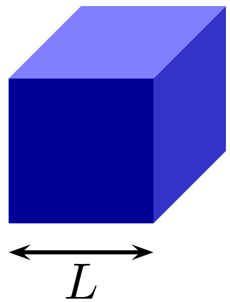
Low Dimensional Systems and Nanotechnology

Judy Bunder

Overview

- Introduction to low dimensional systems:
  - zero dimensions- quantum dots
  - one dimension- quantum wires
  - two dimensions- quantum wells and barriers

Defining low-dimensions

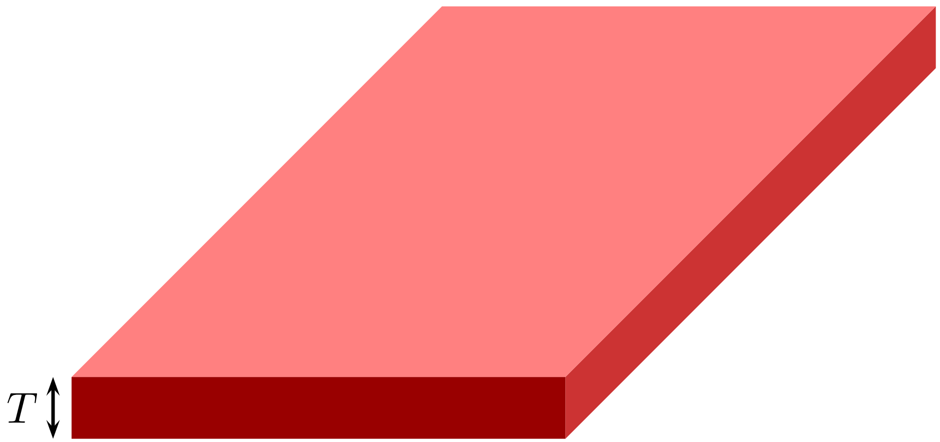


zero dimensions

$L \sim$ few nanometers

one dimension

$W \sim$ few nanometers

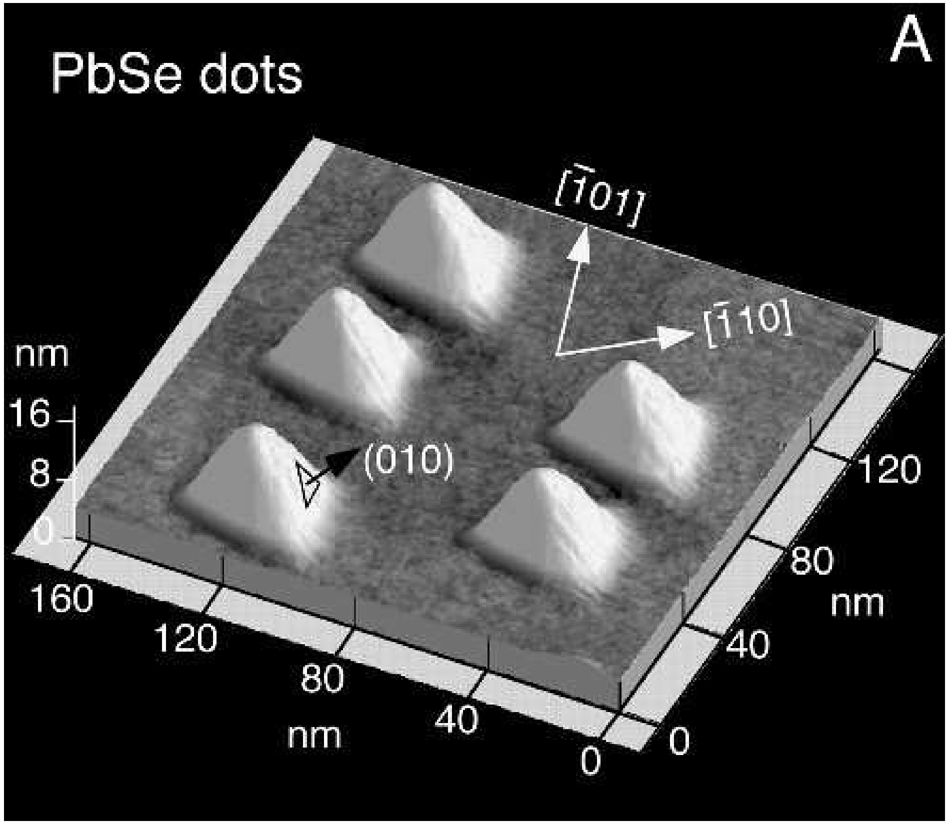


two dimensions

$T \sim$ few nanometers

Quantum dots

- Fabrication
- Applications
- Example of quantum dots as quantum computing qubits.

