow \Psi_2(x) = \sqrt{\frac{2}{L}} \sin\left(2\frac{\pi}{L}x\right) \rightarrow |\Psi_2(x)|^2 = \frac{2}{L} \cdot \sin^2\left(\frac{\pi}{L}2x\right)$$

$$n=3 \rightarrow \Psi_3(x) = \sqrt{\frac{2}{L}} \sin\left(3\frac{\pi}{L}x\right) \rightarrow |\Psi_3(x)|^2 = \frac{2}{L} \cdot \sin^2\left(\frac{\pi}{L}3x\right)$$



① free part,  $\rightarrow E \rightarrow \Psi_E(x) = \frac{1}{\sqrt{2m}} e^{\pm ikx}$   $k = \frac{\sqrt{2mE}}{\hbar}$   $\{E, \Psi_E(x)\}$

Wavefunc.  $\rightarrow \Psi(x,t) = \frac{1}{\sqrt{2m}} e^{\pm ikx - i \frac{E}{\hbar} t}$

3D  $\rightarrow \Psi(\vec{r},t) = \left(\frac{1}{\sqrt{2m}}\right)^3 e^{\pm i \vec{k} \cdot \vec{r} - i \frac{E}{\hbar} t}$

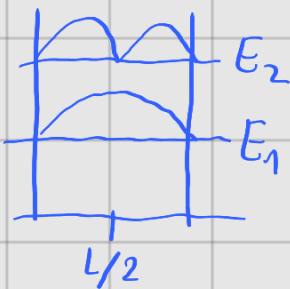
② Potential Well  $\rightarrow E_n = \frac{\hbar^2}{2m} \left(\frac{\pi}{L}\right)^2 n^2$   $\Psi_n(x) = \sqrt{\frac{2}{L}} \cdot \sin \frac{n}{L} nx$



$|\Psi_n(x)|^2 dx \rightarrow$  prob. finding a particle 

$\hookrightarrow$  Prob. finding in a range

$$P_{\text{prob}} = \int_{E_2 - \epsilon}^{E_2 + \epsilon} dx |\Psi_2(x)|^2$$



↳ If we have a quantum well (Q.W.) of:  $L \approx 1 \text{ nm}$ , energy?

$$E_1 = \frac{\hbar^2}{2m} \left(\frac{\pi}{L}\right)^2 \cdot 1 = \frac{(\hbar c)^2}{2mc^2} \approx \frac{(12.4 \cdot 10^3 \text{ eV} \cdot \text{\AA})^2}{10^{-4} \text{ m}^2 \cdot 10^6 \text{ eV}} = \frac{144 \cdot 10^6 \cdot 10^{-20} \text{ m}^2 \cdot 10 \text{ eV}^2}{10^2 \text{ m}^2 \text{ eV}} \approx 10^{-12} \text{ eV}$$

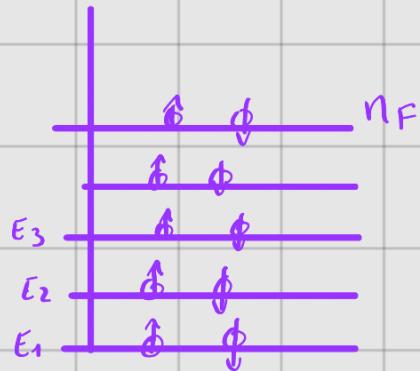
$$E_2 = 4 \cdot E_1$$

$$\Delta E_{21} = E_2 - E_1 = 3 E_1 = 3 \cdot 10^{-12} \text{ eV} \Rightarrow \text{super tiny !!}$$

$$\hookrightarrow \text{If we do with } L \approx 1 \text{ nm} \Rightarrow \Delta E_{21} \approx 1.2 \text{ eV}$$

## {Pauli exclusion principle}

How can we put  $10 e^-$  in energy levels



There can only be  $2 e^-$  (with diff spin) at the same level.

Fermi level ( $n_F$ ): Is the last level filled by  $e^-$   
 $\alpha = \text{total } \# \text{ of } e^- = 2 \times n_F$

$$E_n = \frac{\hbar^2}{2m} \left(\frac{n\pi}{L}\right)^2 n^2$$

$$\text{free p.} \Rightarrow E = \frac{\hbar^2}{2m} k^2$$

density

$$E_F = \frac{\hbar^2}{2m} \left(\frac{\pi}{L}\right)^2 n_F^2 = \frac{\hbar^2}{2m} \underbrace{\left(\frac{\pi}{L}\right)^2}_{k_F^2} \underbrace{\left(\frac{N}{2}\right)^2}_{n_F^2} = \frac{\hbar^2}{2m} \left(\frac{N}{L}\right)^2 \left(\frac{\pi}{2}\right)^2$$

$$K_F = \frac{\pi}{2} \cdot \frac{N}{L}$$

$$V_F = \frac{P_F}{m} = \frac{\hbar k_F}{m} = \frac{\hbar}{m} \left(\frac{\pi}{2} \cdot \frac{N}{L}\right)$$

Fermi velocity

$$V(\vec{r}, t) = V(\vec{r}) = \begin{cases} 0 & \text{inside} \\ \infty & \text{out} \end{cases}$$

$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}, t) = [H] \Psi(\vec{r}, t)$$

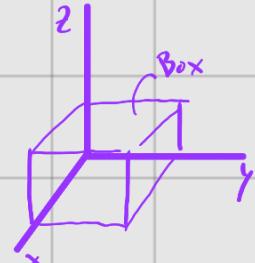
$$\frac{\hbar^2}{2m} \nabla^2 \Psi(\vec{r}) + E \Psi(\vec{r}) = 0$$

Conditions:

outside:  $\Psi(\vec{r}) = 0$

inside:  $\Psi(\vec{r}) = \Psi(x, y, z) = A \sin(k_x x) \cdot \sin(k_y y) \cdot \sin(k_z z)$

↪ Applying  $\Psi(\vec{r})$  in the eq. we get the energy:  $\frac{\hbar^2}{2m} [k_x^2 + k_y^2 + k_z^2] = E$



Now we have conditions for the limits:

$$x: k_x L = \pi n_x \rightarrow k_x = \frac{\pi}{L} n_x$$

$$y: k_y L = \pi n_y \rightarrow k_y = \frac{\pi}{L} n_y$$

$$z: k_z L = \pi n_z \rightarrow k_z = \frac{\pi}{L} n_z$$



$$E_{n_x, n_y, n_z} = \frac{\hbar^2}{2m} \left(\frac{\pi}{L}\right)^2 [n_x^2 + n_y^2 + n_z^2]$$

Orthogonality to compute the constant  $\int d\vec{r} \Psi_E^*(\vec{r}) \Psi_{E'}(\vec{r}) = \delta_{E,E'}$

$$\int dx \int dy \int dz \underbrace{A^* \sin(k_x x) \sin(k_y y) \sin(k_z z)}_{\Psi_E} \underbrace{A \sin(k_x x) \sin(k_y y) \sin(k_z z)}_{\Psi_{E'}} = 1$$

$$|A|^2 \int_0^L dx \sin^2(k_x x) \int_0^L dy \sin^2(k_y y) \int_0^L dz \sin^2(k_z z) = 1$$

$$|A|^2 \left(\frac{L}{2}\right)^3 = 1 \quad \longrightarrow |A| = \left(\frac{2}{L}\right)^{3/2}$$

The wavefunction then →

$$\Psi_{n_x, n_y, n_z}(\vec{r}) = \left(\frac{2}{L}\right)^3 \sin(k_x x) \sin(k_y y) \sin(k_z z)$$

For example for  $\Psi_{1,1,1}$  and  $\Psi_{2,1,1}$  have the same energy  $E_{1,1,1} = E_{2,1,1}$

but the prob. distribution is different. In 1D this does not happen but in 2D and 3D. This is called: Quantum Degeneracy

$$3D \quad E_{\{n_x, n_y, n_z\}} = \begin{cases} \Psi \\ \neq \\ \Psi \end{cases} \quad ] \text{Quantum Degeneracy}$$

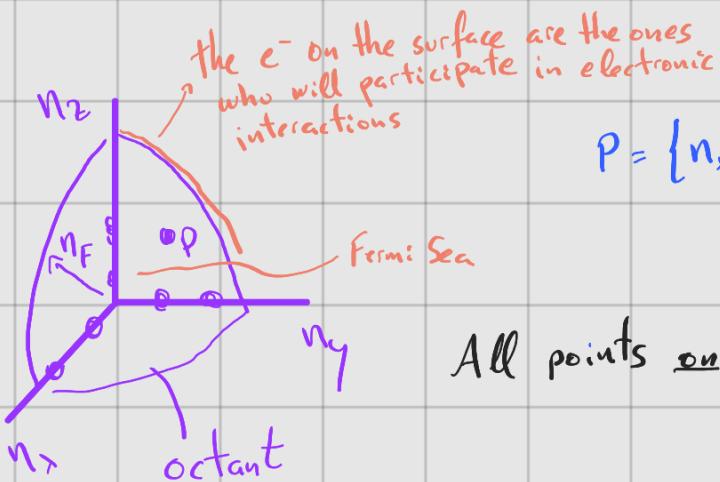
## Recap

3D box

$$E_{n_x, n_y, n_z} = \frac{\hbar^2}{2m} \left(\frac{\pi}{L}\right)^2 (n_x^2 + n_y^2 + n_z^2)$$

$$\psi_{n_x, n_y, n_z}(\vec{r}) = \left(\frac{\sqrt{2}}{L}\right)^3 \sin\left(\frac{\pi}{L}n_x x\right) \sin\left(\frac{\pi}{L}n_y y\right) \sin\left(\frac{\pi}{L}n_z z\right)$$

We can say:  $n^2 = (n_x^2 + n_y^2 + n_z^2)$



$$P = \{n_x, n_y, n_z\} \quad \text{each point is a state}$$

All points on the sphere surface  $\rightarrow$  states with same energy

$$E_n = \frac{\hbar^2}{2m} \left(\frac{\pi}{L}\right)^2 n^2$$

$$n \rightarrow n_F = \text{Fermi level} \rightarrow E_F = \frac{\hbar^2}{2m} \left(\frac{\pi}{L}\right)^2 n_F^2$$

$$E_n \leq E_F$$

$$\frac{4}{3} \pi n_F^3 \times \frac{1}{8} = \text{Total no of points inside sphere with radius } n_F \text{ ('/8')}$$

$\hookrightarrow$  we consider only positive values of  $n_x, n_y, n_z$

2x  $\frac{4}{3} \pi n_F^3 \frac{1}{8} = \text{Tot. no e}^- \text{ when } E \leq E_F = N$

$\hookrightarrow$  bc of Pauli: there are at max. two  $e^-$  in each state

With the previous results we can compute:

$$n_F = \left( \frac{3N}{\pi} \right)^{1/3}$$

3D

$$\bar{E}_F = \frac{\hbar^2}{2m} \left( \frac{\pi}{L} \right)^2 n_F^2 = \frac{\hbar^2}{2m} \left( \frac{\pi}{L} \right)^2 \left( \frac{3N}{\pi} \right)^{2/3} = \frac{\hbar^2}{2m} \left( \frac{\pi^2}{L^3} 3N \right)^{2/3} = \frac{\hbar^2}{2m} \left( 3\pi^2 \frac{N}{L^3} \right)^{2/3}$$

*k<sub>F</sub>*  
volume

$$E_F = \frac{\hbar^2}{2m} k_F^{2/3}$$

$$k_F = \left[ 3\pi^2 \frac{N}{L^3} \right]^{1/3}$$

$$P_F = \hbar k_F = \hbar \left[ 3\pi^2 \frac{N}{L^3} \right]^{1/3}$$

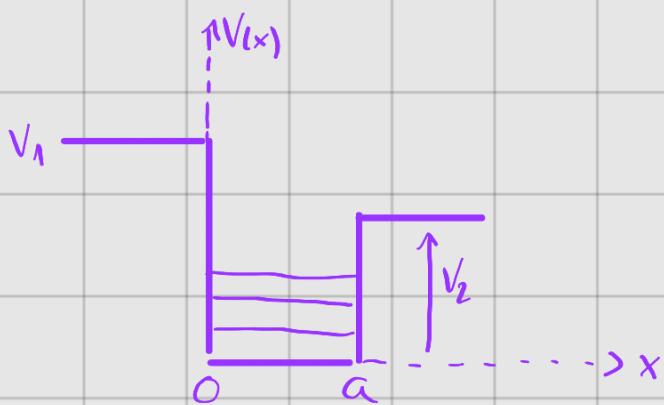
$$V_F = \frac{P_F}{m} = \frac{\hbar}{m} \left[ 3\pi^2 \frac{N}{L^3} \right]^{1/3}$$

# Finite Well

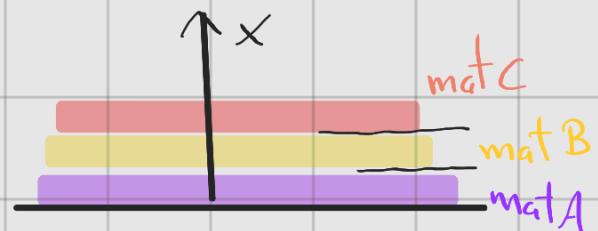
What we have done so far is using Schrödinger eq. to solve:

free part.  $\rightarrow$    $\rightarrow$  

Now finite well:



In materials we have layers



Potential

$$V(x) = \begin{cases} V_1 & x < 0 \\ 0 & 0 \leq x \leq a \\ V_2 & x > a \end{cases}$$

$$\left. \frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi(x) + (E - V_1) \Psi(x) = 0 \right|_{x < 0}$$

$$\left. \frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi(x) + E \Psi(x) = 0 \right|_{0 \leq x \leq a}$$

$$\left. \frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi(x) + (E - V_2) \Psi(x) = 0 \right|_{x > a}$$

Schö Eq for each part

At left side we'll have:  $\Psi(x) \sim e^{ikx}$

$$i\sqrt{\frac{2m(E-V_1)}{\hbar^2}} x = -\frac{i\sqrt{2m(V_1-E)}}{\hbar} x$$

$$k = \frac{\sqrt{2mE}}{\hbar}$$

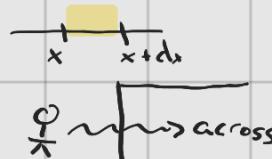
$$K_1 = \frac{i\sqrt{2m(V_1-E)}}{\hbar}$$

$$K_2 = \frac{i\sqrt{2m(V_2-E)}}{\hbar}$$

General Solutions

$$\left\{ \begin{array}{l} \Psi(x) = A_1 e^{-k_1 x} + B_1 e^{+k_1 x} \quad x < 0 \\ \Psi(x) = A e^{-ikx} + B e^{ikx} \quad 0 \leq x \leq a \\ \Psi(x) = A_2 e^{-k_2 x} + B_2 e^{+k_2 x} \quad x > a \end{array} \right.$$

- $\Psi(x)$  has to be finite so:  $A_1 = 0$  and  $B_2 = 0$
- There is a small probability of  $e^-$  to be found after the barrier (tunneling)

Prob of finding the part.  $|\Psi(x)|^2 dx$  in 

↪ for right side  $|A_2|^2 e^{-2k_2 x}$

• Rewriting  $\Psi(x)$ ,  $0 \leq x \leq a$ :

$$A \cos kx - iA \sin kx + B \cos kx + iB \sin kx = (A+B) \cos kx + i(B-A) \sin kx = C \sin(kx + \delta)$$

$C \sin \delta$   
 $C \cos \delta$

↪ Orthogonality cond. for inside region

$$\int_0^a dx C^* \sin(\bar{k}x + \bar{\delta}) \cdot C \sin(kx + \delta) = \delta_{(k, \bar{k})(\delta, \bar{\delta})}$$

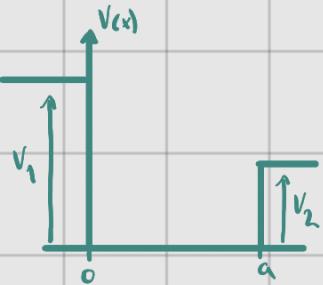
$$|C|^2 \int_0^a dx \sin^2(kx + \delta) = 1 \Rightarrow |C|^2 = \frac{1}{\int_0^a dx} = \frac{4k}{2ka + \sin 2\delta - \sin(2ka + 2\delta)}$$

Now, the constant is not longer a constant it's a function of  $k$

$$C \rightarrow C(k)$$

related with  $E$   $\sqrt{2mE/h}$

## Recap



$$\psi(x) = \begin{cases} B_1 e^{+K_1 x} & x \leq 0 \\ C(k) \sin(Kx + \delta) & 0 \leq x \leq a \\ A_2 e^{-K_2 x} & x \geq a \end{cases}$$

$$K = \frac{\sqrt{2mE}}{\hbar}, \quad K_1 = \frac{\sqrt{2m(V_1 - E)}}{\hbar}, \quad K_2 = \frac{\sqrt{2m(V_2 - E)}}{\hbar}$$

Orthogonality:  $|C(k)|^2 = \frac{4k}{2Ka + \sin 2\delta - \sin(2Ka + 2\delta)}$

\* K is the energy so by changing the energy we change the value of  $C(k)$   
So, every energy level has its own coefficient.

