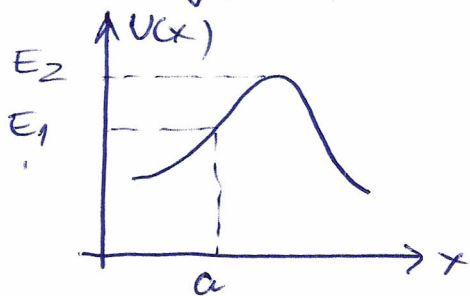


## ⑥ Potential barriers and tunneling

Application: SCANNING TUNNELING MICROSCOPE

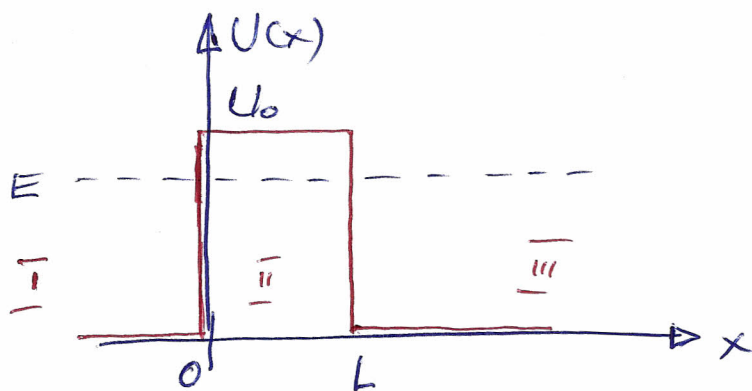
A potential barrier is the opposite of a potential well; its potential energy has a maximum.



According to Newtonian physics, a particle with the energy  $E_1$  initially to the left of the barrier cannot get further than  $x=a$ . If the energy is  $\geq E_2$  the classical particle can pass over the barrier.

In quantum mechanics, the quantum particle which encounter the barrier (with  $E_1 < E_2$ ) can appear on the other side. This phenomenon is called tunneling.

### Tunneling through a rectangular barrier



$$U(x) = \begin{cases} 0 & x < 0, x > L \\ U_0 & 0 < x < L \end{cases}$$

One has to solve the time-independent Schrödinger equation in regions I, II, III and put the continuity conditions for the wave functions and their derivatives in  $x=0$  and  $x=L$ .

The region II represents a potential step with finite  $U_0$  and we have already seen that inside this step the wave function is evanescent and the probability  $|\psi|^2$  has an exponential decay with  $L$ . For small  $L$  the wave function can penetrate the barrier and pass on the other side.

$$\begin{cases} -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi & \text{regions } \underline{i} \text{ and } \underline{iii} \\ -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + U_0\psi = E\psi & \text{region } \underline{ii} \end{cases}$$

$$\Rightarrow \begin{cases} \frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2} \psi = 0 & (\underline{i}, \underline{iii}) \\ \frac{d^2\psi}{dx^2} + \frac{2m(E-U_0)}{\hbar^2} \psi = 0 & (\underline{ii}) \end{cases}$$

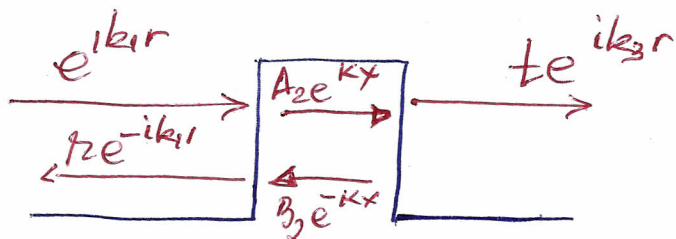
$$k_1 = \sqrt{\frac{2mE}{\hbar^2}} \quad k_2 = \sqrt{\frac{2m(E-U_0)}{\hbar^2}} \in \mathbb{C} \text{ for } E < U_0 = ik$$

$$\Rightarrow \begin{cases} \frac{d^2\psi}{dx^2} + k_i^2 \psi = 0 & i=1,3 \quad (\underline{i}, \underline{iii}) \\ \frac{d^2\psi}{dx^2} + K^2 \psi = 0 & (\underline{ii}) \end{cases}$$

Solutions:

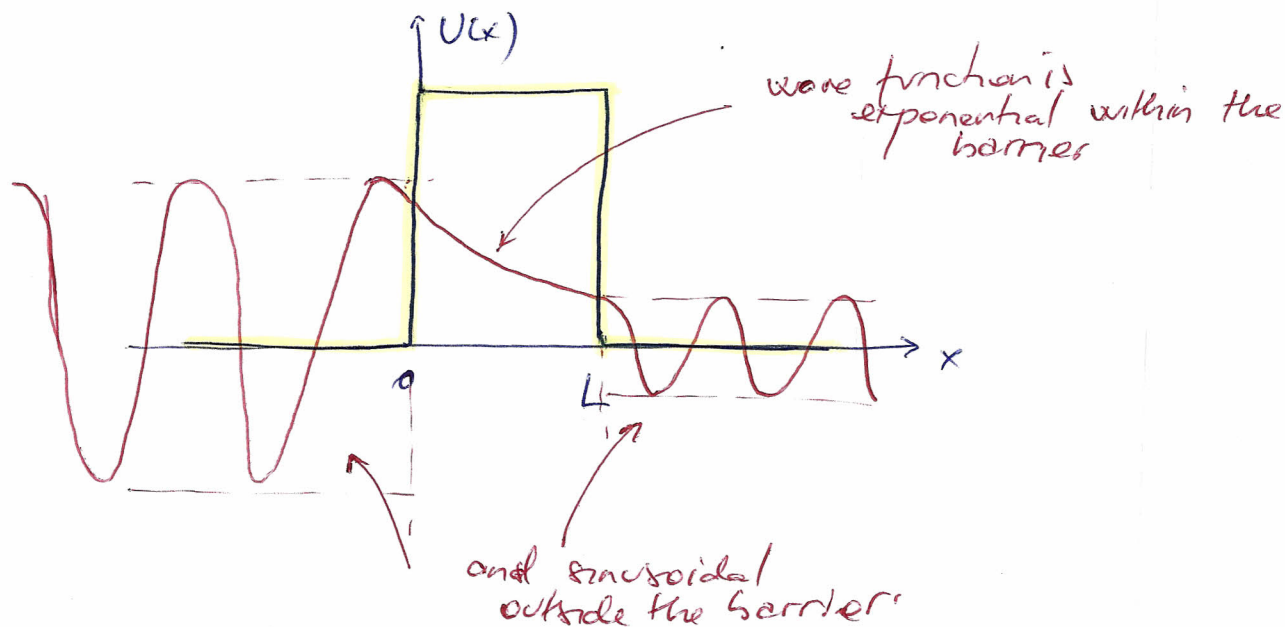
$$\begin{cases} \psi_{\underline{i}}(x) = A_1 e^{ik_1 x} + b_2 e^{-ik_1 x} & x < 0 \\ \psi_{\underline{ii}}(x) = A_2 e^{kx} + b_2 e^{-kx} & 0 < x < L \\ \psi_{\underline{iii}}(x) = A_3 e^{ik_3 x} + b_3 e^{-ik_3 x} & \end{cases}$$

*incident*      *reflected*  
*forward evanescent*      *reflected evanescent*  
*transmitted*      *no reflection in +∞*



One can normalize the incident wave amplitude to 1 ( $A_1 = 1$ ) and then  $|b_2|^2 = R = r^2$  is the reflection coeff. and  $|A_3|^2 = T = t^2$  is the transmission coeff.

The coefficients can be solved by matching the wave function  $\psi(x)$  and its derivative  $\frac{d\psi}{dx}$  in  $x=0$  and  $x=L$ . This requirements lead to a wave function like the one in the figure below:



The function is non-zero inside the barrier (region forbidden by the Newtonian mechanics). Even more remarkable, a particle that is initially to the left of the barrier has a non-zero probability of being found to the right of the barrier.

This probability of tunneling depends on the width  $L$  and on the energy  $E$  of the particle

$$T = \frac{|A_3|^2}{|A_1|^2} = t^2$$

After solving the equations for the coefficients (fairly involved mathematical problem), when  $T$  is much smaller than 1 one gets:

$$T = G e^{-2Kd} \quad \text{where } G = 16 \frac{E}{U_0} \left(1 - \frac{E}{U_0}\right)$$

and  $K = \sqrt{\frac{2m(U_0 - E)}{\hbar^2}}$

This probability exponentially decays with increasing  $L$  and depends with  $\exp(\sqrt{U_0 - E})$  on the energy  $U_0 - E$ .

## APPLICATIONS OF TUNNELING

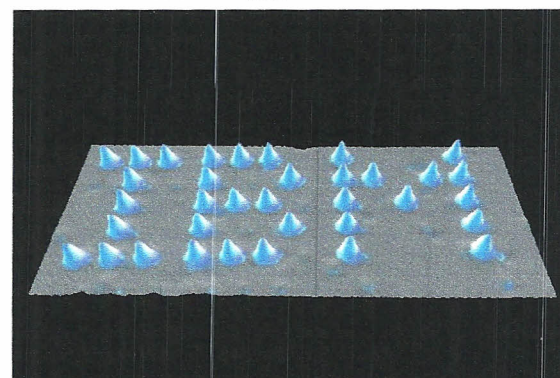
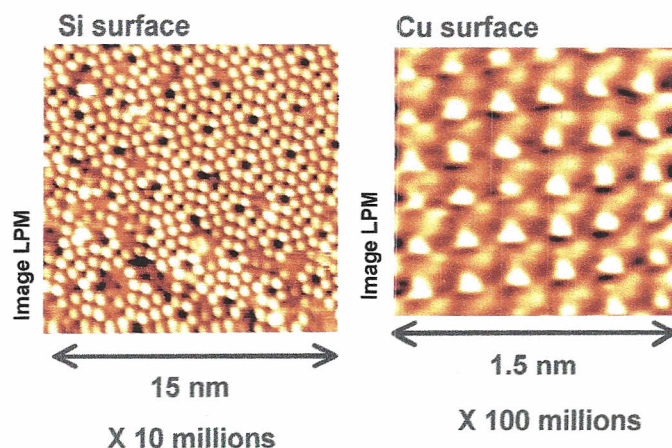
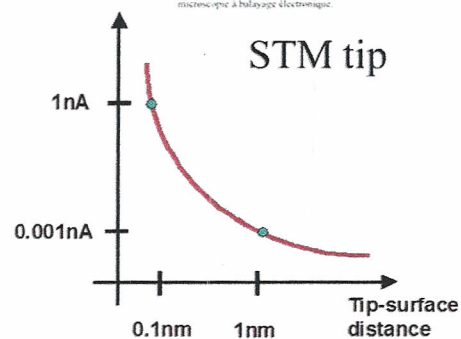
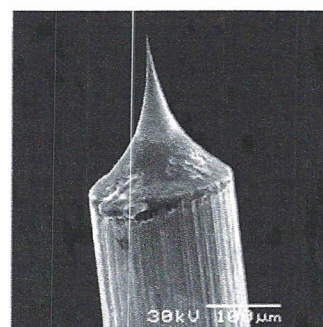
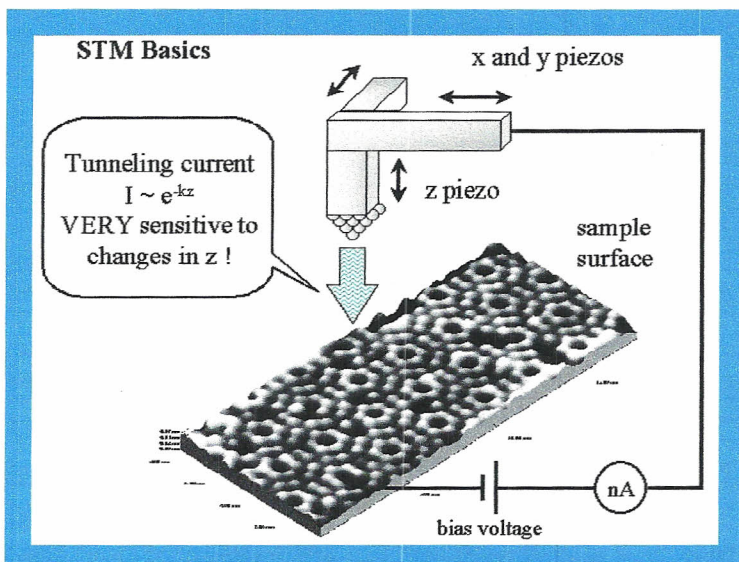
### 1) The scanning tunneling microscope