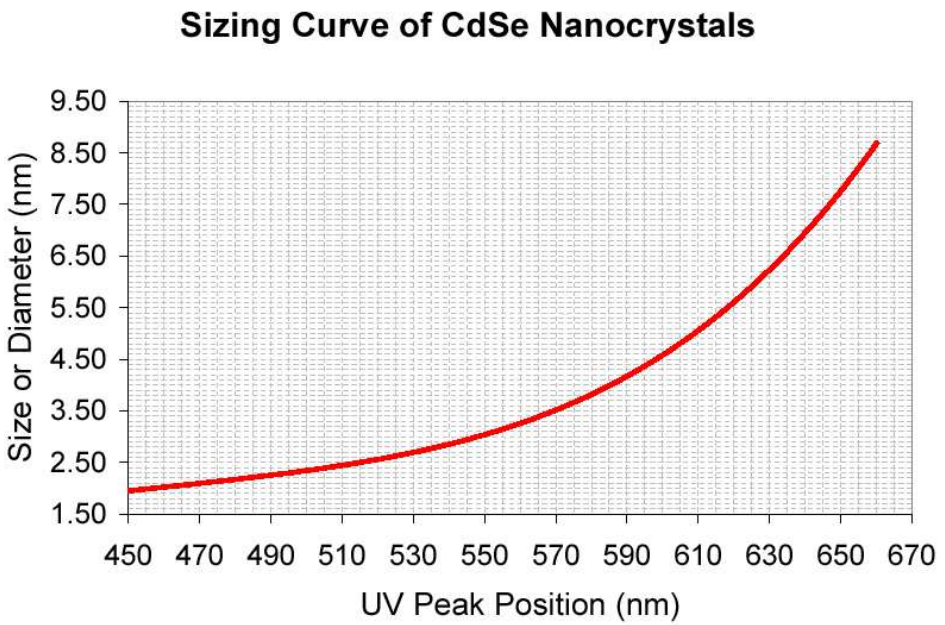


Fabrication

- small crystals (nanocrystals) of one material buried in another material with a larger band gap, e.g., CdSe crystals in ZnSn.
- Lattice mismatch between substrate and deposited material can lead to quantum dot regions, called self-assembled quantum dots.
- Doping or etching can provide individual quantum dots.
- Sizes are typically:
nanocrystals: 2-10nm
self-assembled: 10-50nm

Nanocrystal size and colour

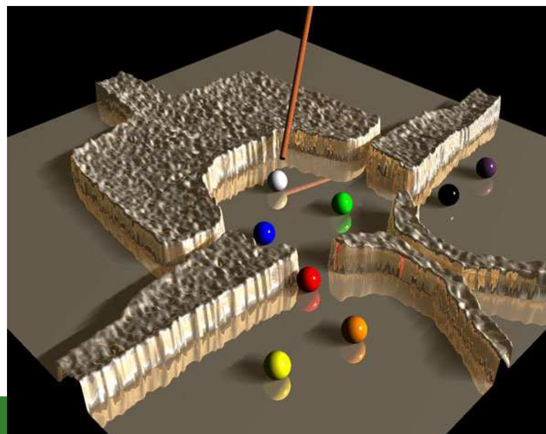
Large dot: red due to
closely spaced energy levels
Small dot: blue due to
widely spaced energy levels