Now we have to impose the two conditions: ① continuity of the function at the boundaries  $[x=0, x=a]$  and ② continuity of the derivative also at the boundaries.

In general:  $f_1 = f_2$  and  $f'_1 = f'_2 \Rightarrow f_1/f'_1 = f_2/f'_2$  which is logarithm derivative. Therefore, it is an easy way to verify impose our conditions and do the calculations.

$x=0$

$$\left. \frac{d}{dx} \left[ \ln(B_1 e^{K_1 x}) \right] \right|_{x=0} = \left. \frac{d}{dx} \left[ \ln(C(k) \sin(Kx + \delta)) \right] \right|_{x=0} \Rightarrow \left. \frac{K_1 B_1 e^{K_1 x}}{B_1 e^{K_1 x}} \right|_{x=0} = \left. \frac{K C(k) \cos(Kx + \delta)}{C(k) \sin(Kx + \delta)} \right|_{x=0}$$

$$\Rightarrow K_1 = K \cdot \frac{\cos \delta}{\sin \delta}$$

$x=a$

$$\left. \frac{d}{dx} \left[ \ln(A_2 e^{-k_2 x}) \right] \right|_{x=a} = \left. \frac{d}{dx} \left[ \ln(C(k) \sin(kx + \delta)) \right] \right|_{x=a} \Rightarrow \left. \frac{-k_2 A_2 e^{-k_2 x}}{A_2 e^{-k_2 x}} \right|_{x=a} = \left. \frac{k(k) \cos(kx + \delta)}{C(k) \sin(kx + \delta)} \right|_{x=a}$$

$$\Rightarrow k_2 = -k \frac{\cos(ka + \delta)}{\sin(ka + \delta)}$$

Now we get the value of  $\delta$

$$① \rightarrow \cot \delta = \frac{k_1}{k} = \sqrt{\frac{2m(V_1 - E)}{2mE}} = \sqrt{\frac{V_1}{E} - 1} = \sqrt{\frac{2mV_1}{\hbar^2 k^2} - 1}$$

$$\cot^2 \delta = \frac{\cos^2 \delta}{\sin^2 \delta} = \frac{2mV_1}{\hbar^2 k^2} - 1 \Rightarrow \frac{\cos^2 \delta}{\sin^2 \delta} + 1 = \frac{2mV_1}{\hbar^2 k^2} \Rightarrow \frac{1}{\sin^2 \delta} = \frac{2mV_1}{\hbar^2 k^2}$$

$$\Rightarrow \sin^2 \delta = \frac{\hbar^2 k^2}{2mV_1} = \underbrace{\sin^2(\delta - \pi n_1)}_{\text{due to periodicity of } \sin^2}$$

$$\Rightarrow \delta(k) = \pi n_1 + \sin^{-1}\left(\frac{\hbar k}{\sqrt{2mV_1}}\right)$$

$$② \rightarrow \cot(ka + \delta) = -\frac{k_2}{k}$$

$$\Rightarrow \delta(k) + ka = \pi n_2 - \sin^{-1}\left(\frac{\hbar k}{\sqrt{2mV_2}}\right)$$

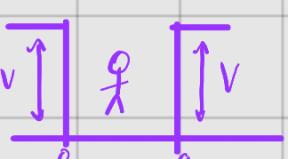
Now if we do  $① = ②$  we get:

$$ka = -\sin^{-1}\left(\frac{\hbar k}{\sqrt{2mV_1}}\right) - \sin^{-1}\left(\frac{\hbar k}{\sqrt{2mV_2}}\right) - \pi(n_2 - n_1) \rightarrow \text{Transcendental equation}$$

Or implicit equation. Solving this, the solutions give us the energy.

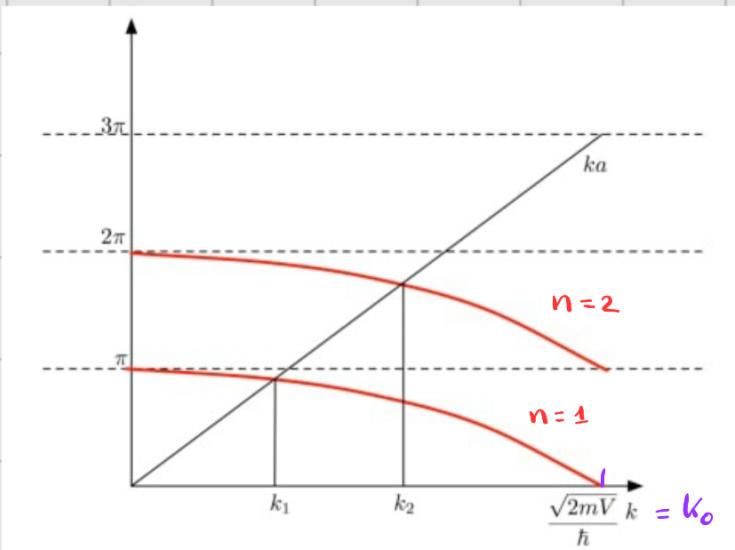
$$f(k) = 0 = f(E)$$

$$n \rightarrow \begin{array}{c|c} n & k \\ \hline 1 & k_1(E_1) \\ 2 & k_2(E_2) \end{array}$$

There is a special case when the both potential barriers have the same value.  So  $V_1 = V_2 = V \Rightarrow$  Symmetric Quantum Well

In this case we have the next equation; with  $n_1 - n_2 = n$  :

$$Ka = -2 \sin^{-1}\left(\frac{\hbar k}{\sqrt{2mV}}\right) + \pi n$$



$$n_1 \rightarrow -2 \sin^{-1}\left(\frac{\hbar k}{\sqrt{2mV}}\right) + \pi$$

$$n_2 \rightarrow -2 \sin^{-1}\left(\frac{\hbar k}{\sqrt{2mV}}\right) + 2\pi$$

Finite number of energy levels inside barrier, after that particle could be free.

Now we are interested in knowing what happens when  $E \ll V$

$$Ka = -2 \sin^{-1}\left(\frac{\hbar k}{\sqrt{2mV}}\right) + \pi n \xrightarrow[V \text{ big}]{\text{Taylor}} Ka = -2 \frac{\hbar k}{\sqrt{2mV}} + n\pi$$

$$K = \frac{\pi n}{a} - \frac{2}{a} \frac{\hbar k}{\sqrt{2mV}} \Rightarrow K \left(1 + \frac{2\hbar}{a\sqrt{2mV}}\right) = \frac{\pi}{a} n \Rightarrow K = \frac{\pi}{a} n \left(1 + \frac{2\hbar}{a\sqrt{2mV}}\right)^{-1}$$

$$K_n = \frac{\pi}{a} \left[1 - \frac{\hbar\sqrt{2}}{a\sqrt{mV}}\right] n$$

↳ When  $V$  big:  
 $(1 + \frac{a}{x})^{-1} \underset{\substack{\text{Taylor} \\ x \rightarrow \infty}}{\approx} 1 - \frac{a}{x}$

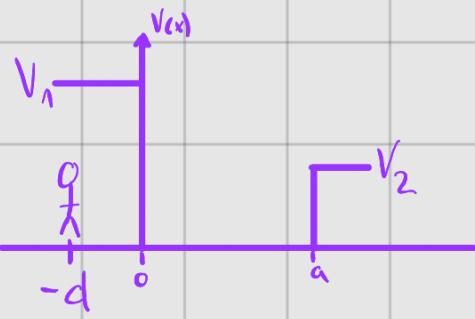
$$\bar{E}_n = \frac{\hbar^2}{2m} K_n^2 \Rightarrow$$

$$\bar{E}_n = \frac{\hbar^2 \pi^2}{2m a^2} \left(1 - \frac{\hbar\sqrt{2}}{a\sqrt{mV}}\right)^2 n^2$$

This is the energy of finite well

If  $V \rightarrow \infty \Rightarrow$  we have infinite well

We now want to calculate the probability of finding a particle outside from the well, on the left.



$$\psi_{(x)} = \begin{cases} B_1 e^{+k_1 x} & x < 0 \\ C(k) \sin(kx + \delta) & 0 \leq x \leq a \\ A_2 e^{-k_2 x} & x > a \end{cases}$$

$$k = \frac{\sqrt{2mE}}{\hbar}$$

$$k_1 = \frac{\sqrt{2m(V_1 - E)}}{\hbar}$$

$$|C(k)|^2 = \frac{4k}{2ka + \sin 2\delta - \sin(2ka + 2\delta)}$$

$$\sin \delta(k) = \frac{\hbar k}{\sqrt{2mV_1}} = \sqrt{\frac{E}{V_1}}$$

We can write the prob as:

$$\int_{-d}^0 |\psi_{(x,t)}|^2 dx = |B_1|^2 \int_{-d}^0 e^{-2k_1 x} dx = |B_1|^2 \frac{1 - e^{2k_1 d}}{2k_1} + \dots$$

at  $x=0$  the eigenfunction has to be continuous  $\Rightarrow B_1 e^{k_1 x} \Big|_{x=0} = C(k) \sin(kx + \delta) \Big|_{x=0}$

$$\Rightarrow B_1 = C(k) \sin \delta(k)$$

Example:

$$E = 4.85 \text{ eV} \quad V_1 = 5 \text{ meV} \quad a = 1 \mu\text{m} \quad d = 10^{-2} \mu\text{m}$$

$$k = \frac{\sqrt{2mE}}{\hbar} = \frac{\sqrt{2mc^2 E}}{\hbar c} = \frac{\sqrt{2 \cdot 0.5 \cdot 10^6 \text{ eV} \cdot 4.85 \cdot 10^{-6} \text{ eV}}}{1973 \text{ eV} \cdot 10^{-10} \text{ m}} = 11.16 \cdot 10^{-6} \text{ m}^{-1}$$

$$\Rightarrow ka = 11.16$$

$$k_1 = \frac{\sqrt{2mc^2(V_1 - E)}}{\hbar c} = 1.96 \cdot 10^6 \text{ m}^{-1}$$

$$\sin(\delta) = \sqrt{\frac{4.85}{5}} = 0.98 \rightarrow \delta = 78.5^\circ \Rightarrow C^2 = 1.9 \cdot 10^6 \text{ m}^{-1} \Rightarrow B_1 = 1.3 \cdot 10^3 \text{ m}^{-1/2}$$

$$\text{Probability} \sim 0.02 \Rightarrow 2\%$$

## Recap

$$\textcircled{1} \text{ Infinite Well} \Rightarrow E_n = \frac{\hbar^2}{2m} \left(\frac{\pi}{a}\right)^2 n^2$$

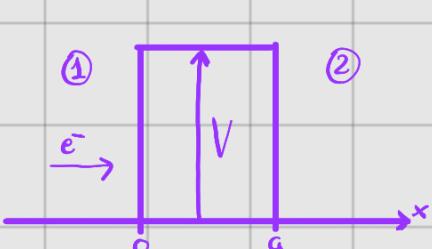
$$\textcircled{2} \text{ Finite Well} \Rightarrow k_a = -\sin^{-1}\left(\frac{\hbar k}{\sqrt{2mV_1}}\right) - \sin^{-1}\left(\frac{\hbar k}{\sqrt{2mV_2}}\right) + \pi n \Rightarrow f(k_n) = 0 \quad \begin{matrix} \text{solve for} \\ \text{each } n \end{matrix}$$

$$\hookrightarrow E_n = \frac{\hbar^2}{2m} k_n^2$$

$n$	1	2	...
$k_n$	$k_1$	$k_2$	...

$$\textcircled{2.1} \text{ When the potential level is the same} = E_n = E_n^0 \left(1 + \frac{1}{\sqrt{V}}\right)$$

## Inverse Barrier



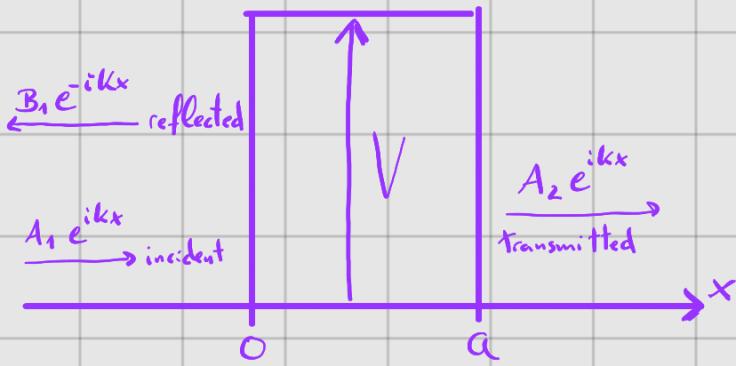
$$V(x) = \begin{cases} V & 0 \leq x \leq a \\ 0 & x < 0, x > a \end{cases}$$

## Schrödinger Equations:

$$\begin{cases} \frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi(x) + (E-V) \Psi(x) = 0 & 0 \leq x \leq a \\ \frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi(x) + E \Psi(x) = 0 & x < 0 \end{cases}$$

We have two situations here: **(A)** outside the barrier where the solution of the free particle is a plane wave and **(B)** inside the barrier.

### (A) Outside



$$\Psi_1(x) = A_1 e^{ikx} + B_1 e^{-ikx}$$

$$\Psi_2(x) = A_2 e^{ikx} + B_2 e^{-ikx}$$

this one makes no sense because out of barrier there is no reflection from anywhere

$$\begin{cases} \Psi_1(x) = A_1 e^{ikx} + B_1 e^{-ikx} \\ \Psi_2(x) = A_2 e^{ikx} \end{cases} \quad k = \frac{\sqrt{2mE}}{\hbar}$$

### (B) Inside

$$\Psi_1(x) = A e^{k_1 x} + B e^{-k_1 x}$$

$$k_1 = \frac{\sqrt{2m(V-E)}}{\hbar}$$

As usual we have to impose continuity of the function and of its derivatives.

$$x=0$$

$$x=a$$

$$(1) \rightarrow A_1 + B_1 = A + B$$

$$(3) \rightarrow A e^{k_1 a} + B e^{-k_1 a} = A_2 e^{i k_1 a}$$

$$(2) \rightarrow i k (A_1 - B_1) = k_1 (A - B)$$

$$(4) \rightarrow A k_1 e^{k_1 a} - B k_1 e^{-k_1 a} = i k A_2 e^{i k_1 a}$$

If we substitute (1) on (2):

$$(I) \rightarrow 2A_1 = A \left( 1 + \frac{k_1}{i k} \right) + B \left( 1 - \frac{k_1}{i k} \right)$$

Sum of (3) and (4):

Diff of (3) and (4)

$$(II) \rightarrow 2A e^{ika} = A_2 e^{ika} \left(1 + \frac{ik}{k_1}\right)$$

$$(III) \rightarrow 2B e^{-ika} = A_2 e^{ika} \left(1 - \frac{ik}{k_1}\right)$$

$$\begin{aligned} \left(1 - \frac{a}{b}\right) \left(1 - \frac{b}{c}\right) &= 2 - \frac{a^2 + b^2}{ab} \\ \left(1 + \frac{a}{b}\right) \left(1 + \frac{b}{c}\right) &= 2 + \frac{a^2 + b^2}{ab} \end{aligned}$$

Now,  $2 \cdot (I)$  and substitute (II) and (III) in (I)

$$\begin{aligned} 4A_1 &= A_2 e^{ika} \cdot e^{-ika} \left(1 + \frac{ik}{k_1}\right) \cdot \left(1 + \frac{k_1}{ik}\right) + A_2 e^{ika} e^{ika} \left(1 - \frac{ik}{k_1}\right) \left(1 - \frac{k_1}{ik}\right) = \\ &= A_2 e^{ika} \left[ e^{-ika} \left(2 + \frac{k_1^2 - k^2}{ik k_1}\right) + e^{ika} \left(2 + \frac{k^2 - k_1^2}{ik k_1}\right) \right] \\ &= A_2 \frac{1}{ik k_1} e^{ika} \left[ e^{-ika} (k_1^2 - k^2 + 2ik k_1) + e^{ika} (k^2 - k_1^2 + 2ik k_1) \right] = \\ &= A_2 \frac{1}{ik k_1} e^{ika} \left[ e^{-ika} (k_1 + ik)^2 + e^{ika} (k + i k_1)^2 \right] \end{aligned}$$

$$\frac{A_2}{A_1} = \frac{4ik k_1 e^{-ika}}{e^{-ika} (k_1 + ik)^2 + e^{ika} (k + i k_1)^2} = \left\{ \begin{array}{l} \sinh x = \frac{e^x - e^{-x}}{2} \\ \cosh x = \frac{e^x + e^{-x}}{2} \end{array} \right\} =$$

$$= \frac{4ik k_1 e^{-ika}}{(k^2 - k_1^2) 2 \sinh(k_1 a) + 4ik k_1 \cosh(k_1 a)} = \frac{2ik k_1 e^{-ika}}{\underbrace{(k^2 - k_1^2)}_a \cdot \sinh(k_1 a) + \underbrace{2ik k_1 \cosh(k_1 a)}_{ib}}$$