“Looking at individual atoms”

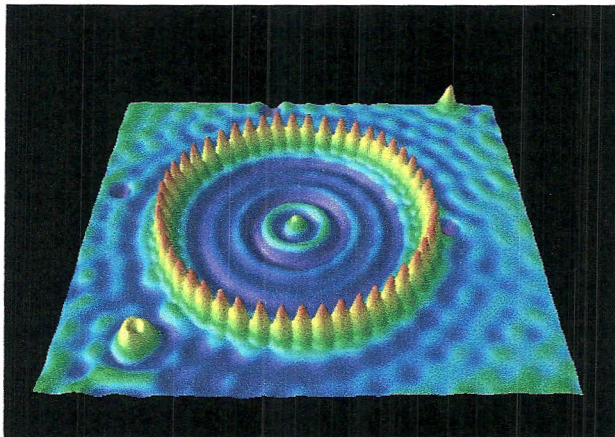
1981: Gerld Binnig, Heinrich Röhrrer, Nobel Prize 1986 ,IBM – Zurich

The scanning tunneling microscope (STM) uses electron tunneling to create images of surfaces down to the scale of individual atoms (**ATOMIC RESOLUTION**).

An extremely sharp conducting needle is brought very close to the surface, within 1 nm or so. When the needle is at a positive potential with respect to the surface, electrons can tunnel through the surface potential-energy barrier and reach the needle.



1988 Donald Eigler IBM Xenon on Nickel (110)



Manipulating individual atoms,  
quantum corrals

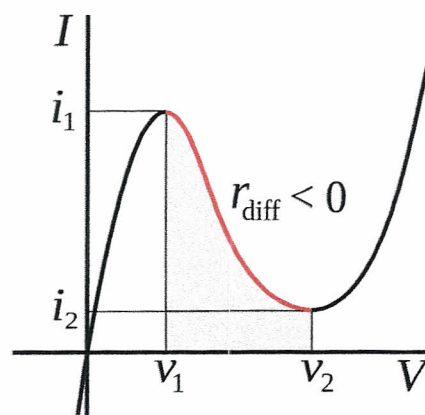
The tunneling probability and hence the *tunneling current* are *very sensitive to changes in the width of the barrier* (the distance between the surface and the needle tip). In one mode of operation the needle is scanned across the surface and at the same time is moved perpendicular to the surface to maintain a constant tunneling current. The needle motion is recorded, and after many parallel scans, an image of the surface can be reconstructed. Extremely precise control of needle motion, including isolation from vibration, is essential.

The discovery of the STM represent a huge step in developing of the surface science.

## 2) Tunneling diodes (Esaki)

A tunnel diode is a semiconductor device in which electrons tunnel through a potential barrier. The current can be switched on and off very quickly (within a few picoseconds) by varying the height of the barrier (by biasing voltage).

*IV* curve similar to a tunnel diode characteristic curve. It has negative resistance in the shaded voltage region, between  $v_1$  and  $v_2$

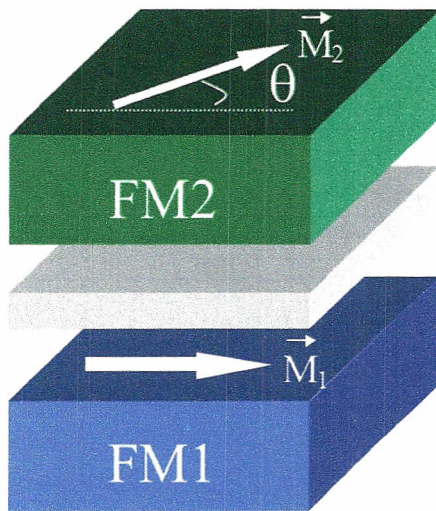


## 3) Josephson junctions

A Josephson junction consists of two superconductors separated by an oxide layer a few atoms (1 to 2 nm) thick. Electron pairs in the superconductors can tunnel through the barrier layer, giving such a device unusual circuit properties. Josephson junctions are useful for establishing precise voltage standards and measuring tiny magnetic fields, and they play a crucial role in the developing field of quantum computing.