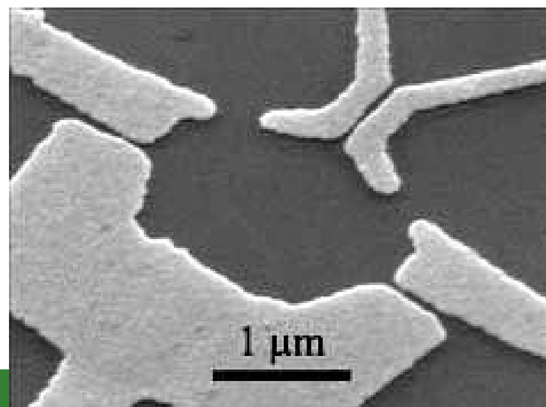


bang gap $\propto$ 1/size^2

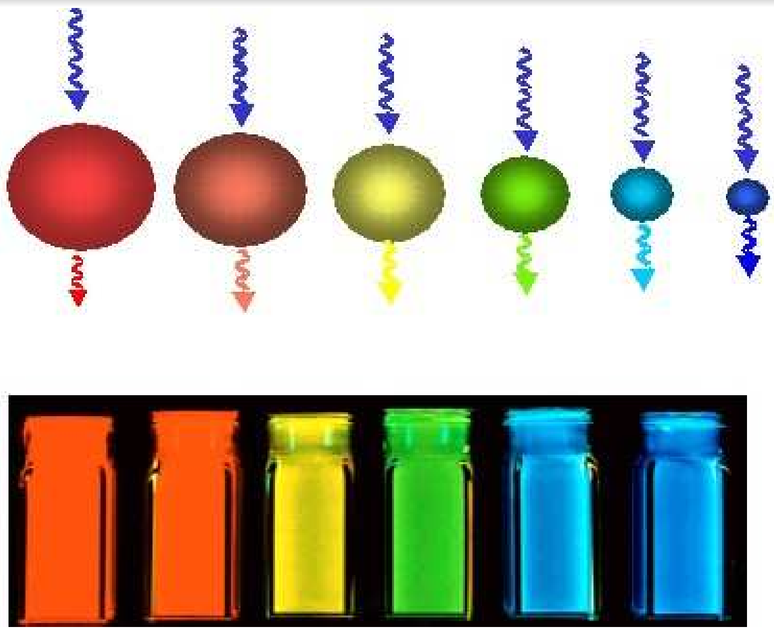
Applications of quantum dots

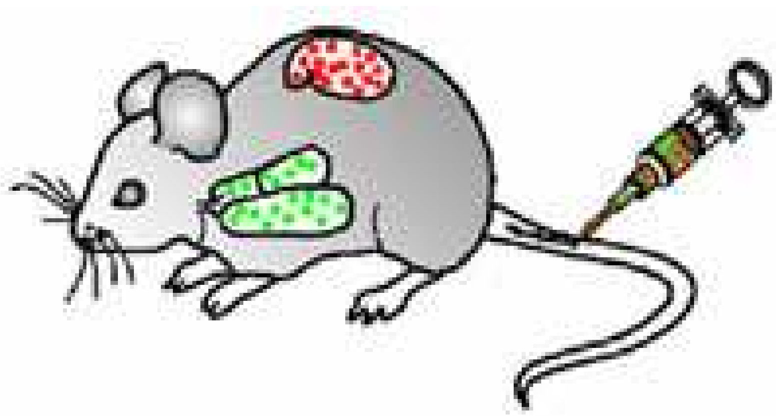
➪ lasers, amplifiers and sensors: zero-dimensional systems have sharp DOS giving them superior transport and optical properties.
➪ Solar cells: more efficient than conventional cells.
➪ Colour displays: LCDs require colour filters so a large proportion of energy is lost, unlike quantum dots.
➪ Cosmetics: some nanocrystals are transparent to visible light but reflect UV light (Titanium dioxide and Zinc oxide)
➪ Medical uses such as cancer treatment.