Transmittance is defined as:  $\left| \frac{A_2}{A_1} \right|^2$ . So, if we get the modulus square of the previous equation:

$$\left| \frac{A_2}{A_1} \right|^2 = \frac{4k^2 k_1^2}{(k^2 - k_1^2)^2 \sinh^2(k_1 a) + 4k^2 k_1^2 \cosh^2(k_1 a)} = \frac{4k^2 k_1^2}{(k^2 - k_1^2)^2 \sinh^2(k_1 a) + 4k^2 k_1^2 (1 + \sinh^2(k_1 a))} =$$

$$= \frac{4k^2 k_1^2}{(k^2 + k_1^2)^2 \sinh^2(k_1 a) + 4k^2 k_1^2} = \left[ 1 + \frac{(k^2 + k_1^2)^2 \sinh^2(k_1 a)}{4k^2 k_1^2} \right]^{-1} = T$$

Using now the expression of  $K$  and  $k_1$  in terms of  $E$  and  $V$ :

• Check that the behaviour of a transmittance corresponds with what we obtained

$$\textcircled{*} \quad a \rightarrow 0 \Rightarrow T = 1$$

$$\textcircled{*} \quad V \rightarrow 0 \Rightarrow T = 1$$

$$\textcircled{*} \quad V \rightarrow \infty \Rightarrow T = 0$$

$$\textcircled{*} \quad a \rightarrow \infty \Rightarrow T = 0$$

Transmission function of a particle across the barrier  
(probability)

Let's focus now on the reflectance, we need to find  $\left| \frac{B_1}{A_1} \right|^2$

$$\frac{|B_1|^2}{|A_1|^2} = \frac{(k^2 + k_1^2)^2 \sinh^2(k_1 a)}{(k^2 + k_1^2)^2 \sinh^2(k_1 a) + 4k^2 k_1^2} \Rightarrow$$

$$R = \left[ 1 + \frac{4E(V-E)}{V^2} \cdot \frac{1}{\sinh^2(k_1 a)} \right]^{-1}$$

To see everything more clear let's define:  $\xi = \frac{V^2}{4E(V-E)} \sinh^2 \left( \frac{\sqrt{2m(V-E)}}{\hbar} \cdot a \right)$

So we have:

$$T = (1 + \xi)^{-1} \quad R = \left( 1 + \frac{1}{\xi} \right)^{-1}$$

Therefore:

$$T + R = \frac{1}{1+\xi} + \frac{1}{1+\frac{1}{\xi}} = 1 \Rightarrow \boxed{T + R = 1}$$

**Note:** In photonics  $T + R = 1$  is the ideal case because we have to take into consideration that the photons can be absorbed.

In our case  $T + R = 1$  is real because particles are not lost.

We consider now the particular case where a particle has an energy slightly above the barrier  $E > V$

$$\textcircled{a) } \alpha k_1 = \alpha \frac{\sqrt{2m(V-E)}}{\hbar} = \alpha \frac{\sqrt{2m(E-V)}}{\hbar} \quad i$$

$$\textcircled{b) } \frac{\sinh(ix)}{i} = \frac{e^{ix} - e^{-ix}}{2i} = \sin(x)$$

$$\Rightarrow R = \left[ 1 + \frac{4E(E-V)}{V^2} \cdot \frac{1}{\sin^2\left(\frac{\sqrt{2m(E-V)}}{\hbar} a\right)} \right]^{-1}$$

$$\text{If we have: } k_1 a = \frac{\sqrt{2m(E-V)}}{\hbar} = \pi n \Rightarrow R=0, T=1$$

↓  
Transmission Resonance

$$\text{and the energy} \Rightarrow \frac{2m(E-V)}{\hbar^2} = \frac{\pi^2 n^2}{e} \rightarrow E_{III} = \frac{\hbar^2}{2m} \left(\frac{\pi n}{a}\right)^2 + V$$

↳ energy of resonance where the incident e- with an energy above the barrier behaves as a free electron.

The reflection across a barrier is very small when we are slightly above the barrier. It is zero when we are far above the barrier

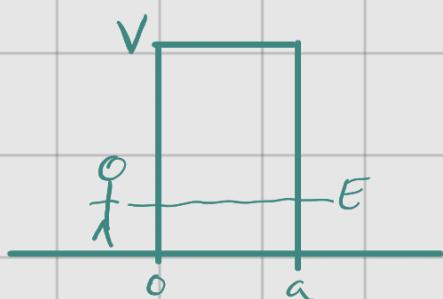
## Recap

Reflectance R:

- )  $E < V$
- )  $E > V$  (unusual)

Transmittance T:

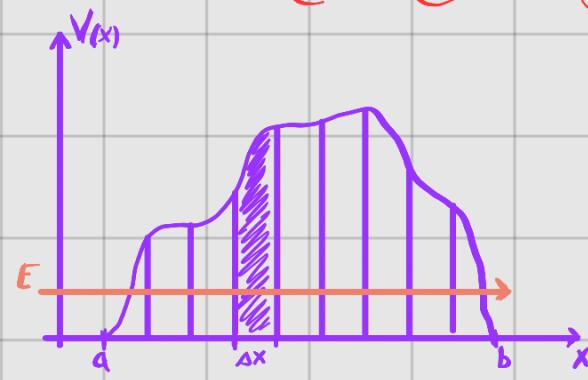
- )  $E < V$
- )  $E > V$



$$T = \frac{|A_2|^2}{|A_1|^2} = \left[ 1 + \frac{V^2}{4E(V-E)} \cdot \sinh^2(k_1 a) \right]^{-1}$$

$$k_1 = \frac{\sqrt{2m(V-E)}}{\hbar}$$

## Generic Barrier



We study now the case where an  $e^-$  travels from the left to the right as is shown in the drawing. We can divide this barrier in several thin barriers of  $\Delta x$  width.

We use the previous result of T we had and also we impose that the potential  $V(x)$  is big enough so:

$$V - E \gg \frac{\hbar^2}{2ma^2} \Rightarrow k_1 a \gg 1$$

$$\text{Therefore: } \sinh^2(k_1 a) = \left( \frac{e^{k_1 a} + e^{-k_1 a}}{2} \right)^2 \approx \frac{e^{2k_1 a}}{4}$$

Then for the transmittance:

$$T \approx \frac{16 k^2 k_1^2}{(k^2 + k_1^2)^2} e^{-2k_1 a} \approx T_0 e^{-2k_1 a}$$

prob of crossing the barrier

$T_0 = \frac{16 k^2 k_1^2}{(k^2 + k_1^2)^2}$

This quantity doesn't depend on a

① For a generic situation  $V$  is not longer a constant it depends on  $x$ .  
 Because  $V$  changes at different positions. Now the width of a single barrier  
 is  $\Delta x$  and we indicate the position of the barrier  $x_i$

•)  $K_1 \rightarrow K_1(x_i) = \frac{\sqrt{2m(V(x_i) - E)}}{\hbar}$

•)  $e^{-2K_1 a} \rightarrow e^{-2K_1(x_i)\Delta x} \equiv P(x_i)$  Prob. of  $e^-$  crossing the barrier  $x_i$

② Probability of crossing boxes is not correlated if the events are independent  
 as individual boxes.

$$P_{\text{Total}} = n\text{-independent events} = \prod_i P(x_i) = \prod_i e^{-2K_1(x_i)\Delta x} = e^{-2 \sum_i K_1(x_i)\Delta x}$$

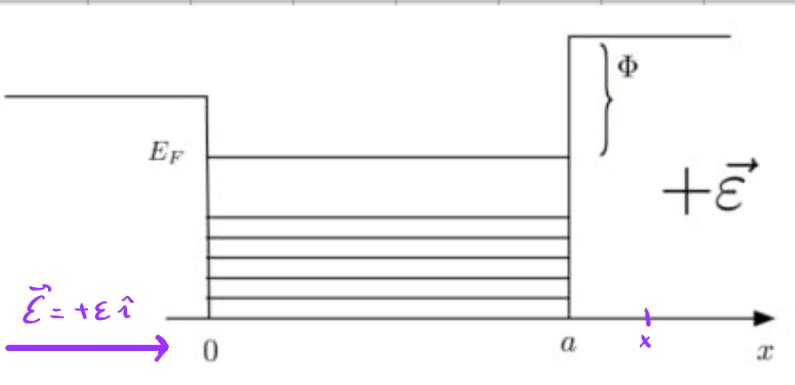
when  $\Delta x \rightarrow 0$  we integrate

$$\exp \left\{ -2 \int_a^b K(x) dx \right\} = \exp \left\{ -2 \int_a^b \frac{\sqrt{2m(V(x) - E)}}{\hbar} dx \right\}$$

$$P_{\text{Total}} = \exp \left\{ -2 \sqrt{\frac{2m}{\hbar^2}} \int_a^b \sqrt{|V(x) - E|} dx \right\}$$

where  $V(x)$  is a generic potential that  
 can take any value.

Let's apply the result we got to a finite potential well immersed in an electric field  $\vec{E}$  with an electron with a charge  $q = -|e|$



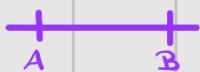
$$V_0 = E_F + \Phi$$

$$V(x) = \begin{cases} 0 & 0 \leq x \leq a \text{ (inside)} \\ V_0 & x > a, x < 0 \text{ (outside)} \end{cases}$$

The electric force is:  $\vec{F} = q \vec{E} = q \epsilon \hat{i}$

The work done by the electric field  $\vec{E}$  on the charge "q" from A to B is:

$$W = \int_A^B \vec{F} \cdot d\vec{s} = \int_A^B \vec{F} \cdot d\vec{x} = \int_A^B -|e|\epsilon dx = q \epsilon (x_B - x_A)$$

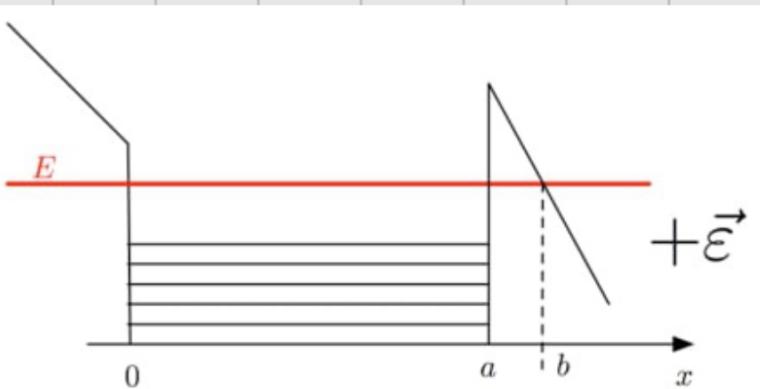


So, the general form of the potential we obtain is:

$$V(x) = V_0 + q \epsilon (x - a) \rightarrow \text{when } x > a$$

$$V(x) = V_0 + q \epsilon (-x) \rightarrow \text{when } x < 0$$

Taking into account that  $q = -|e|$  what we obtain is the next:



$$V(x) = \begin{cases} V_0 - |e|\epsilon(x-a) & x > a \\ 0 & 0 \leq x \leq a \\ V_0 + |e|\epsilon x & x < 0 \end{cases}$$

To calculate the probability of the  $e^-$  to tunneling we have to compute the integral  $\int_a^b \sqrt{V(x) - E} dx$ , but first some considerations. If we take a generic energy  $E$  we will have the next:

$$V(a) = V_0 = E_F + \phi$$

$$V(b) = E \Rightarrow V_0 - |e|E(b-a) = E \Rightarrow b = a + \frac{V_0 - E}{|e|E}$$

So we calculate the integral:

$$\int_a^{a + \frac{V_0 - E}{|e|E}} \sqrt{V_0 - |e|E(x-a) - E} dx \rightarrow \begin{cases} V_0 - E - |e|E(x-a) = y \\ -|e|E dx = dy \end{cases} \rightarrow -\frac{1}{|e|E} \int_{V_0 - E}^0 \sqrt{y} dy = \frac{1}{|e|E} \int_0^{V_0 - E} \sqrt{y} dy =$$

$$= \frac{2}{3|e|E} (V_0 - E)^{3/2}$$

Therefore:

$$P_T = \exp \left\{ -\frac{4}{3|e|E} \sqrt{\frac{2m}{\hbar^2}} (V_0 - E)^{3/2} \right\} = e^{-\frac{E_0}{E}} \quad \text{with} \quad E_0 = \frac{4}{3|e|} \sqrt{\frac{2m}{\hbar^2}} (V_0 - E)^{3/2}$$

By turning the  $E$  field we change the probability of the tunnelling. So if we increase the strength of the  $E$  field  $\Rightarrow$  We increase the probability of tunnelling.

Also, modifying the  $E$ -field will change the slope of  $V(x)$ .

① If we use Fermi Level energy:

$$E = E_F \Rightarrow V_0 - E = V_0 - E_F \equiv \phi$$

$$E_0 = \frac{4}{3} \sqrt{\frac{2m\phi^3}{\hbar^2|e|^2}}$$

② Tunnelling condition:  $\rightarrow V_0 - E = (b-a)|e|E$

$$P_T = \exp \left( -\frac{4}{3} \sqrt{\frac{2m|e|E}{\hbar^2}} (b-a)^{3/2} \right) \xrightarrow{\text{d = distance!!}} \text{Scanning Tunneling Microscope (STM)}$$

③ Using Fermi Level energy and tunnelling condition

$$\begin{aligned} V_0 - E_F &= (b-a)|e|E = d|e|E \\ \phi &= |e|E d \end{aligned}$$

$$\sqrt{\frac{2m|e|E}{\hbar^2}} (b-a)^{3/2} = \sqrt{\frac{2m|e|E d^2 d}{\hbar^2}} = \sqrt{\frac{2m\phi^3}{\hbar^2}} d$$

$$P_T = \exp \left( -\frac{4}{3} \sqrt{\frac{2m\phi^3}{\hbar^2}} d \right)$$

## Recap

Probability of tunnelling in presence of an electric field

- Depending on the energy:  $P_T(E) = \exp \left\{ -\frac{4}{3} \sqrt{\frac{2m}{\hbar^2 |e| \epsilon^2}} (V_0 - E)^{3/2} \right\}$

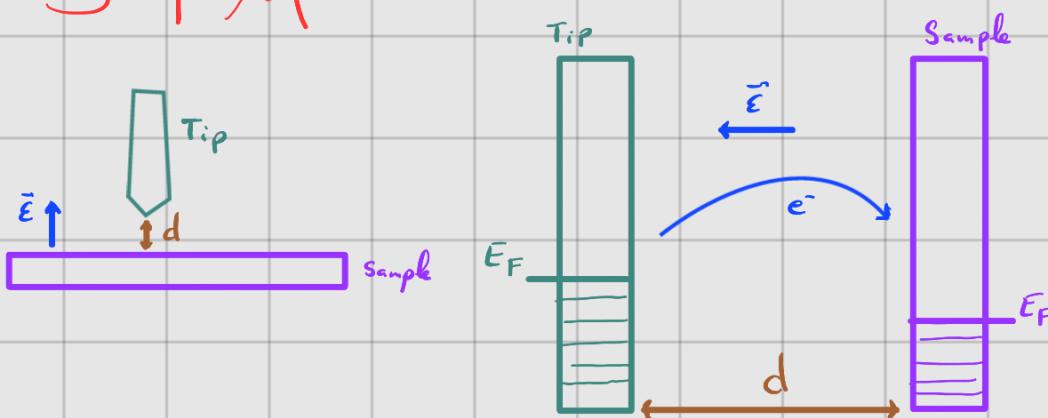
- Depending on Tunnelling distance:  $\exp -\frac{4}{3} \sqrt{\frac{2m |e| E}{\hbar^2}} d^{3/2}$

If we are in the Fermi Level  $\Rightarrow E = E_F$

- $P_T(E_F) = \exp \left\{ -\frac{4}{3} \sqrt{\frac{2m \phi^{3/2}}{\hbar^2 |e| \epsilon^2}} \right\}$