#### 4) Magnetic tunnel junctions/ Data storage and sensors

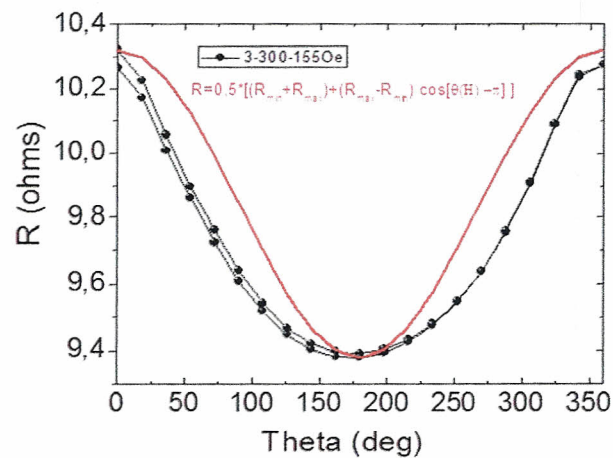
A magnetic tunnel junctions consists in two ferromagnetic layers separated by a thin insulating barrier. The tunnel transmission and the tunnel current depend on the relative orientation of the magnetization of the junction's electrodes, defining the so-called spin valve effect. This effect has huge application potential in sensors and non-volatile data-storage technologies.



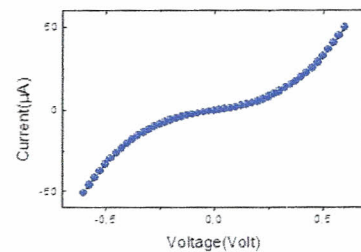
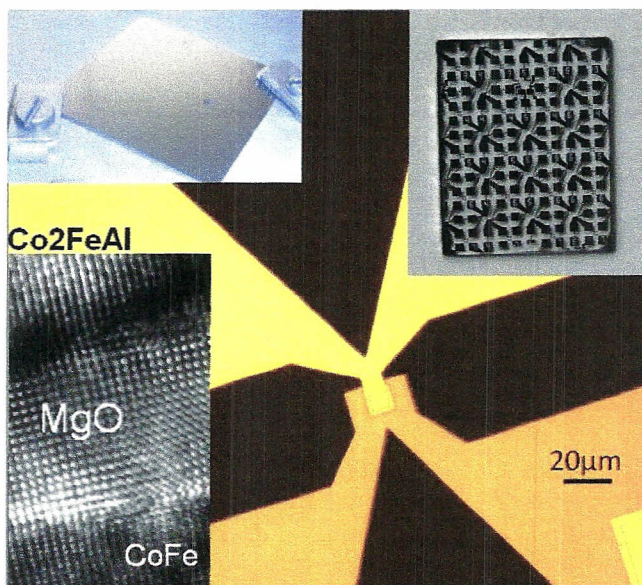
$$R = \frac{R_p + R_{ap}}{2} + \frac{R_p - R_{ap}}{2} \cos(\theta),$$

$$\theta = (\vec{M}_1, \vec{M}_2)$$

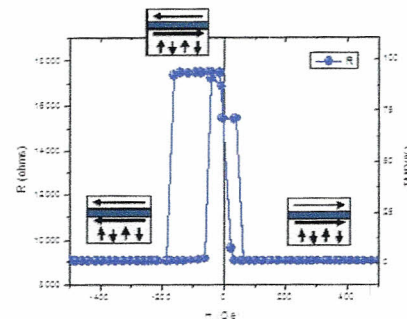
Si/SiO<sub>2</sub>//Ta/NiFe/CoFe/Cu/CoFe/IrMn



The MTJ devices are produced from multilayer thin film structures by clean micro-electronic patterning technologies (UV lithography + Ion Beam Etching).



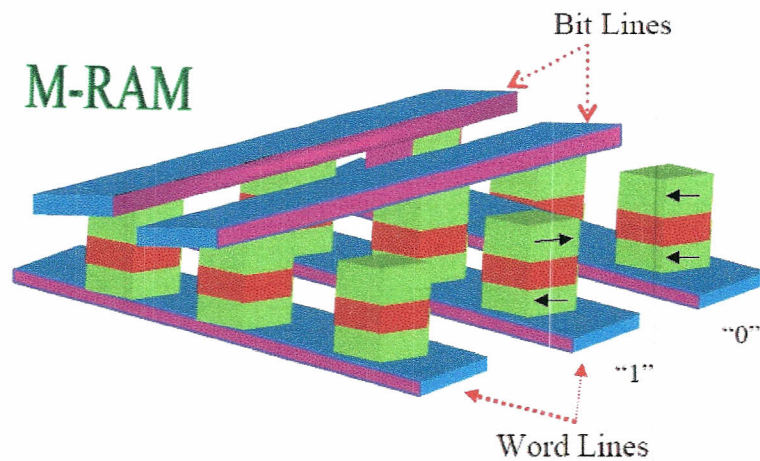
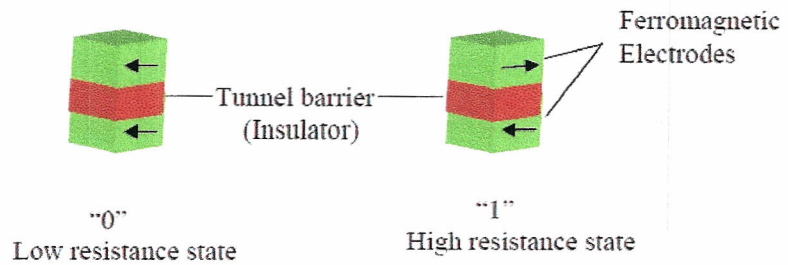
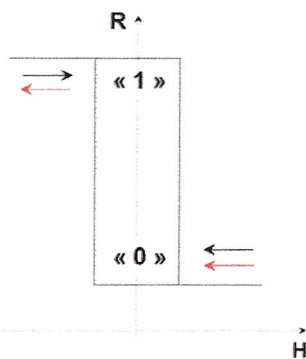
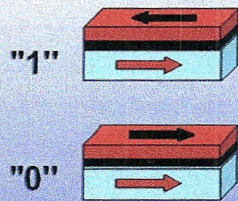
Nonlinear I(V) characteristics