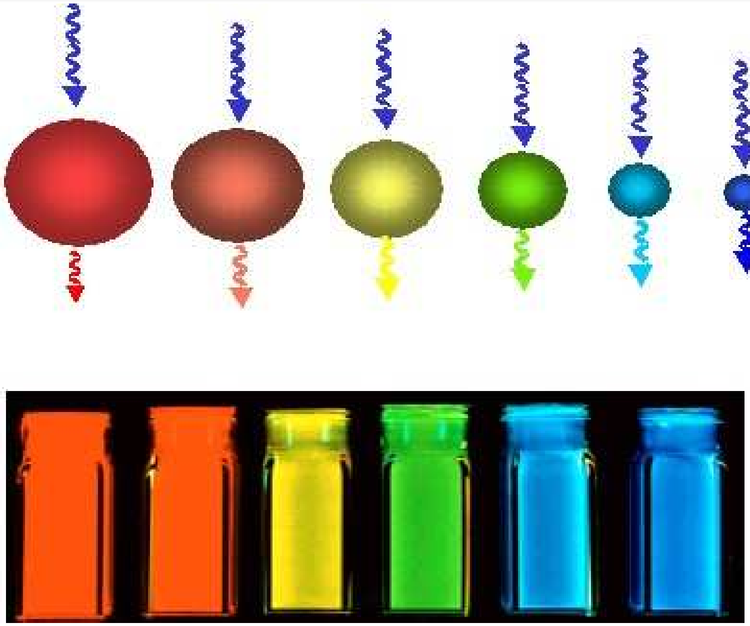


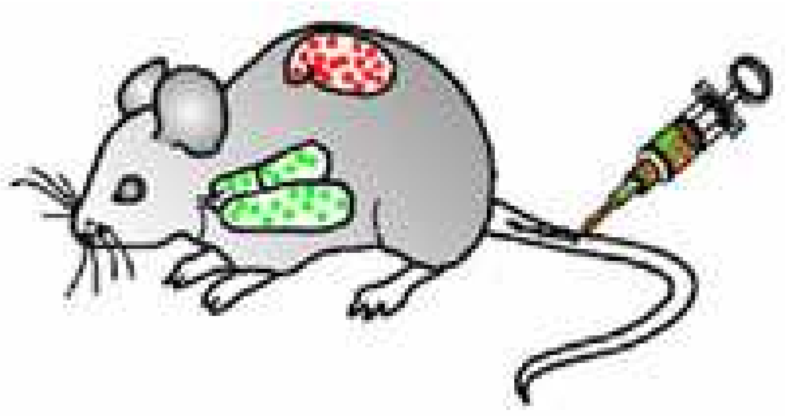
Medical applications





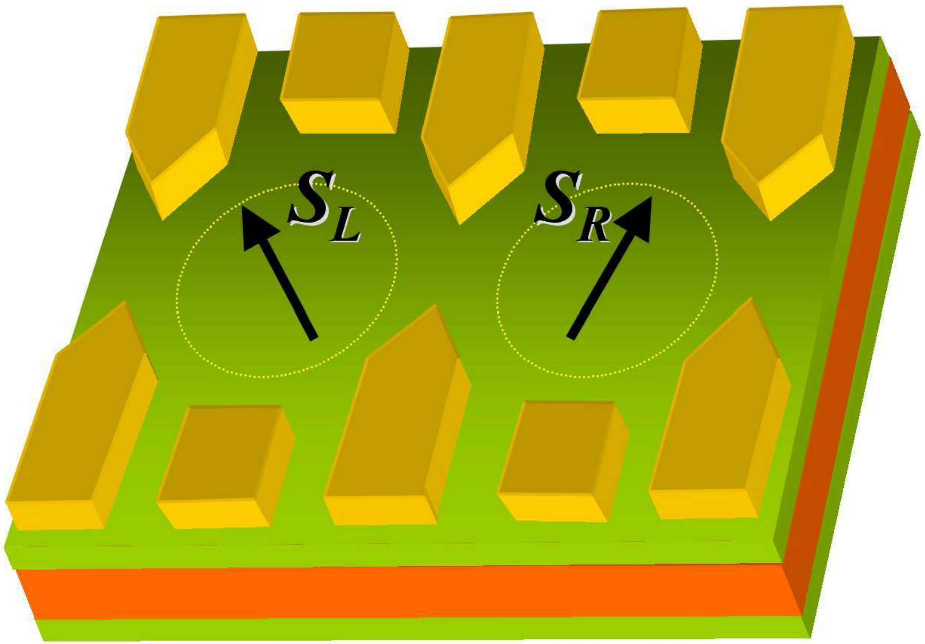
Medical applications





Quantum computing

➪ Any computation controlled by quantum mechanical processes.
➪ Data is defined by qubits (Quantum bits).
➪ The 0 and 1 states (0 volts and 5 volts) of conventional computers become $|0\rangle$ and $|1\rangle$ quantum states.
➪ Any observable A which has two time-independent easily distinguishable eigenstates is a suitable qubit candidate



Why qubits are better than bits

- A standard 3 bit computer can describe one of 8 configurations,
000, 001, 010, 011, 100, 101, 110, 111.
- A 3 qubit computer can describe these 8 configurations all at the same time,

$$|\psi\rangle = a_1|000\rangle + a_2|001\rangle + a_3|010\rangle + a_4|011\rangle + a_5|100\rangle + a_6|101\rangle + a_7|110\rangle + a_8|111\rangle$$

- N qubits $\Rightarrow 2^N$ configurations.
- Quantum computers should be vastly faster than conventional computers.