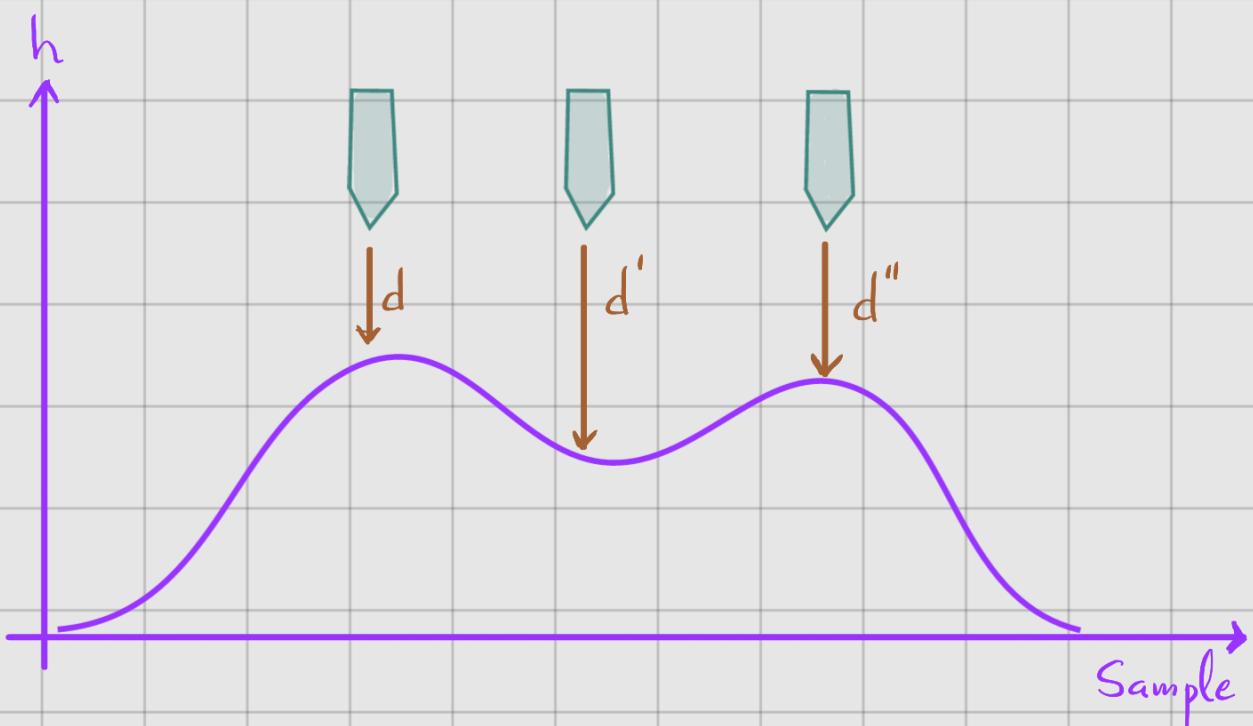
- $P_T(d) = \exp \left\{ -\frac{4}{3} \sqrt{\frac{2m \phi^{1/2}}{\hbar^2}} d \right\} \rightarrow \text{STM}$

## STM

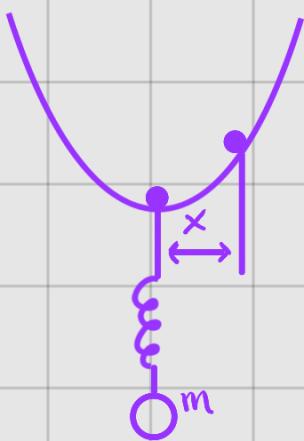


The distance between the tip and the sample is very small, in the range of nanometers. The electric field is applied in the direction of the tip, and the electron tunnel from the tip to the sample.

When the tunnelling gets to saturation, that is the sample has been charged such that it repels electron and no electron can tunnel from the tip to the sample. We change the direction of the electric field such that the  $e^-$  will tunnel backwards.



## Confinement of a particle in a Parabolic Well



The potential of the particle:  $V(x) = \frac{1}{2} kx^2$

The force:  $F(x) = kx$

The Schrödinger Equation:  $\left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} kx^2 \right] \psi(x) = E \psi(x)$

$$\hookrightarrow \text{spring constant } k \Rightarrow \omega_0 = \sqrt{\frac{k}{m}}$$

We rearrange the equation as:

$$\begin{aligned} \left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega_0^2 x^2 \right] \psi = E \psi &\Rightarrow \left[ -\frac{d^2}{dx^2} + \left( \frac{m \omega_0}{\hbar} \right)^2 x^2 \right] \psi = \frac{2mE}{\hbar^2} \psi \Rightarrow \\ \Rightarrow \left[ -\frac{d^2}{dx^2} + \left( \frac{x}{\hbar/m \omega_0} \right)^2 \right] \psi &= \frac{2mE}{\hbar^2} \psi \quad \rightarrow \bar{x} = \frac{x}{\hbar/m \omega_0} \Rightarrow dx = d\bar{x} \sqrt{\frac{\hbar}{m \omega_0}}, \bar{E} = \frac{E}{m \omega_0} \\ \Rightarrow \left[ -\frac{d^2}{d\bar{x}^2} + \bar{x}^2 \right] \psi(\bar{x}) &= 2\bar{E} \psi(\bar{x}) \end{aligned}$$

Finally we get the S. eq.

$$\left[ \frac{d^2}{dx^2} + (2\bar{E} - \bar{x}^2) \right] \Psi(\bar{x}) = 0$$

We can try a solution like:  $\Psi(\bar{x}) = e^{-\frac{\bar{x}^2}{2}} U(\bar{x})$  and we get:

$$\frac{d^2}{dx^2} U(\bar{x}) - 2\bar{x} \frac{dU(\bar{x})}{dx} + (2\bar{E} - 1) U(\bar{x}) = 0 \rightarrow \text{Hermite Equation}$$

o) It can only be solved if  $2\bar{E} - 1 = 2 \cdot n$

o) The solutions are Hermite polynomials  $H_0 = 1, H_1 = 2\bar{x}, H_2 = 4\bar{x}^2 - 2$

Therefore

$$E_n = \hbar\omega_0 \left( n + \frac{1}{2} \right) \rightarrow \text{The energy level is equidistance}$$

(unlike hydrogen atom:  $E_n = -\frac{1}{n^2}$  and finite well:  $E_n = E_1 \cdot n^2$ )

$$\Psi(\bar{x}) = A e^{-\frac{\bar{x}^2}{2}} H_n(\bar{x}) \rightarrow \Psi(x) = A e^{-\frac{x^2}{2\hbar\omega_0}} H\left(\sqrt{\frac{\hbar\omega_0}{m}}x\right)$$

The solution is:

$$E_n = \hbar\omega_0 \left( n + \frac{1}{2} \right)$$

$$\Psi_n(x) = A_n e^{-\frac{m\omega_0}{2\hbar} x^2} H_n\left(\sqrt{\frac{m\omega_0}{\hbar}}x\right)$$

Gaussian  $\rightarrow e^{-x^2/2\sigma^2}$

$\sigma = \sqrt{\frac{\hbar}{m\omega_0}}$

polynomial

$$\text{First electronic state: } \Psi_0(x) = A_0 e^{-\frac{m\omega_0}{2\hbar} x^2}$$

$$\text{Second electronic state: } \Psi_1(x) = A_1 e^{-\frac{m\omega_0}{2\hbar} x^2} 2x \sqrt{\frac{m\omega_0}{\hbar}}$$

In general we have:

↳ Eigenfunction ( $\Psi_{(n)}$ ) = Hermite Polynomial \* Gaussian function

↳ Energy has equal spacing

The subsequent states after the first electronic state are multiples of a gaussian state. The second state is like multiplying the gaussian by straight line.

Let's compute the constant  $A_0$  for the fundamental state.

$$\psi_0(x) = A_0 e^{-\frac{m\omega_0}{2\hbar}x^2}$$

Orthonormality:  $\int_{-\infty}^{+\infty} \psi_0^*(x) \psi_0(x) dx = 1$

$$\int_{-\infty}^{+\infty} A_0^* e^{-\frac{m\omega_0}{2\hbar}x^2} A_0 e^{-\frac{m\omega_0}{2\hbar}x^2} dx = |A_0|^2 \int_{-\infty}^{+\infty} e^{-\frac{m\omega_0}{\hbar}x^2} dx = \begin{cases} \frac{\sqrt{m\omega_0}}{\hbar} x = y \\ \frac{m\omega_0}{\hbar} dx = dy \end{cases}$$

$$= |A_0|^2 \sqrt{\frac{\hbar}{m\omega_0}} \int_{-\infty}^{+\infty} e^{-y^2} dy = |A_0|^2 \sqrt{\frac{\hbar}{m\omega_0}} \sqrt{\pi}$$

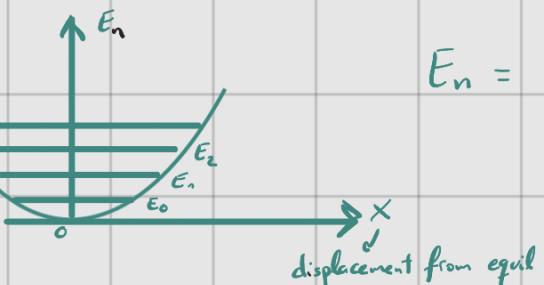
$\underbrace{\qquad}_{= \sqrt{\pi}}$

$$|A_0|^2 \sqrt{\frac{\hbar}{m\omega_0}} \sqrt{\pi} = 1 \Rightarrow A_0 = \left( \frac{m\omega_0}{\hbar\pi} \right)^{1/4}$$

## Recap

We saw the very important parabolic confinement

$$V(x) = \frac{1}{2} k x^2$$



$$E_n = \hbar \omega_0 \left( \frac{1}{2} + n \right) \rightarrow \Psi_n(x) = A_n e^{-\frac{m\omega_0}{2\hbar} x^2} H_n \left( x \sqrt{\frac{m\omega_0}{\hbar}} \right)$$

$$E_n = -\frac{R}{n^2}$$

gaussian x Pol. Hermite

$$H_0(x) = 1$$

$$H_1(x) = 2x$$

$$\Psi_0(x) = \text{ground state} = A_0 e^{-\frac{m\omega_0}{2\hbar} x^2} = \left( \frac{m\omega_0}{\hbar\pi} \right)^{1/4} e^{-\frac{m\omega_0}{2\hbar} x^2}$$

using:  $\int dx |\Psi_0(x)|^2 = 1$

$$\Psi_0(x, t) = \Psi_0(x) e^{-i \frac{E_0 t}{\hbar}}$$

Position expectation value: at ground state  $E_0$

$$\langle x(t) \rangle_0 = \int dx \Psi_{0(t)}^* x \Psi_{0(t)} = \int dx |\Psi_{0(t)}|^2 x = 0 \rightarrow \text{at origin!}$$

Expectation value of  $x^2$  at ground state  $E_0$

$$\langle x^2(t) \rangle_0 = \int dx \Psi_{0(t)}^* x^2 \Psi_{0(t)} = \int_{-\infty}^{\infty} dx |\Psi_{0(t)}|^2 x^2 = \sqrt{\frac{m\omega_0}{\hbar\pi}} \int_{-\infty}^{\infty} dx x^2 e^{-\frac{m\omega_0}{2\hbar} x^2} =$$

$= \frac{\hbar}{2m\omega_0} \longrightarrow x^2 \text{ account of the fluctuations of the wavefunction at the origin}$

$$\text{Variance: } \Delta x(t) = \sqrt{\langle x^2(t) \rangle - \langle x(t) \rangle^2} = \sqrt{\frac{\hbar}{2m\omega_0}}$$

Now we compute  $\langle p \rangle$  for  $E_0$

$$\langle p(t) \rangle_0 = \int dx \Psi_0^*(x) \left[ -i\hbar \frac{d}{dx} \right] \Psi_0(x) = 0$$

$$\langle p^2(t) \rangle = \int dx \Psi_0^*(x) \left[ -i\hbar \frac{d}{dx} \right]^2 \Psi_0(x) = \frac{\hbar \omega_0 m}{2}$$

$$\text{Variance} = \Delta p(t) = \sqrt{\langle p^2(t) \rangle - \langle p(t) \rangle^2} = \sqrt{\frac{\hbar \omega_0 m}{2}}$$

Now we take the product of these two variances:

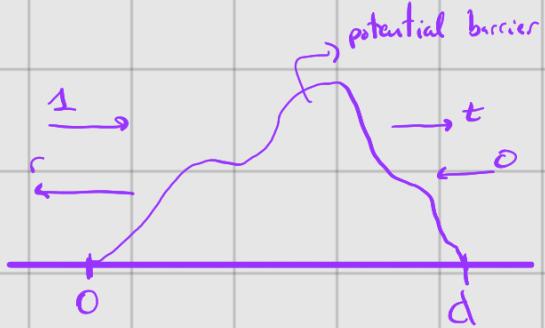
$$\Delta x(t) \cdot \Delta p(t) = \sqrt{\frac{\hbar}{2m\omega_0}} \cdot \sqrt{\frac{\hbar \omega_0 m}{2}} = \frac{\hbar}{2}$$

This is the Heisenberg uncertainty principle:

$$\boxed{\Delta x \Delta p \geq \frac{\hbar}{2}}$$

In the ground state where we are, we have MUS (minimum uncertainty state) that is where we have the equal in the Heisenberg relation. We cannot go below that value.

# Transfer Matrix



$$\bar{u}(o) = \begin{pmatrix} 1 \\ o \end{pmatrix} \quad \text{moving direction: } \rightarrow$$

$$\bar{u}(d) = \begin{pmatrix} t \\ 0 \end{pmatrix} \quad \text{moving direction: } \leftarrow$$

$$\bar{u}(d) = M \bar{u}(o)$$

Transfer Matrix (2x2)

$r$  = complex reflection coefficient =  $|r| e^{i\phi}$

$t$  = complex transfer coefficient

So we have expanded the matrix.  $\begin{pmatrix} t \\ o \end{pmatrix} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \begin{pmatrix} 1 \\ r \end{pmatrix}$

This matrix should describe the direct process and also time reverse

process  $\Rightarrow$  Transpose + Complex Conjugate

For the time reverse process:



$$\bar{u}(d) = \begin{pmatrix} 0 \\ t^* \end{pmatrix} \quad \bar{u}(o) = \begin{pmatrix} r^* \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} 0 \\ t^* \end{pmatrix} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \begin{pmatrix} r^* \\ 1 \end{pmatrix}$$

In the end we have 4 eqs. and 4. unknowns

$$t = m_{11} + m_{12} r$$

$$0 = m_{21} + m_{22} r$$

$$0 = m_{11} r^* + m_{12}$$

$$t^* = m_{21} r^* + m_{22}$$

$$M = \begin{pmatrix} \frac{1}{1-|r|^2} & -\frac{t r^*}{1-|r|^2} \\ -\frac{t^* r}{1-|r|^2} & \frac{t^*}{1-|r|^2} \end{pmatrix} = \frac{1}{1-|r|^2} \begin{pmatrix} t & -t r^* \\ -t^* r & t^* \end{pmatrix}$$

# The transfer Matrix

$$M = \frac{1}{1-|r|^2} \begin{pmatrix} t & -tr^* \\ -t^*r & t^* \end{pmatrix}$$

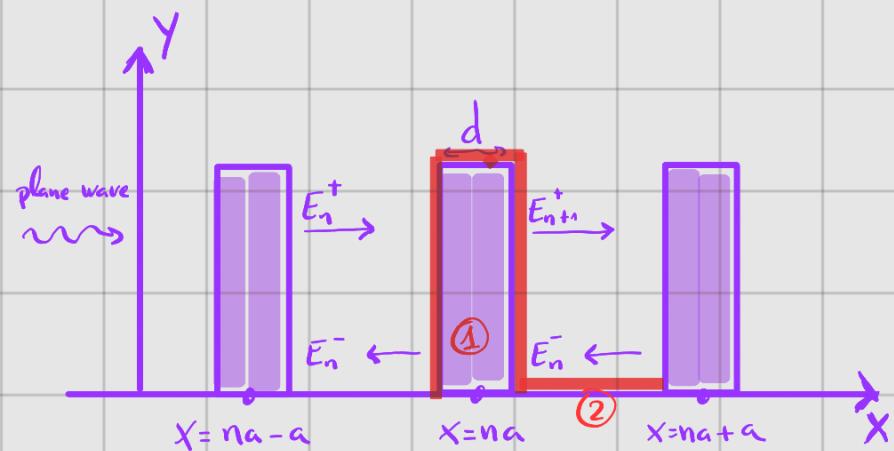
The determinant

$$\det M = \frac{|t|^2}{(1-|r|^2)^2} - \frac{|t|^2|r|^2}{(1-|r|^2)^2} \Rightarrow \det M = \frac{|t|^2}{1-|r|^2}$$

① No Absorption :  $1 = |r|^2 + |t|^2 \Rightarrow \det M = 1$

② Absorption :  $1 \neq |r|^2 + |t|^2 \Rightarrow \det M \neq 1$

## Block Modes in a Periodic Structure



$a$  = period

$w = ck$

$$k_n = \frac{w}{c} = k$$

$a$  = period

$$\vec{E}(\vec{r}, t) = \vec{E}(x, t) = \hat{\vec{y}} \left[ E_n^+(\vec{r}) + E_n^-(\vec{r}) \right] e^{-iwt} = \hat{\vec{y}} \left[ E_n^+ e^{ikx} + E_n^- e^{-ikx} \right] e^{-iwt}$$