MTJ represents the elementary brick of non-volatile Magnetic **Random Access Memories (MRAM)**.

**Principle :**

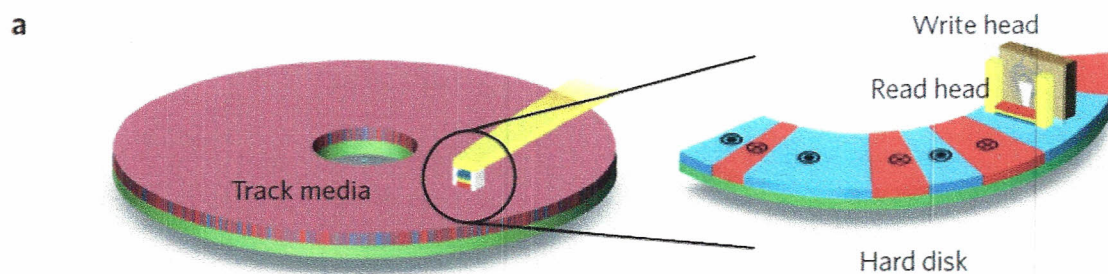
Store data by the direction (parallel or antiparallel) of magnetic layers in MTJ



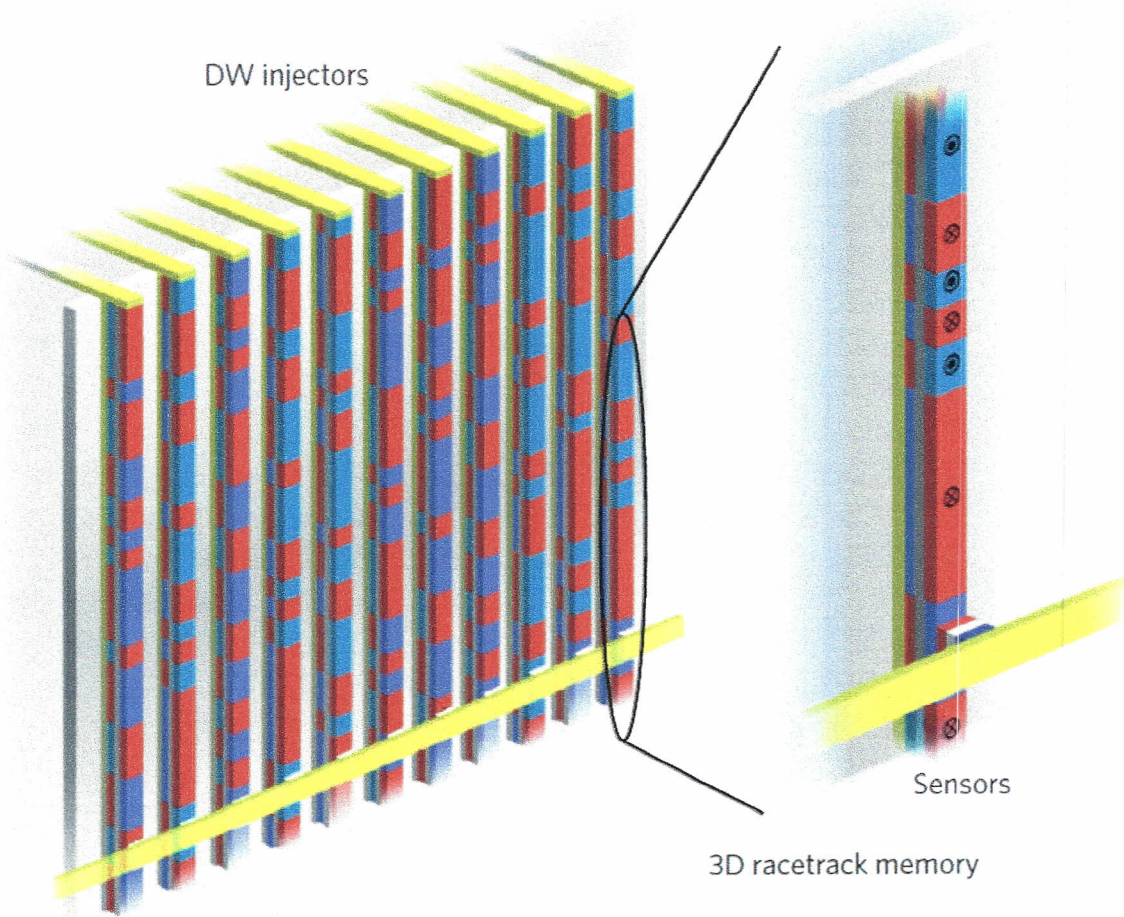
The advantages of MRAMs:

- non volatile
- low power consumption (no mechanical pieces), compared to hard-disk
- stable against radiation
- high speed (competitive with SRAM) and large density (competitive with DRAM)

MTJS represent the read-head sensor in the high-density hard disk drives



From S.S. Parkin, S-H. Yang, *Nature Nanotechnology*, **10**,195–198, (2015)



Or 3D next generation of memories (RACE-TRACKS)...  
From S.S. Parkin, S-H. Yang, *Nature Nanotechnology*, **10**,195–198, (2015)



# The Quantum Harmonic Oscillator

Systems that oscillate are extremely important in the physical world. Simple harmonic motion is exceptionally important in classical physics where it serves as prototype for more complex oscillations.

Oscillations are equally important for particles at microscopic scale where quantum effects dominate. Here we deal with the quantum harmonic oscillator - as model of oscillations at the atomic level

The defining characteristic of simple harmonic motion is the LINEAR RESTORING FORCE.

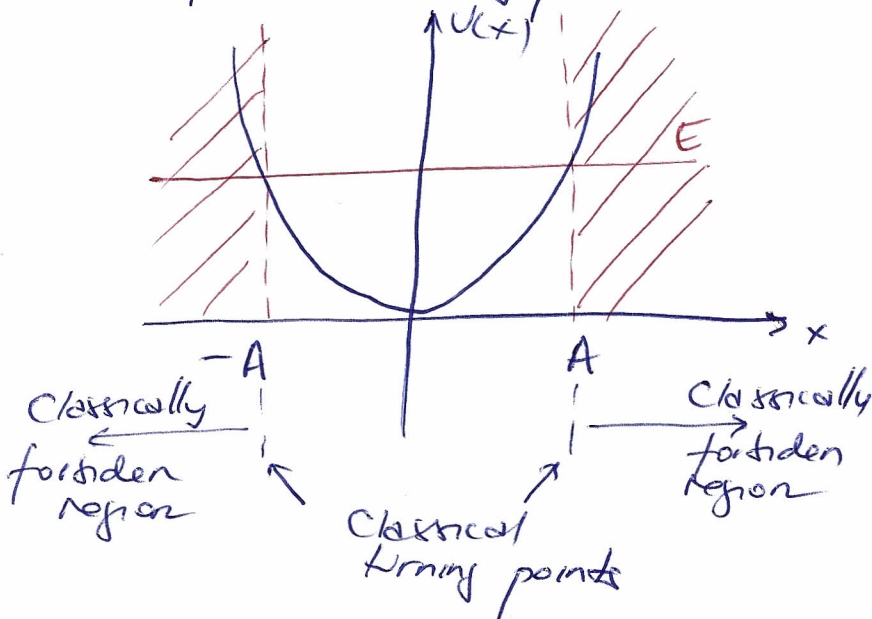
$$F = -kx \quad \text{where } k \text{ is the force (spring) constant.}$$

The corresponding potential energy is:

$$U(x) = \frac{1}{2} kx^2$$

where we assume that the equilibrium position is  $x_e = 0$ .

The potential energy  $U(x)$  is represented below:



The particle is "restricted" for a total energy  $E$  between  $x = -A$  and  $+A$  (classical turning points)

$U(x)$  is a parabolic potential well. A particle of mass  $m$  classically oscillates with frequency  $\omega$

$$\omega = \sqrt{\frac{k}{m}}$$

between two turning points  
 $x = -A$  and  $x = +A$

This description fails for an atomic particle which has to be described using wave quantum mechanics. It means that we have to solve the Schrödinger equation to find the wave functions and energies for  $U(x) = \frac{1}{2}kx^2$

$$\Rightarrow -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + \frac{1}{2} kx^2 \psi = E \psi \quad \Rightarrow$$

$$\boxed{\frac{d^2 \psi}{dx^2} + \frac{2m}{\hbar^2} \left( E - \frac{1}{2} kx^2 \right) \psi(x) = 0}$$

We will assert, without deriving them, that the wave functions of the first three states are:

$$\begin{cases} \psi_1(x) = A_1 e^{-x^2/2b^2} \\ \psi_2(x) = A_2 \frac{x}{b} e^{-x^2/2b^2} \\ \psi_3(x) = A_3 \left( 1 - \frac{2x^2}{b^2} \right) e^{-x^2/2b^2} \end{cases}$$

Hermite  
functions

"  
exponential fct.  
multiplied by a  
polynomial in  $x$ .

where  $b = \sqrt{\frac{\hbar}{m\omega}}$  has a dimension of length.