General execution

- Initialize all qubits to $|0\rangle$.
- Run the algorithm.
- Read each qubit.

General execution

- Initialize all qubits to $|0\rangle$.
- Run the algorithm.
- Read each qubit.
- Store the read data.
- Run the above 4 steps several times and determine the correct solution statistically.

Eg: at the end of the algorithm a qubit has the state

$$|\psi\rangle = \frac{8}{10}|0\rangle + \frac{6}{10}|1\rangle$$

The state of this qubit can be read as either $|0\rangle$ or $|1\rangle$, but most of the readings will be $|0\rangle$ so $|0\rangle$ is the correct result.

What can quantum computers do?

➩ Not every type of calculation will be best performed by quantum computers.

➩ Simple example- the password cracker

- Find a solution to a problem, where the only way to solve the problem is choose a solution and check it.
- There are n possible solutions which take equal time to check.
- On average we would need to check $n/2$ times but a quantum computer needs to check $\sqrt{n}$ times.

DiVincenzo criteria for quantum computers

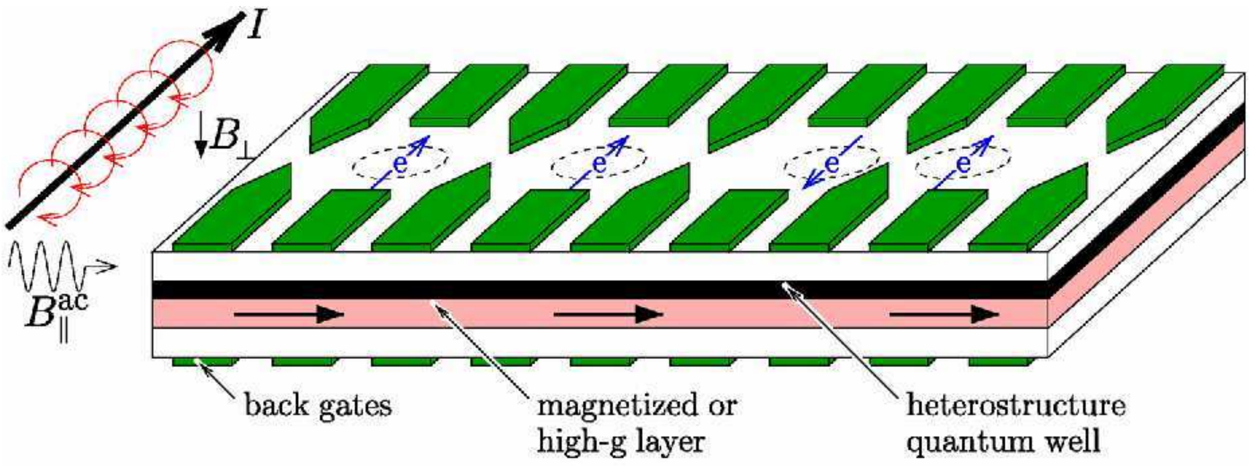
- **Information storage**: need a large number of qubits.
- **Initial state**: must be able to set all qubits to $|0\rangle$ at the end of every computation.
- **Isolated**: to prevent decoherence.
- **Gate implementation**: need a method to change the state of the qubit in a precise way in a limited time period.
- **Read out**: need a method to read the final result.

Control the coupling between qubits

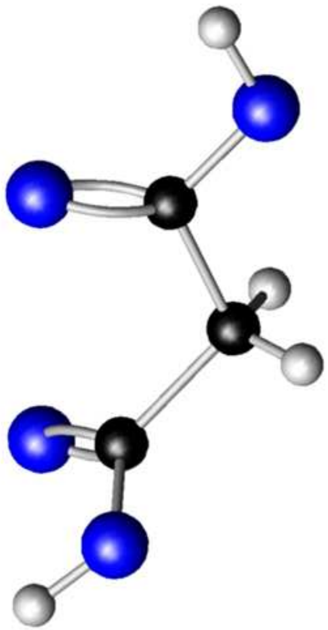
Heisenberg Hamiltonian between two spins