↳ field amplitude      ↳ plane wave

① Through the barrier

$$\begin{pmatrix} E_{n+1}^+(x) \\ E_{n+1}^-(x) \end{pmatrix} = \frac{1}{1-|r|^2} \begin{pmatrix} t & -r^*t \\ -rt^* & t^* \end{pmatrix} \begin{pmatrix} E_n^*(x) \\ E_n^-(x) \end{pmatrix} \quad x = na - \frac{d}{2}$$

② Travelling from the end of barrier to the beginning of the next barrier

$$\begin{pmatrix} E_{n+1}^+(x) \\ E_{n+1}^-(x) \end{pmatrix} = \begin{pmatrix} e^{ik(a-d)} & 0 \\ 0 & e^{-ik(a-d)} \end{pmatrix} \begin{pmatrix} E_n^*(x) \\ E_n^-(x) \end{pmatrix}$$

$x = na + \frac{d}{2}$

Computing the chain of matrix:

$$\begin{pmatrix} E_{n+1}^+(x) \\ E_{n+1}^-(x) \end{pmatrix} = \begin{pmatrix} e^{ik(a-d)} & 0 \\ 0 & e^{-ik(a-d)} \end{pmatrix} \frac{1}{1 - |r|^2} \begin{pmatrix} t & -r^*t \\ -r^*t^* & t^* \end{pmatrix} \begin{pmatrix} E_n^*(x) \\ E_n^-(x) \end{pmatrix}$$

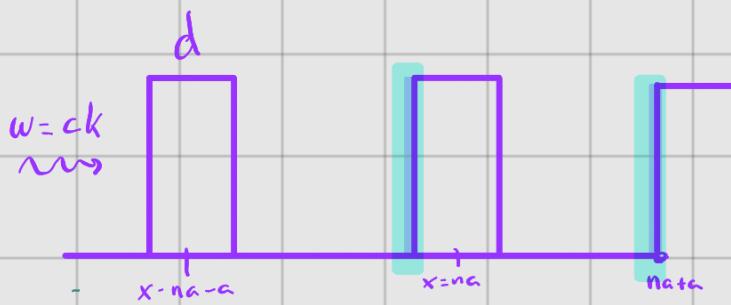
$x = na + a - \frac{d}{2}$

$$M = \frac{1}{1 - |r|^2} \begin{pmatrix} t & -rt^* \\ -r^*t & t^* \end{pmatrix}$$

$r$  and  $t$  complex functions



## Block Theorem



$$\textcircled{1} \quad \begin{pmatrix} E_{n+1}^+(x) \\ E_{n+1}^-(x) \end{pmatrix}_{x=na + \frac{d}{2}} = \begin{pmatrix} e^{ik(a-d)} & 0 \\ 0 & e^{-ik(a-d)} \end{pmatrix} [M] \begin{pmatrix} E_n^+(x) \\ E_n^-(x) \end{pmatrix}_{x=nc - \frac{d}{2}}$$

$\rightarrow$  straight wavevector  
 $w/c = 2\pi/\lambda \neq k$

$$E_{n+1}(x+a) = e^{ika} E_n(x)$$

Block wavevector  $\rightarrow$  it is the wavevector inside the structure

Using block theorem we get:

$$\textcircled{2} \quad \begin{pmatrix} E_{n+1}^+(x) \\ E_{n+1}^-(x) \end{pmatrix}_{x=na + \frac{d}{2}} = \begin{pmatrix} e^{ika} & 0 \\ 0 & e^{-ika} \end{pmatrix} \cdot \begin{pmatrix} E_n^+(x) \\ E_n^-(x) \end{pmatrix}_{x=nc - \frac{d}{2}}$$

$$\begin{pmatrix} e^{ik(a-d)} & 0 \\ 0 & e^{-ik(a-d)} \end{pmatrix} \frac{1}{D} \begin{pmatrix} t & -tr^* \\ -t^r & t^* \end{pmatrix} - \begin{pmatrix} e^{ika} & 0 \\ 0 & e^{-ika} \end{pmatrix} \begin{pmatrix} E_n^+(x) \\ E_n^-(x) \end{pmatrix} = 0$$

Determinant of

$$\frac{1 - |r|^2}{|t|^2} e^{2ika} - 2 \operatorname{Re} \left[ \frac{e^{ik(a-d)}}{t^*} \right] e^{ika} + 1 = 0$$

Equation for the structure  
 $f(k, k) = 0$

We can solve it analytically for some specific cases:

(A) Vacuum:

$$e^{2ika} - 2 \operatorname{Re} [e^{ik(a-d)}] e^{ika} + 1 = 0$$

$$e^{ika} - 2 \cos(ka) + e^{-ika} = 0$$

$$2 \cos ka = 2 \cos ka \quad \longrightarrow \quad k = \ell_k = \frac{\omega}{c}$$

(B) When we have  $\boxed{\begin{matrix} \epsilon \\ d \\ \epsilon \end{matrix}}$  the same medium (refractive index  $n$ ) so:  $d \rightarrow a$

$$w = ck \\ \sim n$$



Fresnel:

$$r = \frac{(n^2 - 1)(e^{2ika} - 1)}{(n+1)^2 - (n-1)^2 e^{2ika dn}}$$

$$t = \frac{4n e^{ikdn}}{\text{same}} \rightarrow \frac{u}{t} = \frac{(n+1)^2 e^{-ikdn}}{4n} - \frac{(n-1)^2 e^{+ikdn}}{4n}$$

We also take  $n = \text{real}$  and  $\alpha_0$  absorption

$$e^{izka} - 2\operatorname{Re} \left[ \frac{-(n+1)^2 e^{ikdn}}{4n} - \frac{(n-1)^2 e^{-ikdn}}{4n} \right] e^{ika} + 1 = 0$$

$$-2 \cos kdn \left( \frac{(n+1)^2}{4n} - \frac{(n-1)^2}{4n} \right)$$

$$e^{izka} - 2 \cos kdn e^{ika} + 1 = 0$$

$$e^{ika} - 2 \cos kdn + e^{-ika} = 0$$

$$\cos ka = \cos kdn \quad \rightarrow \quad k = kn \quad \omega = \frac{c}{n} k$$

(C)  $\alpha_0$  absorption

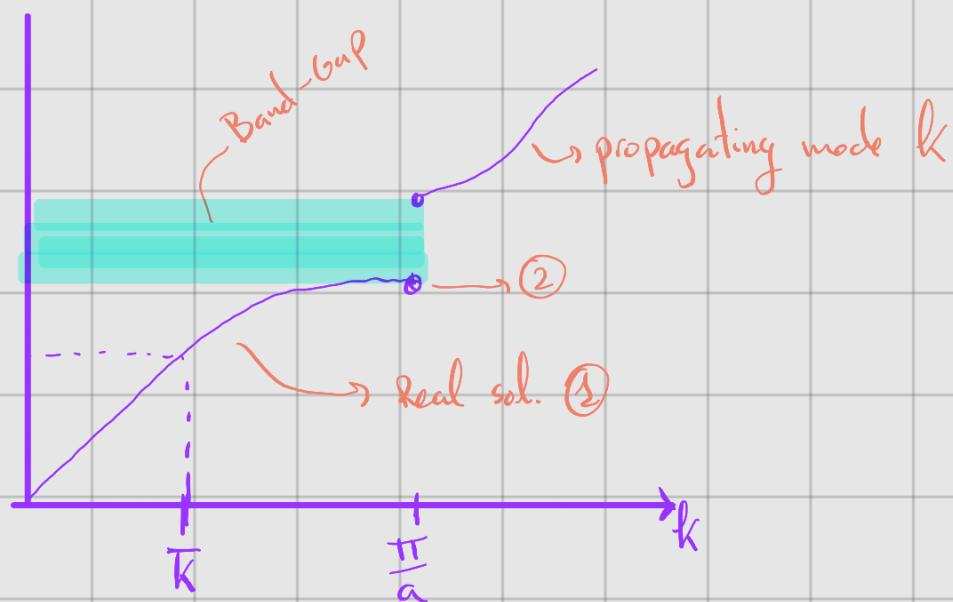
$$\cos ka = \operatorname{Re} \left[ \frac{e^{ik(a-d)}}{t^*} \right]$$

(Case 1)  $-1 < \operatorname{Re}[ ] < 1 \Rightarrow$  Real solution  $k$

(Case 2)  $\operatorname{Re}[ ] = 1 \Rightarrow$  Real sol.  $k$

(Case 3)  $\operatorname{Re}[ ] > 1$  or  $< -1 \Rightarrow$  Imaginary Solution  $k$

Bloch dispersion  
for a photonic  
periodic structure



Bloch Theorem for  $e^- \Rightarrow$

$$\Psi(x+a) = e^{ika} \Psi(x)$$

here  $k$  is de Broglie wavevector

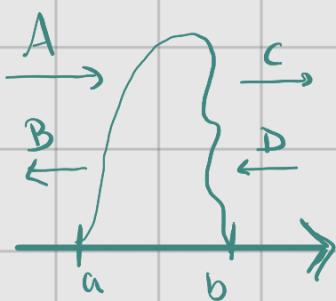
Creating defects in the structure we can trap a photon. In the place of the defect the photon will see a periodic structure but choosing the correct frequency we trap the photon

## Recap

S.E.

$$i\hbar \partial_t \Psi(x,t) = \frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi(x,t) + V(x_1) \Psi(x,t) \rightarrow \Psi(x,t) = \Psi(x_1) e^{-i \frac{E}{\hbar} t}$$

S.S. | S.E.



$$\Psi(x) = A e^{ikx} + B e^{-ikx} \quad x < a$$

$$\Psi(x) = \Psi_{ab}(x)$$

$$\Psi(x) = C e^{ikx} + D e^{-ikx} \quad x > b$$

Boundary Conds.  $\rightarrow \{A, B, C, D\}$

$$\vec{u}(b) = M \vec{u}(a)$$

↓ transfer matrix

$$\begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix}$$

wave direct  $\rightarrow$   
wave direct.  $\leftarrow$

Applying time reversal:  $t \rightarrow -t$

Now  $\Psi(x, -t)$  doesn't satisfy the original S.E.  $i\hbar \partial_t \Psi \rightarrow -i\hbar \partial_t \Psi$

We use:  $\Psi^*(x, -t)$

Original

$$\Psi(x,t) = e^{-i \frac{E}{\hbar} t} \cdot \begin{cases} A e^{ikx} + B e^{-ikx} & x < a \\ \Psi_{ab}(x) & \\ C e^{ikx} + D e^{-ikx} & x > b \end{cases}$$

Time reversal

$$\psi_{(x,-t)}^* = e^{-\frac{iE}{\hbar}t} \cdot \begin{cases} A^* e^{-ikx} + B^* e^{+ikx} & x \leq a \\ \psi_{ab}^*(x) & \\ C^* e^{-ikx} + D^* e^{+ikx} & x > b \end{cases}$$

$$\begin{pmatrix} D^* \\ C^* \end{pmatrix} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \begin{pmatrix} B^* \\ A^* \end{pmatrix}$$

Expanding the matrix and doing the complex conjugate

$$C = m_{21}^* B + m_{22}^* A$$

$$D = m_{11}^* B + m_{12}^* A$$

$$\Rightarrow \begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} m_{22}^* & m_{21}^* \\ m_{12}^* & m_{11}^* \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix}$$

$\underbrace{\phantom{m_{11}^* m_{12}^*}}_M$

So now we know:

$$m_{11} = m_{22}^*$$

$$m_{21}^* = m_{12}$$

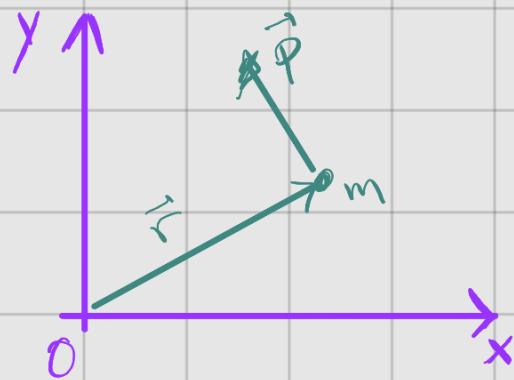
$$\Rightarrow M = \boxed{\begin{pmatrix} m_{11} & m_{12} \\ m_{12}^* & m_{11}^* \end{pmatrix}}$$

Previously in the notes we said that transmission and reflection were connected. We did in the notes: transpose and conjugate.

Here in time reversal we did it.

# Angular Momentum

$$\vec{L} = \vec{r} \times \vec{p}$$



① Highschool level to compute  $\vec{L}$

Magnitude:  $|L| = |r| |p| \sin\theta$

Direction: pulgar:  $r$ , índice:  $p$ , corazón:  $L$

② Bachelor's level to compute  $\vec{L}$

$$\vec{r} = (x, y, z)$$

$$\vec{p} = (p_x, p_y, p_z)$$

$$\vec{L} = \begin{pmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ p_x & p_y & p_z \end{pmatrix}$$

$$L_x = y p_z - z p_y$$

$$L_y = z p_x - x p_z$$

$$L_z = x p_y - y p_x$$

We have to go to quantum world:  $P_x = m V_x \longrightarrow \left( -i\hbar \frac{\partial}{\partial x} \right)$

$$\hat{L}_x = -i\hbar (y \partial_z - z \partial_y)$$

$$\hat{L}_y = -i\hbar (z \partial_x - x \partial_z)$$

$$\hat{L}_z = -i\hbar (x \partial_y - y \partial_x)$$

Some operators will commute but not all

Commutator:  $[\hat{A}, \hat{B}] = \hat{A} \cdot \hat{B} - \hat{B} \cdot \hat{A}$

$$[Ex1]: [\hat{x}, \hat{p}] = \hat{x} \hat{p} - \hat{p} \hat{x} = x (-i\hbar \partial_x) - (-i\hbar \partial_x) x$$

$$[\hat{x}, \hat{p}] f = x (-i\hbar) \partial_x f - (-i\hbar) \partial_x (x f) = -i\hbar [x \partial_x f - f - x \partial_x f] = i\hbar f(x)$$

$$[\hat{x}, \hat{p}] = i\hbar$$

$$[Ex2]: [\hat{L}_x, \hat{L}_y] = \hat{L}_x \hat{L}_y - \hat{L}_y \hat{L}_x = (y \hat{p}_z - z \hat{p}_y)(-x \hat{p}_z + z \hat{p}_x) - (-x \hat{p}_z + z \hat{p}_x)(y \hat{p}_z - z \hat{p}_y) = i\hbar (x p_y - y p_x) i\hbar \hat{L}_z$$

$$[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$$

We can see the cyclic property of the commutator of the angular moment

$$[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$$

X ↘

$$[\hat{L}_y, \hat{L}_z] = i\hbar \hat{L}_x$$

②

Y

$$[\hat{L}_z, \hat{L}_x] = i\hbar \hat{L}_y$$

Theorem: If two operators commute then there is always a common set of eigenfunctions that describes both

$$[\hat{A}, \hat{B}] = 0 \rightarrow \begin{aligned} \hat{A} \Psi &= a \Psi \\ \hat{B} \Psi &= b \Psi \end{aligned} \begin{matrix} \text{same } \Psi \\ \text{(eigenfunc)} \end{matrix} \quad \text{set of eigenfunc } \{\Psi, \Phi, \Psi\}$$

I cannot measure simultaneously two observables when they don't commute.

$$\hat{K} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}$$

$$\hat{A} \rightarrow \hat{P}$$

$$\hat{B} \rightarrow \hat{K} \text{ (kinetic energy)}$$

$$[\hat{P}, \hat{K}] = 0$$

The common eigenfunction is the one of free particle (plane wave)

So we get  $\Psi = A e^{ikx} \Rightarrow$  We can measure both

$$\begin{aligned} \hat{P} e^{ikx} &= a e^{ikx} \\ \hat{K} e^{ikx} &= b e^{ikx} \end{aligned} \quad \left. \begin{array}{l} a = \hbar k \\ b = \frac{\hbar^2}{2m} k^2 \end{array} \right\}$$

More commutators:

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

$$[\hat{L}^2, \hat{L}_x] = [\hat{L}_x^2, \hat{L}_x] + [\hat{L}_y^2, \hat{L}_x] + [\hat{L}_z^2, \hat{L}_x]$$

$$\hookrightarrow [\hat{L}_y, \hat{L}_x] + [\hat{L}_y, \hat{L}_x] \hat{L}_y$$

$$[\hat{A} \hat{B}, \hat{C}] = \hat{A} [\hat{B}, \hat{C}] + [\hat{A}, \hat{C}] \hat{B}$$

$$[\hat{L}^2, \hat{L}_x] = [\hat{L}^2, \hat{L}_y] = [\hat{L}^2, \hat{L}_z] = 0$$

So we can find a common base

$$\{\Psi_{lm}\}$$

$\downarrow$   
common set of eigenfunt.