One can easily show that  $b$  is exactly the classical turning point (AMPLITUDE OF OSCILLATOR) of the oscillator in the  $n=1$  ground state. The constants  $A_1, A_2, A_3$  are normalization constants. They can be calculated from:

$$\int_{-\infty}^{+\infty} |\psi_1(x)|^2 dx = A_1^2 \int_{-\infty}^{+\infty} e^{-\frac{x^2}{b^2}} dx = 1$$

on so on for  $A_2, A_3, \dots$

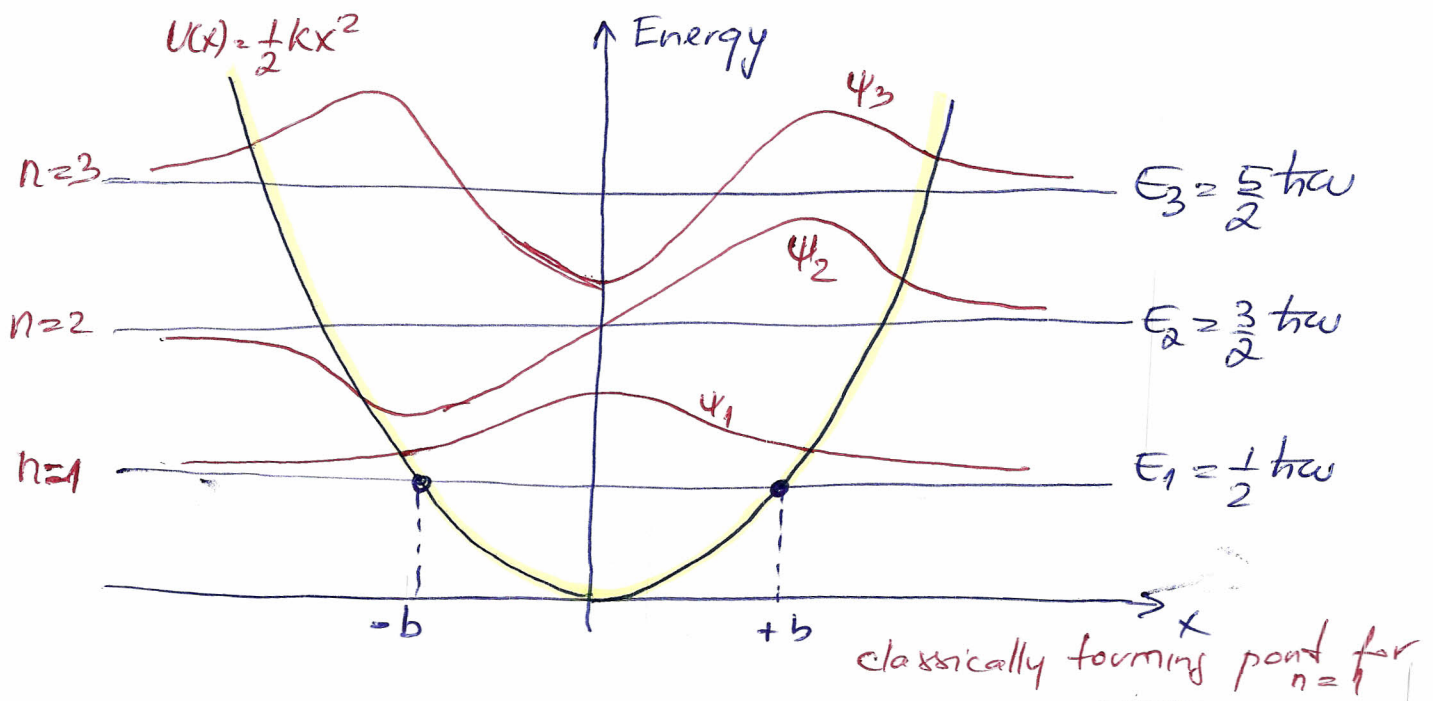
As expected, as for any particle in a quantum well, stationary states of the quantum harmonic oscillator exist only for certain discrete energy levels, the quantum states of the oscillator. The allowed energies are given by the simple equation

$$E_n = \left(n - \frac{1}{2}\right) \hbar \omega \quad n = 1, 2, 3, \dots$$

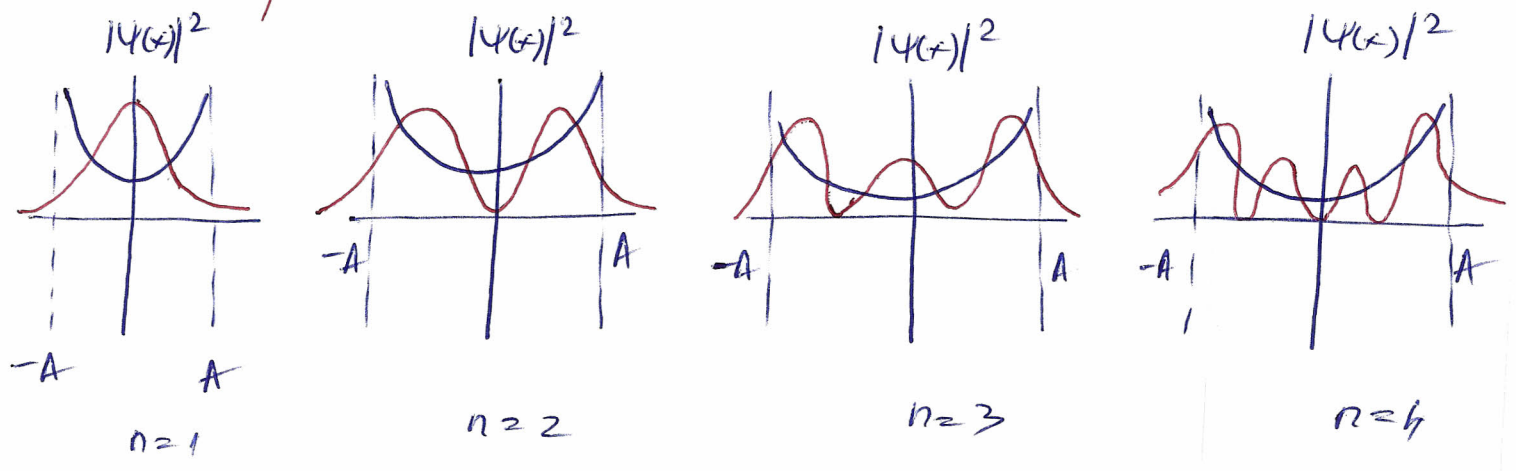
where  $\omega = \sqrt{\frac{k}{m}}$  is the classical angular frequency  
 $n = 1, 2, 3, \dots$  is the quantum number.

ok ① The ground state of the quantum harmonic oscillator is  $E_1 = \frac{1}{2} \hbar \omega$ . An atomic mass on a spring can not be brought in rest. This is a direct consequence of the uncertainty principle.