$$\hat{L}^2, \hat{L}_z$$

$$\hat{L}^2 \Psi_{lm} = \hbar^2 l(l+1) \Psi_{lm}$$

$$\hat{L}_z \Psi_{lm} = \hbar m \Psi_{lm}$$

We will start with this equation

$$\left\{ \begin{array}{l} L^2 \Psi_{lm} = \hbar^2 l(l+1) \Psi_{lm} \\ L_z \Psi_{lm} = \hbar m_l \Psi_{lm} \end{array} \right. \quad \begin{array}{l} l = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \dots, n-1 \\ m_l = -l, \dots, 0, \dots, l-1, l \end{array}$$

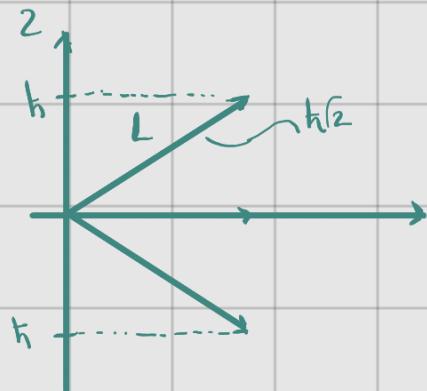
energy level minus one

So we can see that we can only have a certain values of the angular momentum. It is discrete or quantized  $\Rightarrow L = \hbar \sqrt{l(l+1)}$

The value  $l=0 \Rightarrow m=0 \Rightarrow$  Is a particle with no angular momentum

Example:

a)  $l=1 \Rightarrow m = \begin{cases} \hbar \\ \hbar \\ \hbar \\ \hbar \end{cases}$   
 $L = \hbar \sqrt{2}$



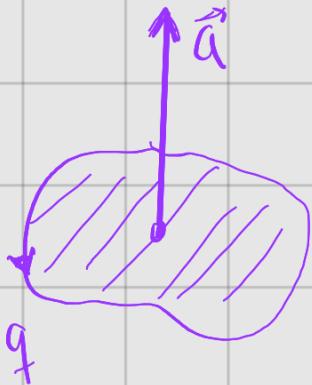
b)  $l = \frac{1}{2} \Rightarrow m = -\frac{1}{2}, \frac{1}{2}$

$$L = \frac{\hbar}{2} \sqrt{3}$$

So in the nanoworld we cannot change the angular momentum continuously, it will change in units of  $\hbar$  ( $\hbar, 2\hbar, 3\hbar, \dots$ )

# Orbital Angular Momentum

No  $\frac{1}{2}$  integer values:  $\cancel{\frac{1}{2}}, \cancel{\frac{3}{2}}, \dots$



$$I = \text{current} = q \cdot v \quad (\omega = 2\pi v)$$

$v$  = frequency

Magnetic momentum:  $\bar{\mu} = I \bar{a} = \text{Orbital magnetic momentum}$

$$\begin{aligned} \bar{\mu} &= I \bar{a} = I a \cdot \hat{a} = qv \cdot a \hat{a} = qv \pi r^2 \hat{a} = \\ &= -1e \nu \pi r^2 \hat{a} \end{aligned}$$

area enclosed by loop

Calculating  $\vec{L}$  we know that  $\vec{r} \perp \vec{p}$

$$\vec{L} = \vec{r} \times \vec{p} = rp = rmv = rm\omega r \hat{a} = 2\pi \nu m r^2 \hat{a}$$

Using both results:

$$\boxed{\bar{\mu} = -\frac{1e}{2m} \vec{L}}$$

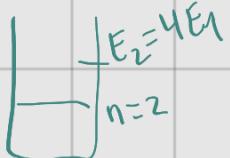
Now applying quantum we get that the directions of  $\bar{\mu}$  are also discrete.

$$|\bar{\mu}| = \frac{1e}{2m} |\vec{L}| = \frac{1e}{2m} \hbar \sqrt{l(l+1)} = \mu_B \sqrt{l(l+1)}$$

$$\boxed{|\bar{\mu}| = \mu_B \sqrt{l(l+1)}}$$

Bohr's magneton:  $\mu_B = 5,79 \cdot 10^{-5} \text{ eV/T}$

Example

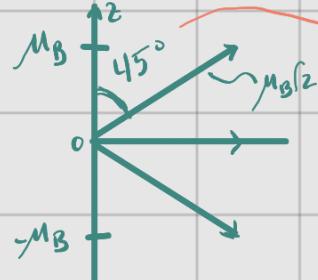


$$n=2 \Rightarrow l=0, 1$$

$$\circ l=0 \Rightarrow \mu=0$$

$$\circ l=1 \Rightarrow |\bar{\mu}| = \mu_B \sqrt{(l+1) \cdot 1} = \sqrt{2} \mu_B \neq 0$$

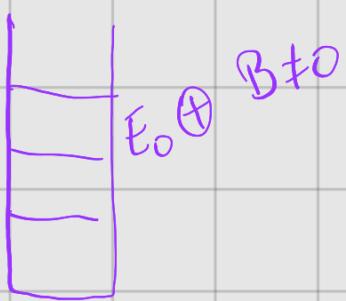
$$\begin{aligned} m &= 1, 0, -1 \\ L &= -\mu_B \cdot 1 \\ &- \mu_B \cdot 0 \\ &- \mu_B \cdot (-1) \end{aligned}$$



It is  $45^\circ$  because

$$\begin{aligned} \cos \theta &= \frac{\mu_B}{\sqrt{2} \mu_B} \\ \theta &= 45^\circ \end{aligned}$$

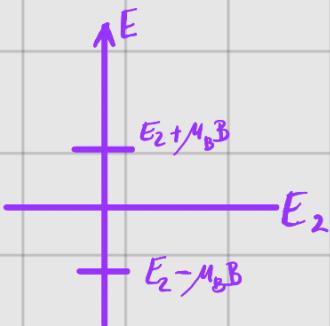
Now if we put a magnetic field



$$\text{Interaction} \rightarrow E_0 - \vec{\alpha} \cdot \vec{B} = E_0 + \frac{|e|}{2m} \vec{L} \cdot \vec{B} = E_0 + \frac{|e| h m_e}{2m} B = E_0 + \mu_B B m_e$$

$$E = E_0 + \mu_B B m_e$$

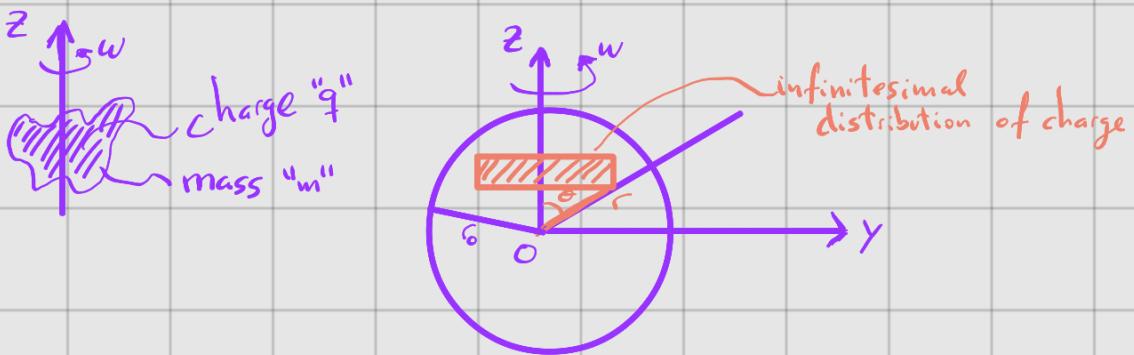
Zeeman



22/11/2022

# Electron Intrinsic Angular Momentum SPIN

Each particle has his own orbital angular momentum. The  $e^-$  is a distribution of charge rotating about some direction



$$\text{Rotation} \Rightarrow d\vec{\mu} = (\nu q) \cdot \text{surface } \hat{k} = (\nu dq) \cdot (\pi r^2) \hat{k}$$

$$dq = g \cdot dv = g r^2 dr \sin\theta d\theta d\varphi$$

$$g = \frac{q}{\frac{4}{3} \pi r_0^3} \quad \begin{matrix} \text{tot. charge} \\ \text{sphere} \end{matrix}$$

$$\text{Magnetic moment due rotation } \boxed{\text{||||}} \Rightarrow d\vec{\mu} = \nu dq (\pi r^2) \hat{k} = \pi \nu g r^4 dr \sin^3 \theta d\theta d\varphi \hat{k}$$

$$\text{Total is: } \vec{\mu} = \int d\vec{\mu} = \nu \pi g \frac{r_0^5}{5} 2\pi \int_0^\pi d\theta \sin^3 \theta = \frac{8}{3} \pi^2 \nu g \cdot \frac{r_0^5}{5} \hat{k}$$

Magnetic momentum induced by ROTATION in z axis

$$\Rightarrow \boxed{\vec{\mu} = \frac{8}{3} \pi^2 \nu g \frac{r_0^5}{5} \hat{k}}$$

Now, we have to compute the angular momentum of the sphere

$$\vec{S} = I\omega = \frac{2}{5}m r_0^2 2\pi D \hat{k}$$

If we compare both we get:

$$\vec{\mu} = \frac{q}{2m} \vec{S}$$



magnetic moment due to the intrinsic rotation  
angular momentum due to rotation

Remember:  $\vec{\mu} = \frac{q}{2m} \cdot \vec{L}$  → magnetic moment due to orbital momentum



IMPORTANT: The right value is  $\vec{\mu}_s = -\frac{1e1}{m} \vec{S}$  for the electron

the discrepancy comes from the fact that the  $e^-$  is not a ball but a wavefunction. Also, to find the right solution we have to take into account that the  $e^-$  is a relativistic particle.

Right values:

$$\vec{\mu} = -\frac{1e1}{2m} \vec{L}$$

$$\vec{\mu}_s = -\frac{1e1}{m} \vec{S}$$

Coming back to the orbital equations:

$$\begin{cases} L^2 \Psi_{lm} = h^2 l(l+1) \Psi_{lm} \\ L_z \Psi_{lm} = h m_l \Psi_{lm} \end{cases}$$

For the electron

$$\begin{cases} S^2 \chi_{s,m_s} = \hbar^2 s(s+1) \chi_{s,m_s} \\ S_z \chi_{s,m_s} = \hbar m_s \chi_{s,m_s} \end{cases} \Rightarrow m_s = -\frac{1}{2}, m_s = +\frac{1}{2}$$

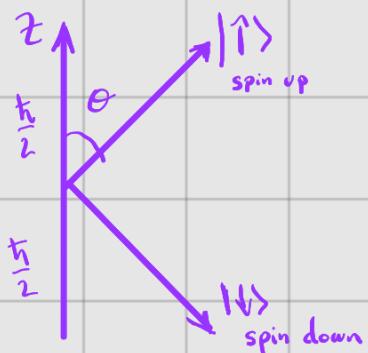
the value of  $s = \frac{1}{2}$  (experiments)

$$\chi_{\frac{1}{2}, \frac{1}{2}} \rightarrow | \uparrow \rangle$$

$$\chi_{\frac{1}{2}, -\frac{1}{2}} \rightarrow | \downarrow \rangle$$

Calculating the angles of orientation:

$$S = \hbar \sqrt{s(s+1)} = \hbar \frac{\sqrt{3}}{2}$$



$$\frac{\hbar}{2} = \frac{\hbar}{2} \sqrt{3} \cos \theta \Rightarrow \theta =$$

Therefore the full wavefunction of an electron inside the quantum well is:

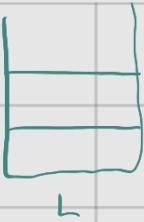
spatial part, orbital part, spin part

$$\text{space} \rightarrow \psi(x) = \sqrt{\frac{2}{L}} \sin \frac{\pi}{L} 2x$$

$$\text{orbital: } \varphi_{l,m_l}$$

$$\text{spin: } \chi_{s,m_s}$$

$$\psi = A \sqrt{\frac{2}{L}} \sin \left( \frac{\pi}{L} 2x \right) \varphi_{l,m_l} \chi_{s,m_s}$$

Example :   $n=2 \rightarrow E_2 = 4E_1$

Orbital angular momentum:  $\ell=0$ ,  $\ell=1$

$$\downarrow$$

$$L=0$$

$$|\vec{m}|=0$$

$$\downarrow$$

$$L=\hbar\sqrt{2}$$

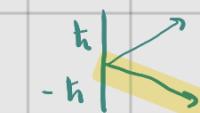
$$|\vec{m}| = \frac{|e|}{2m} \hbar\sqrt{2} = \sqrt{2}/\mu_B$$

$$\downarrow$$



3 possible orientation  $\vec{m}_z$

$$S = \frac{1}{2} \rightarrow \chi_{\frac{1}{2}, \frac{1}{2}} \\ \chi_{\frac{1}{2}, -\frac{1}{2}}$$



2 possible spin

The wavefunction in case of — is :  $\Psi \sim \sqrt{\frac{2}{L}} \sin \varphi_{1,1} \chi_{\frac{1}{2}, \frac{1}{2}}$

## Recap

## Spin

$$\begin{aligned} S^2 \chi_{s,m_s} &= \hbar^2 s(s+1) \chi_{s,m_s} \\ S_z \chi_{s,m_s} &= \hbar m_s \chi_{s,m_s} \end{aligned} \Rightarrow \begin{aligned} \text{spin } e^- = \frac{1}{2} &\Rightarrow \chi_{\frac{1}{2}, \frac{1}{2}} \text{ spin up} \\ m_s = -\frac{1}{2}, \frac{1}{2} &\Rightarrow \chi_{\frac{1}{2}, -\frac{1}{2}} \text{ spin down} \\ \Rightarrow \vec{\mu}_s = -\frac{|e|}{m} \vec{S} &\Rightarrow \vec{\mu} = -\frac{|e|}{2m} \vec{L} \end{aligned}$$

We have now an electron with no orbital angular momentum ( $l=0$ )

(A) No magnetic field  $B=0$

$$\vec{E} = E_0$$

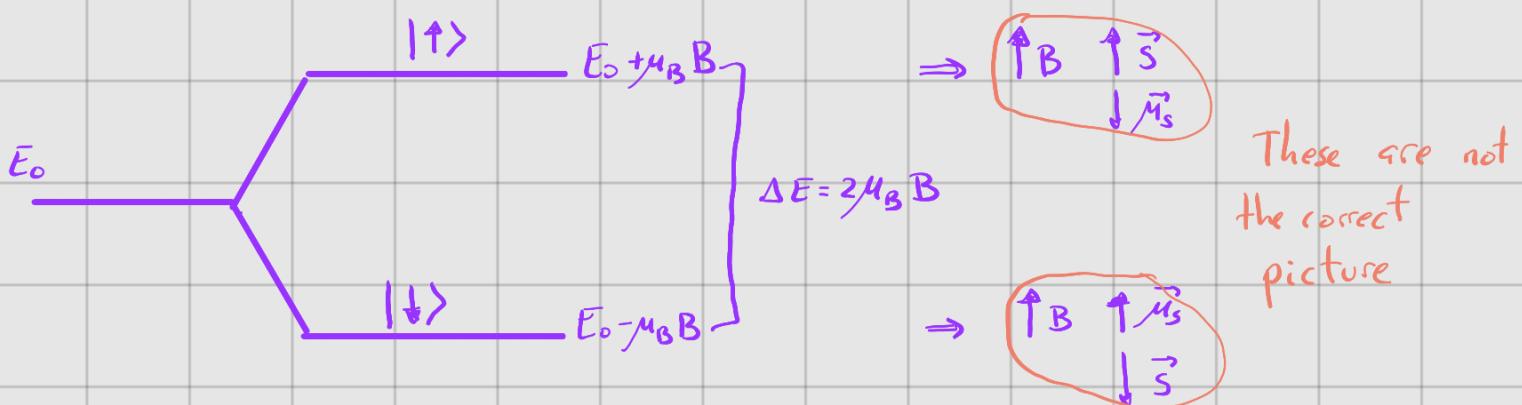
(B) Constant magnetic field  $\vec{B} = B \hat{k}$

$$\begin{aligned} E &= E_0 - \vec{\mu} \cdot \vec{B} = E_0 - \left( -\frac{|e|}{m} \vec{S} \right) \cdot \vec{B} = E_0 + \frac{|e|}{m} [S_z] B = \\ &= E_0 + \frac{|e|}{m} \hbar m_s B = E_0 + \frac{\hbar |e|}{2m} 2 m_s B = 2 \text{ possibilities} \end{aligned}$$

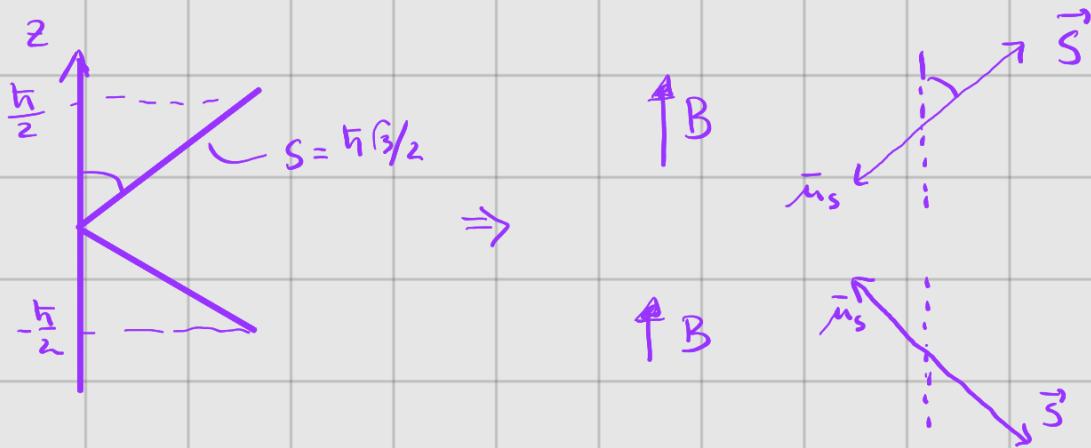
$$\boxed{1} \Rightarrow E_0 + \frac{\hbar |e|}{2m} B = E_0 + \mu_B B$$

$$\boxed{2} \Rightarrow E_0 - \frac{\hbar |e|}{2m} B = E_0 - \mu_B B$$

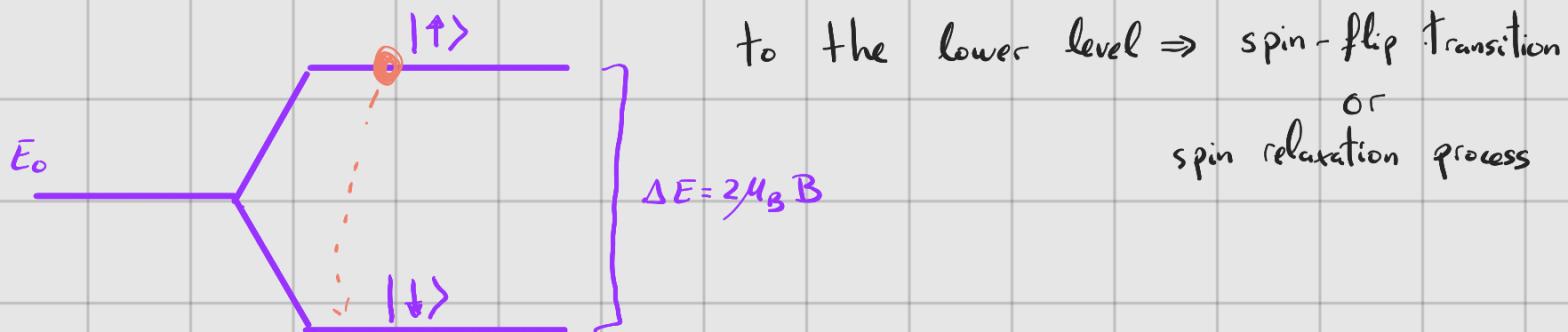
So, we will have the energy level splitted in two levels



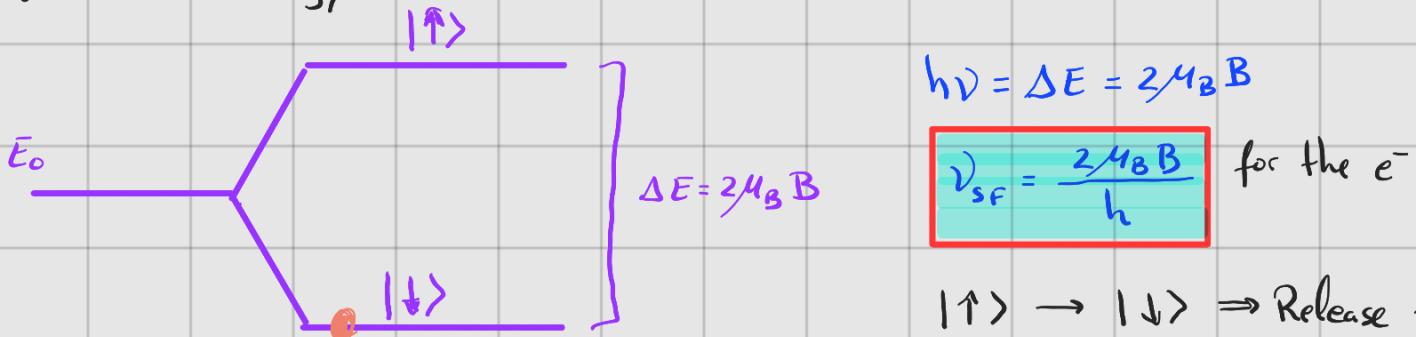
In fact, the spin has this direction



If we have an  $e^-$  in the level shown, after a while it can decay



If we are in the lower state and we want to go back to the upper level we need energy



$|↑⟩ \rightarrow |↓⟩ \Rightarrow$  Release photon

Using some numbers:

$$\nu_{SF} = \frac{2 \cdot 5,79 \cdot 10^{-5} \frac{\text{eV}}{\text{T}} \cdot 1 \text{T}}{10^{-15} \text{ eV} \cdot \text{s}} = 3 \cdot 10^{10} \text{ Hz} \longrightarrow \text{microwaves frequency}$$

The photon is a microwave photon when we put 1 Tesla

## {Nuclear Magnetic Resonance}

NMR is the previous situation but for the proton. Also, the proton does not have orbital ang. moment. and its spin is like  $e^-$

$$\rightarrow l=0, \quad s=\frac{1}{2}$$

So everything is like with the  $e^-$  in the previous case. We can introduce the gyro magnetic factor:  $g_s$

$$(\text{electron}) \rightarrow \vec{\mu} = -\frac{1e1}{m} \vec{S} = -g_s \frac{1e1}{2m} \vec{S} \Rightarrow g_s = 2$$

$$(\text{proton}) \rightarrow \vec{\mu} = \dots = +g_p \frac{1e1}{2m_p} \vec{S} \Rightarrow g_p = 5,597 \rightarrow \text{Nobel prize for measuring}$$

This very strange number appears for the fact of the proton is made by 3 quarks.

If we compare both magnetic moments:

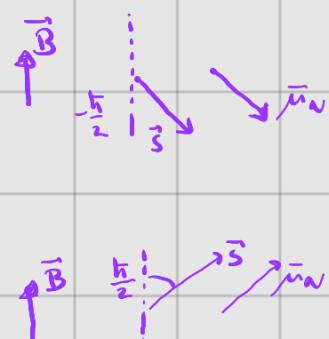
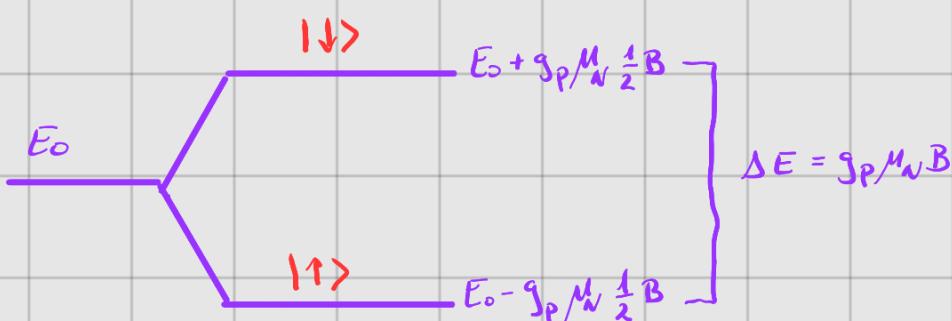
$$\frac{|\mu_p|}{|\mu_e|} = \frac{g_p}{m_p} \cdot \frac{m_e}{g_e} \approx \frac{6}{2} \cdot \frac{1}{2 \cdot 10^3} = 1,5 \cdot 10^{-3}$$

Now we put a nucleus in a magnetic field

$$E = E_0 - \vec{\mu}_p \cdot \vec{B} = E_0 - \left( g_p \frac{1e1}{2m_p} \vec{S} \right) \cdot \vec{B} = E_0 - g_p \frac{1e1}{2m_p} [S_z] B = E_0 - g_p \frac{1e1}{2m_p} \hbar m_s B = \\ = E_0 - g_p \frac{\hbar 1e1}{2m_p} m_s B = E_0 - g_p \underline{\mu_N m_s B} = 2 \text{ possibilities}$$

$$\boxed{1} \Rightarrow E_0 + g_p \mu_N \frac{1}{2} B \quad m_s = -\frac{1}{2} \quad (\text{spin down}) \quad \frac{\hbar 1e1}{2m_p} = \mu_N = \frac{\text{nuclear magneton}}{\text{T}} = 3,15 \cdot 10^{-8} \frac{\text{esu}}{\text{T}}$$

$$\boxed{2} \Rightarrow E_0 - g_p \mu_N \frac{1}{2} B \quad m_s = \frac{1}{2} \quad (\text{spin up})$$



The angle is the same as we had with the electron

If we do the same calculation as before of the spin-flip frequency:

$$\Delta E = g_p \mu_N B \cong 6 \cdot 3,15 \cdot 10^{-8} \frac{\text{eV}}{\text{T}} \cdot 1 \text{T} \cong 10^{-7} \text{ eV} = h D_{SF}$$

$$\nu_{SF} = \frac{\Delta E}{\hbar} \simeq 40 \text{ MHz} \rightarrow \text{Radio waves}$$

$$V_{SF} = \frac{g_p / M_p B}{h}$$

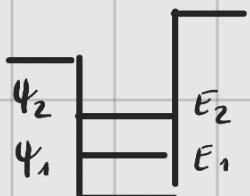
An application of this is to find if a biological tissue is healthy or not.

The spin-flip transition is different when the tissue is healthy.

# Quantum BIT

$q$ -bit = quantum system with 2 distinct states

→ i.e. quantum well with 2 energy levels:



The two states are orthogonal

c) i.e. single photon  $\xrightarrow{\quad} |V\rangle$   $\xrightarrow{\quad} |H\rangle \}$  flying q. bit

V → vertical polarization  
H → horizontal polariz.

So we have:  $\{4_0, 4_1\} \xrightarrow{\text{classical encoding}} \begin{matrix} \{4_0\} \\ \downarrow \\ 0 \end{matrix} \quad \begin{matrix} \{4_1\} \\ \downarrow \\ 1 \end{matrix}$

→ quantum encoding:  $a_0 \Psi_0(x) + a_1 \Psi_1(x) = a_0 |0\rangle + a_1 |1\rangle$

## Operation with q-bit

$$I = |0\rangle\langle 0| + |1\rangle\langle 1|$$

$\downarrow \Psi_0$      $\downarrow \Psi_0^*$      $\downarrow \Psi_1$      $\downarrow \Psi_1^*$

→ Identity operator

$$\sigma_x = |0\rangle\langle 1| + |1\rangle\langle 0|$$

$$\sigma_y = i(|1\rangle\langle 0| - |0\rangle\langle 1|)$$

$$\sigma_z = |0\rangle\langle 0| - |1\rangle\langle 1|$$

q-bit basis states

$$\{|0\rangle, |1\rangle\}$$

Example:

$$\sigma_x |0\rangle = (|0\rangle\langle 1| + |1\rangle\langle 0|) |0\rangle = |0\rangle\langle 1|0\rangle + |1\rangle\langle 0|\overbrace{0\rangle}^{\text{BRAKET}} = |1\rangle$$

$$\Rightarrow \langle 0|0\rangle = \int \Psi_0^*(x) \Psi_0(x) dx = \int |\Psi_0(x)|^2 dx = 1$$

$$\Rightarrow \langle 1|1\rangle = 1$$

$$\Rightarrow \langle 0|1\rangle = \int \Psi_0^*(x) \Psi_1(x) dx = \delta_{10} = 0 \rightarrow \text{the two states are orthogonal}$$

$\sigma_x$  is the flip operator

$$\sigma_x |0\rangle = |1\rangle$$

$$\sigma_x |1\rangle = |0\rangle$$

## Recap

A q-bit is having two states system. These states have to be orthogonal

## Important Operators

•) Identity:  $I = |0\rangle\langle 0| + |1\rangle\langle 1|$

•) Flip:  $\hat{\sigma}_x = |0\rangle\langle 1| + |1\rangle\langle 0|$

•)  $\hat{\sigma}_y = i(|1\rangle\langle 0| - |0\rangle\langle 1|)$

•)  $\hat{\sigma}_z = |0\rangle\langle 0| - |1\rangle\langle 1|$

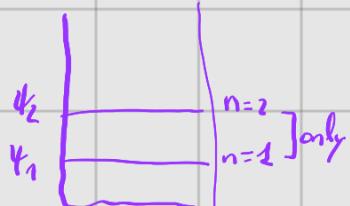
Notation: Dirac representation

$|\alpha\rangle \rightarrow$  Dirac quantum state  $\rightarrow$  ket

Formal q-bit representation:  $a_0|0\rangle + a_1|1\rangle$

with  $|0\rangle, |1\rangle$  the two basis states and  $\{a_0, a_1\} \in \mathbb{C}$

Also  $a_0\psi_0(x) + a_1\psi_1(x) =$  Solution of Schrödinger Equation



Computation:  $\hat{\sigma}_y |\alpha\rangle$

$$\hat{\sigma}_y |0\rangle = i(|1\rangle\langle 0| - |0\rangle\langle 1|)|0\rangle = i|1\rangle = e^{i\pi/2}|1\rangle$$

$$\hat{\sigma}_y |1\rangle = \dots = -i|0\rangle = e^{-i\pi/2}|0\rangle$$

Flip and add a phase

Computation:  $\hat{\sigma}_z |\alpha\rangle$

$$\hat{\sigma}_z |0\rangle = (|0\rangle\langle 0| - |1\rangle\langle 1|)|0\rangle = |0\rangle \rightarrow \text{Maintain the state}$$

$$\hat{\sigma}_z |1\rangle = \dots = -|1\rangle = e^{i\pi}|1\rangle \rightarrow \text{add a phase}$$

## Commutation:

•)  $[\hat{\sigma}_x, \hat{\sigma}_y] = 2i\hat{\sigma}_z \rightarrow$  They don't commute, they will NOT have common set of eigenstates

$$\begin{aligned} \hat{\sigma}_x \hat{\sigma}_y &= (\lvert 10 \rangle \langle 11 + \lvert 11 \rangle \langle 01 \rangle) \cdot i(\lvert 11 \rangle \langle 01 - \lvert 10 \rangle \langle 11 \rangle) = i(\lvert 10 \rangle \langle 01 - \lvert 11 \rangle \langle 11 \rangle) \\ \hat{\sigma}_y \hat{\sigma}_x &= i(\lvert 11 \rangle \langle 01 - \lvert 10 \rangle \langle 11 \rangle) \cdot (\lvert 10 \rangle \langle 11 + \lvert 11 \rangle \langle 01 \rangle) = i(\lvert 11 \rangle \langle 11 - \lvert 10 \rangle \langle 01 \rangle) \end{aligned} \quad \left. \begin{array}{c} 2i\hat{\sigma}_z \\ \text{ } \end{array} \right\}$$

•)  $\hat{O} \Psi = \lambda \Psi$

$$\hat{\sigma}_x \left[ \frac{1}{\sqrt{2}} (\lvert 10 \rangle + \lvert 11 \rangle) \right] = \frac{1}{\sqrt{2}} (\lvert 10 \rangle \langle 11 + \lvert 11 \rangle \langle 01 \rangle) (\lvert 10 \rangle + \lvert 11 \rangle) = \frac{1}{\sqrt{2}} (\lvert 10 \rangle + \lvert 11 \rangle) (+1) \quad \begin{array}{c} \text{Eigenvalue for} \\ \text{THIS eigenstate} \\ \lambda = 1 \end{array}$$

$$\hat{\sigma}_y \frac{1}{\sqrt{2}} (\lvert 10 \rangle + i\lvert 11 \rangle) = \dots = \frac{1}{\sqrt{2}} (\lvert 10 \rangle + i\lvert 11 \rangle) (-1)$$

So we have:

$$\left. \begin{array}{c} \text{Eigenstate of } \hat{\sigma}_x \rightarrow \frac{1}{\sqrt{2}} (\lvert 10 \rangle \pm \lvert 11 \rangle) \\ \text{Eigenstate of } \hat{\sigma}_y \rightarrow \frac{1}{\sqrt{2}} (\lvert 10 \rangle \pm i\lvert 11 \rangle) \end{array} \right\} \text{Different set of eigenstates}$$

## Operation with q-bit "matrices"

•)  $\lvert 10 \rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \rightarrow$  matrix of single state  
 $\lvert 11 \rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$$a_0 \lvert 10 \rangle + a_1 \lvert 11 \rangle = a_0 \begin{pmatrix} 1 \\ 0 \end{pmatrix} + a_1 \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} a_0 \\ a_1 \end{pmatrix}$$

matrix of the superposition q-bit state!