② The energy are equally spaced by  $\Delta E = \hbar \omega$ . Notice that the wave functions, like those of a finite potential well extend beyond turning points into the classically forbidden region (tunneling)



# Probability distribution function



The blue curve represents the corresponding probability distributions for the Newtonian motion. Red curves represent the quantum  $|\psi(x)|^2$ . As  $n$  increases, the averaged-out quantum mechanical functions resemble more and more the Newtonian ones.

OK The classical probability density  $P_{class}(x)$  notes that a classical particle is most likely to be found where it is moving slowest.

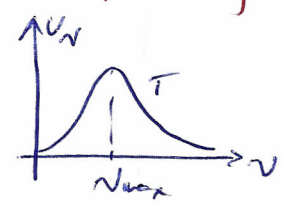
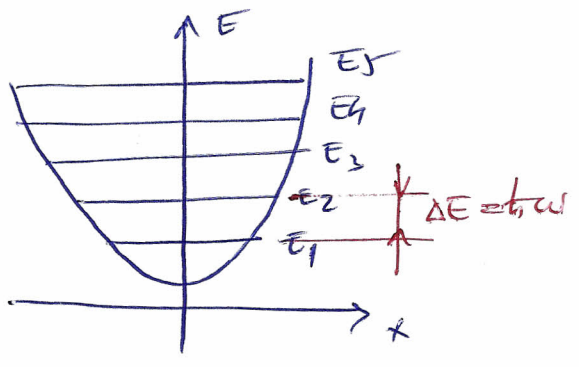
→ in agreement with the Correspondence Principle

Niels Bohr : The average behaviour of a quantum system should begin to look like a classical solution in the limit of large quantum number ( $n \rightarrow \infty$ )

↳ quantum world should smoothly blend into the classical world for high quantum numbers.

Obs :  $E_n = (n - \frac{1}{2}) h\nu$   $n = 1, 2, \dots$

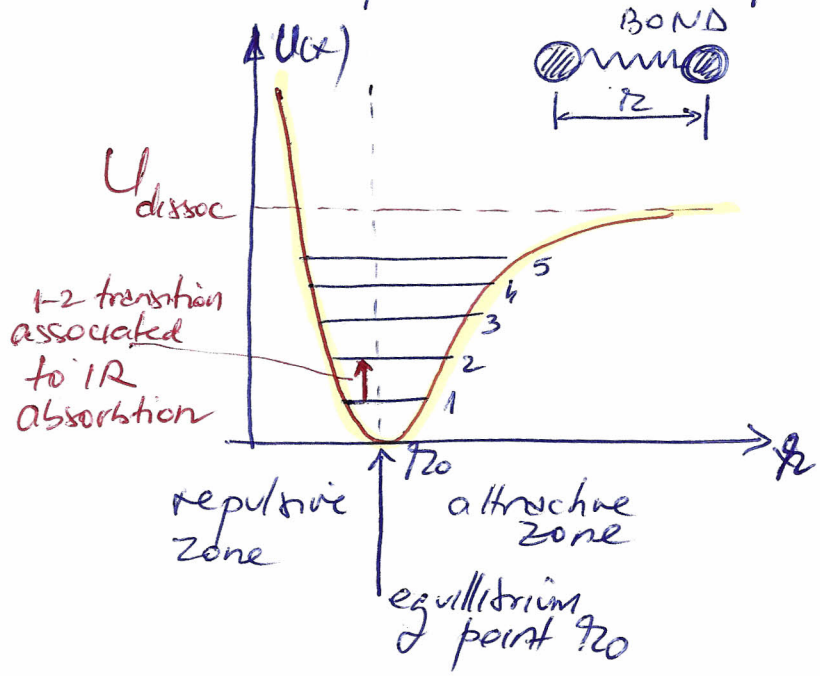
contrasts the assumption of Planck (1900) that the energy levels of the quantum oscillator are quantified and separated by  $\Delta E = h\nu$  to explain the black-body radiation spectral density  $U_r(\nu) = f(\nu, T)$



Molecular vibration, IR Spectroscopy

We use the idea that atoms in a molecule are held together by spring-like molecular bonds. These bonds can be modeled by quantum harmonic oscillator

The potential energy for a molecular bond is:



$U_{dissoc}$  it is the energy at which the molecule will dissociate and the two atoms will fly apart.

In the lower part of the quantum well the system is likewise in a parabolic quantum well  $\Rightarrow$  quantified energy levels

$\Rightarrow$  quantified energy

$E_{vib} \approx (n - \frac{1}{2}) h\nu$

vibrational energy levels

At room temperature, most molecules are in the ground  $E_0$  level

Their vibrational motion can be excited by absorbing photons with  $\Delta E = h\nu$

The frequency is typically in the infrared region of the spectrum and these vibrational transitions give each molecule a unique distinct IR absorption spectrum  $\Rightarrow$  IR spectroscopy.

ex acetone absorption spectrum