•)  $\hat{\sigma}_x [\lvert 10 \rangle + \lvert 11 \rangle] = a_0 \lvert 11 \rangle + a_1 \lvert 10 \rangle$

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} = \begin{pmatrix} a_1 \\ a_0 \end{pmatrix} \Rightarrow \begin{array}{l} a_0 A + a_1 B = a_1 \\ a_0 C + a_1 D = a_0 \end{array} \Rightarrow \begin{array}{l} A=0, B=1 \\ C=1, D=0 \end{array}$$

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Matrix representation of  $\hat{\sigma}_x$  operator

$$\hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Matrix form of  $\sigma_x, \sigma_y, \sigma_z$  are called Pauli spin matrices

Computation:

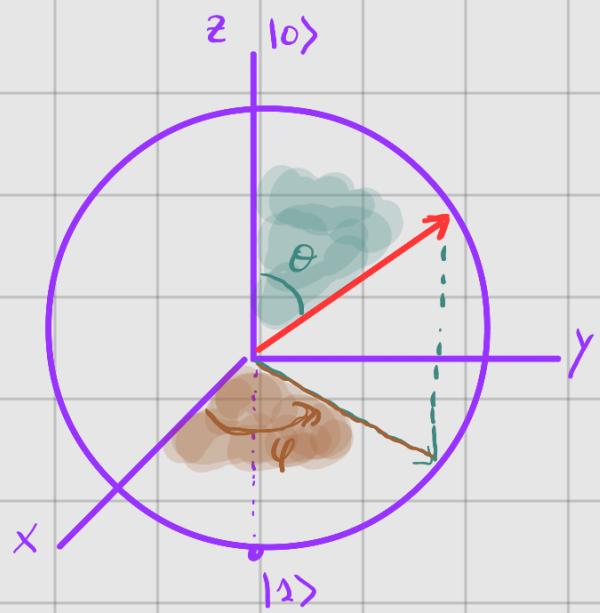
$$\langle 0| \sigma_x | 0 \rangle = \langle 0| (|0\rangle\langle 1| + |1\rangle\langle 0|) |0\rangle = 0 \rightarrow \text{matrix } (\sigma_x)_{00}$$

$$\langle 0| \sigma_x | 1 \rangle = \langle 0| (|0\rangle\langle 1| + |1\rangle\langle 0|) |1\rangle = 1 \rightarrow \text{matrix } (\sigma_x)_{01}$$

$$\langle 1| \sigma_x | 0 \rangle = \dots 1 \rightarrow \text{matrix } (\sigma_x)_{10}$$

$$\langle 1| \sigma_x | 1 \rangle = \dots 0 \rightarrow \text{matrix } (\sigma_x)_{11}$$

Bloch Sphere



The most general form of q-bit is:

$$|\Psi\rangle = \cos \frac{\theta}{2} |0\rangle + e^{i\phi} \sin \frac{\theta}{2} |1\rangle$$

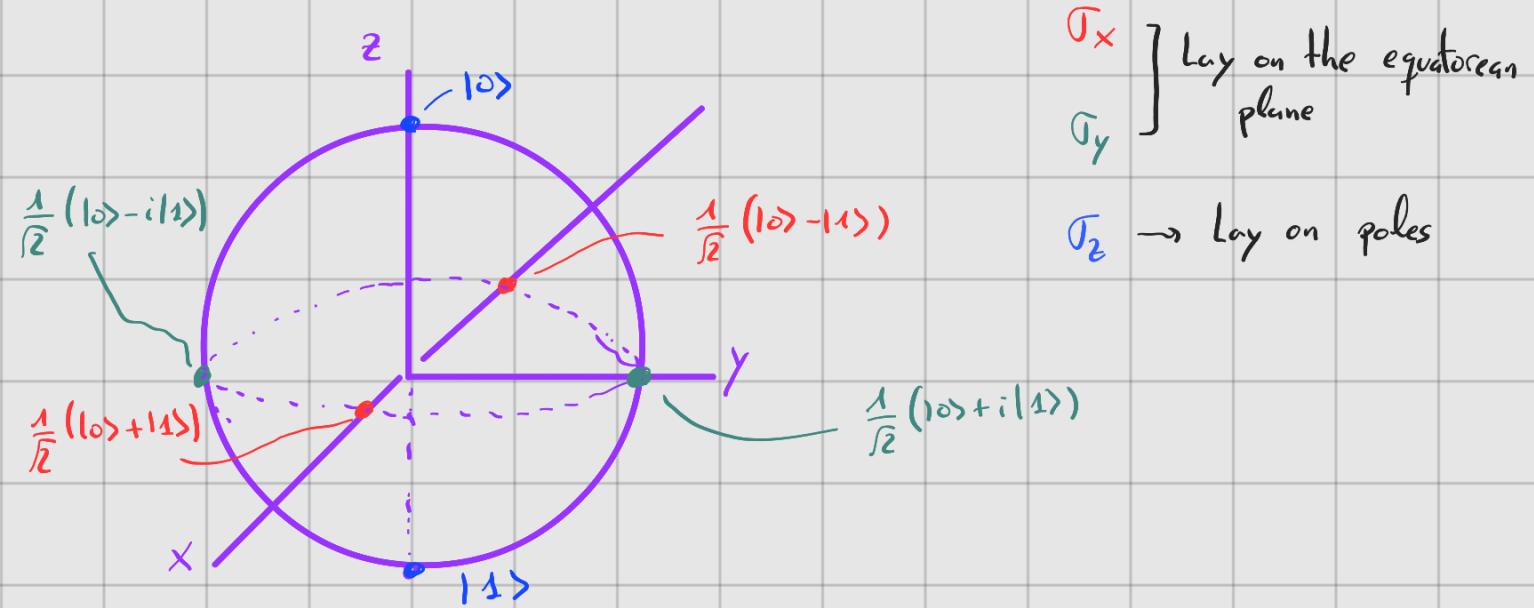
$$\text{If we remember: } \int dx |\Psi(x)|^2 \rightarrow \langle \Psi | \Psi \rangle = (a_0^* \langle 0| + a_1^* \langle 1|)(a_0 |0\rangle + a_1 |1\rangle) =$$

$$\text{We have to normalise} \Rightarrow = |a_0|^2 + |a_1|^2 = 1$$

$$\text{Using bloch representation: } \langle \Psi | \Psi \rangle = (\cos \theta \langle 0| + e^{-i\phi} \sin \theta \langle 1|)(\cos \theta |0\rangle + e^{i\phi} |1\rangle) = 1$$

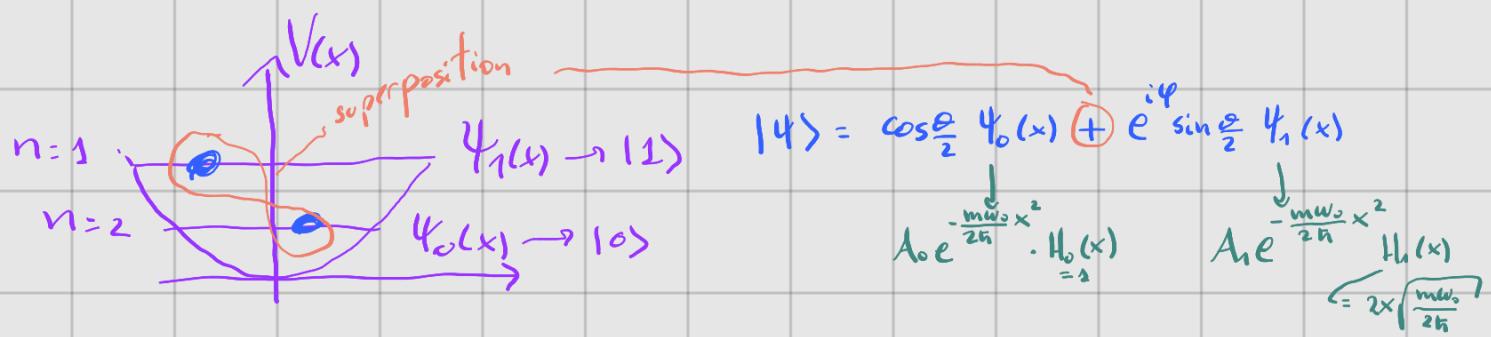
It is naturally normalised!

The different states of  $\sigma_x, \sigma_y, \sigma_z$  are located in the sphere like this



The points in the opposite position with respect to the centre are always orthogonal.

Let's take for instance the harmonic oscillator



Here we have that the  $c^-$  is in a superposition of two states so we don't initialise the  $c^-$  in  $|\psi_0\rangle$  (bit 0) or  $|\psi_1\rangle$  (bit 1), that is classical.

## Entanglement

Particles at some point will decay, what means they will break. If it breaks in two and it has neutral charge, the two obtained particles can have neutral charges or opposite charges. The spin is also maintained:  $\pi^+$ -on has  $\text{spin} = 0$  when it decays the particles will have spin up and the other spin down

$$\begin{array}{ccc} \text{General particle} & \xrightarrow{\text{decay}} & |\uparrow\rangle_R |\downarrow\rangle_L + |\downarrow\rangle_R |\uparrow\rangle_L \\ \text{with spin} = 0 & & \underbrace{\hspace{10em}}_{\text{2 possibilities}} \end{array}$$

Making it more formal

$$|\Psi\rangle = |\lambda\rangle_a |\phi\rangle_b$$

two particle system

$\lambda \perp \phi$  states

$|\lambda\rangle_a$  = state system "a"

$|\phi\rangle_b$  = state system "b"

For instance

$$|\Psi\rangle = \frac{1}{2} (|0\rangle_a |0\rangle_b + |0\rangle_a |1\rangle_b + |1\rangle_a |0\rangle_b + |1\rangle_a |1\rangle_b) =$$

$$= \frac{1}{2} (|0\rangle_b (|0\rangle_a + |1\rangle_a) + |1\rangle_b (|0\rangle_a + |1\rangle_a)) = \frac{1}{2} (|0\rangle_b + |1\rangle_b) \frac{1}{2} (|0\rangle_a + |1\rangle_a)$$

$\Rightarrow$  Not an entangled state

4 Bell states

$$\left\{ \begin{array}{l} |\Psi\rangle = \frac{1}{\sqrt{2}} (|0\rangle_a |0\rangle_b \pm |1\rangle_a |1\rangle_b) \neq |\lambda\rangle_a \otimes |\phi\rangle_b \Rightarrow \text{Definition of entangled state} \\ |\Psi\rangle = \frac{1}{\sqrt{2}} (|0\rangle_a |1\rangle_b \pm |1\rangle_a |0\rangle_b) \neq |\lambda\rangle_a |\phi\rangle_b \end{array} \right.$$

2 states

The superposition state is said to be entangled when you can't split the superposition into the product of two independent states.

The general form of an entangled state:

$$|4\rangle = \alpha |\phi_1\rangle_a |\phi_2\rangle_b + \beta |\phi_2\rangle_a |\phi_1\rangle_b$$

2 particles                    2 particles

$\{|\phi_1\rangle_a, |\phi_2\rangle_a\} = 2 \perp$  states  $\rightarrow$  part. "a"

$\{|\phi_1\rangle_b, |\phi_2\rangle_b\} = 2 \perp$  states  $\rightarrow$  part. "b"

## SPDC [II]

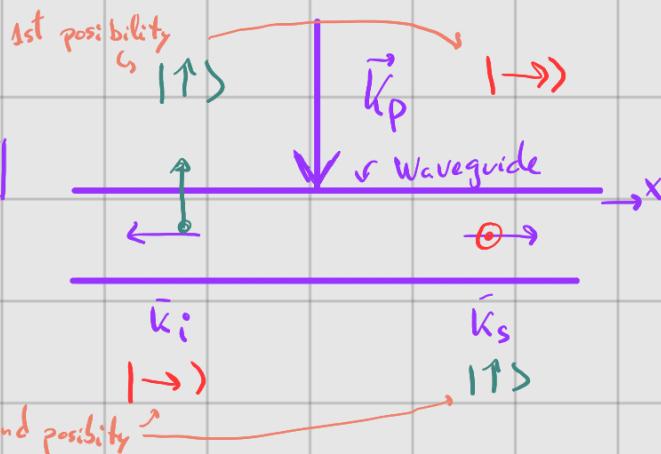
$$w_p \longrightarrow w_i \quad w_s$$

$$w_p = w_i + w_s$$

$$\vec{k}_p = \vec{k}_s + \vec{k}_i$$

If I pump with  $\vec{k}_p$  the momentum will conserve  
here the initial momentum is zero.

one of them have vertical polarization the other has horizontal



$|↑\rangle$  = photon Vertical Polariz. (Linear)  $\hat{E} \uparrow$

$|→\rangle$  = photon Horizontal Polariz. (Linear)  $\hat{E} \rightarrow$

$a \rightarrow$  signal photon       $|0\rangle \rightarrow$  Vertical  $|↑\rangle$   
 $b \rightarrow$  idler photon       $|1\rangle \rightarrow$  Horizontal  $|→\rangle$

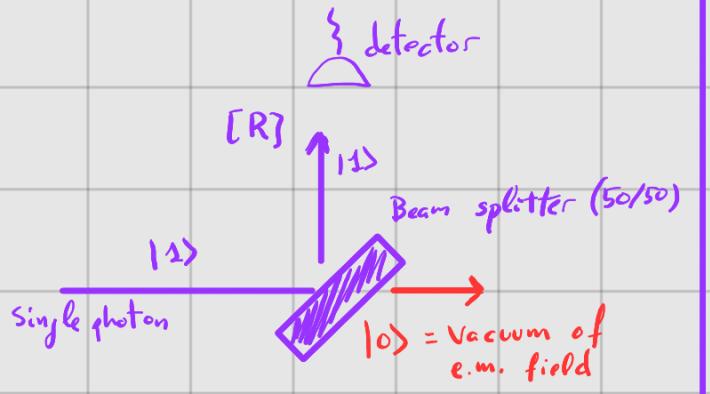
State of whole system:  $|4\rangle = \alpha |↑\rangle_i |→\rangle_s + \beta |→\rangle_i |↑\rangle_s \neq |\lambda\rangle_a |\phi\rangle_b$

This is an entangled state of two photons: idler and signal with two polarization states Vertical and Horizontal

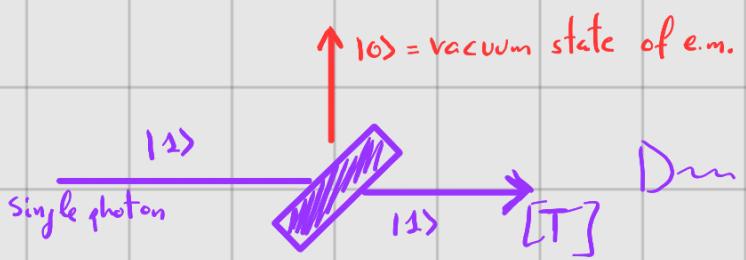
Known as: Two photon polarization entangled state

We have a beam splitter, 50% reflected and 50% transmitted. If we have a single photon it cannot break up so it will be either transmitted or reflected

## Possibility 1



Possibility 2



This is: one photon entangled state

$$|14\rangle = \alpha |1\rangle_R |0\rangle_T + \beta |0\rangle_R |1\rangle_T$$

## No-cloning Theory

$|4\rangle \rightarrow$  particle quantum state to be cloned

$|x\rangle \rightarrow$  Register  $\rightarrow$  clone quantum state

$|4\rangle |x\rangle \xrightarrow{\text{"cloning"}} |4\rangle |4\rangle$

If this cloning process is true for two q-states it should work for the super

$$\text{position } \{ |4_1\rangle, |4_2\rangle \} \rightarrow [\alpha|4_1\rangle + \beta|4_2\rangle]$$

$$\textcircled{2} \rightarrow (\alpha|4_1\rangle + \beta|4_2\rangle) |x\rangle \stackrel{\text{linearity}}{=} \alpha|4_1\rangle|x\rangle + \beta|4_2\rangle|x\rangle \stackrel{\text{cloning}}{=} |\psi_1\rangle|4_1\rangle + |\psi_2\rangle|4_2\rangle$$

We can also write:

We can also write:

$$\textcircled{2} \rightarrow (\alpha|4_1\rangle + \beta|4_2\rangle) |x\rangle \stackrel{\text{cloning}}{=} (\alpha|4_1\rangle + \beta|4_2\rangle) (\alpha|4_1\rangle + \beta|4_2\rangle) =$$

$$= \alpha^2|4_1\rangle|4_1\rangle + \beta^2|4_2\rangle|4_2\rangle + \alpha\beta(|4_1\rangle|4_2\rangle + |4_2\rangle|4_1\rangle)$$

① and ② should be equivalent, the conditions for that to happen are:

$$\alpha^2 = \alpha \quad \beta^2 = \beta$$

$$\alpha\beta = 0$$

But if we have  $\alpha=0$  or  $\beta=0$  we don't have superposition, we have a single state

Therefore superposition is not consistently cloned  $\Rightarrow$

We cannot clone a superposition state

You CAN copy a single particle state

This is a very interesting because we can encode a message in a superposition quantum state and be sure that it cannot be cloned.

Alice  $\xrightarrow{\text{Eve}}$  Bob If Alice sends a message to Bob encoded in a superposition then Eve cannot clone (copy) and it will be secret.