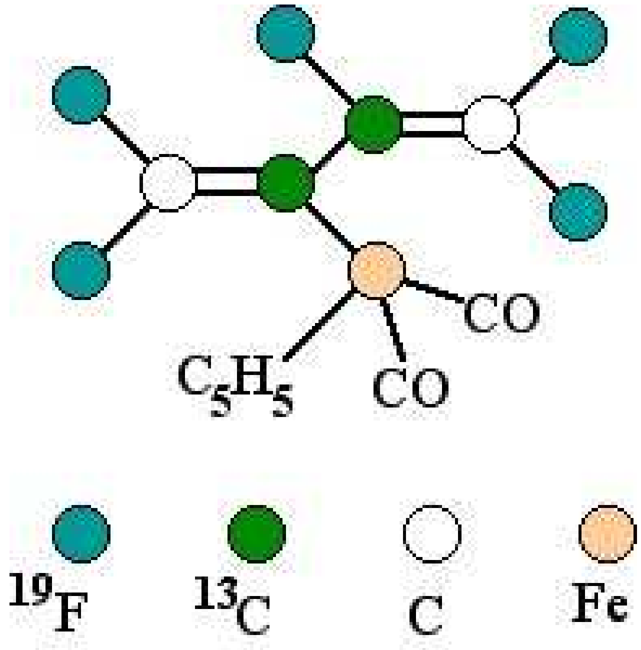
$$H = J(t)\mathbf{S}_L.\mathbf{S}_R$$

where the coupling is controlled by J.
On: $J \neq 0$. Off: $J = 0$.



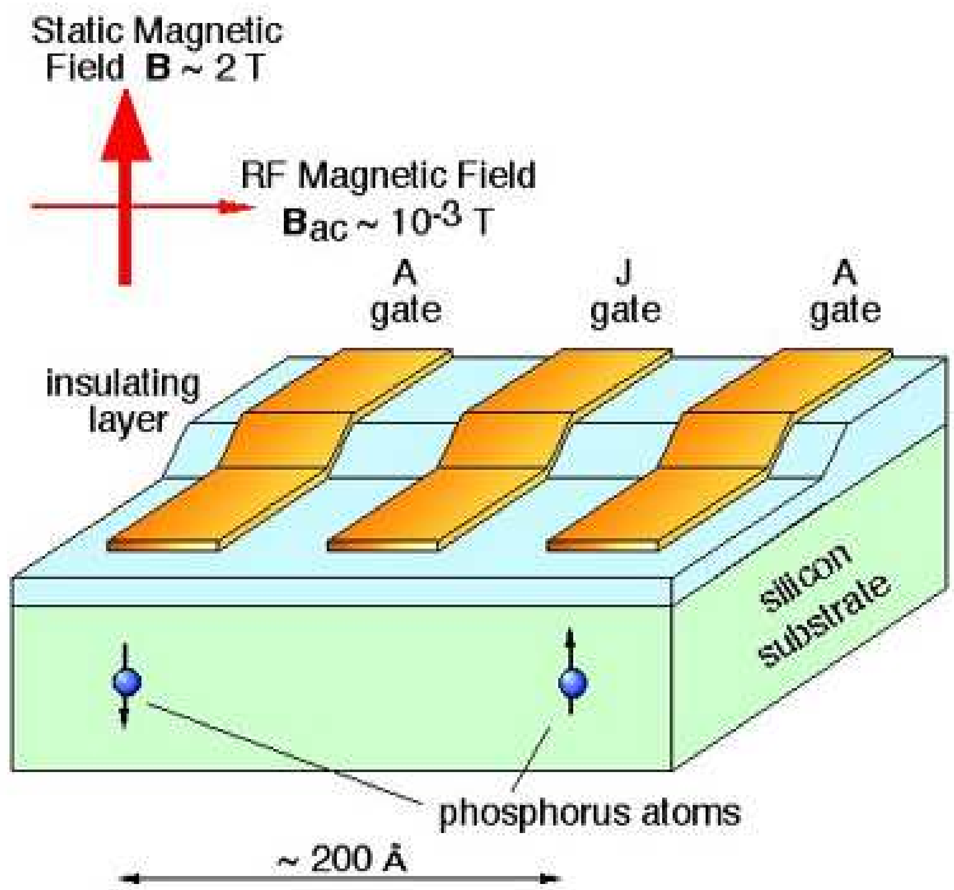
Molecular quantum computers





Malonic acid
Blue: O, White: H
Black: ^{13}C

Solid state quantum computer

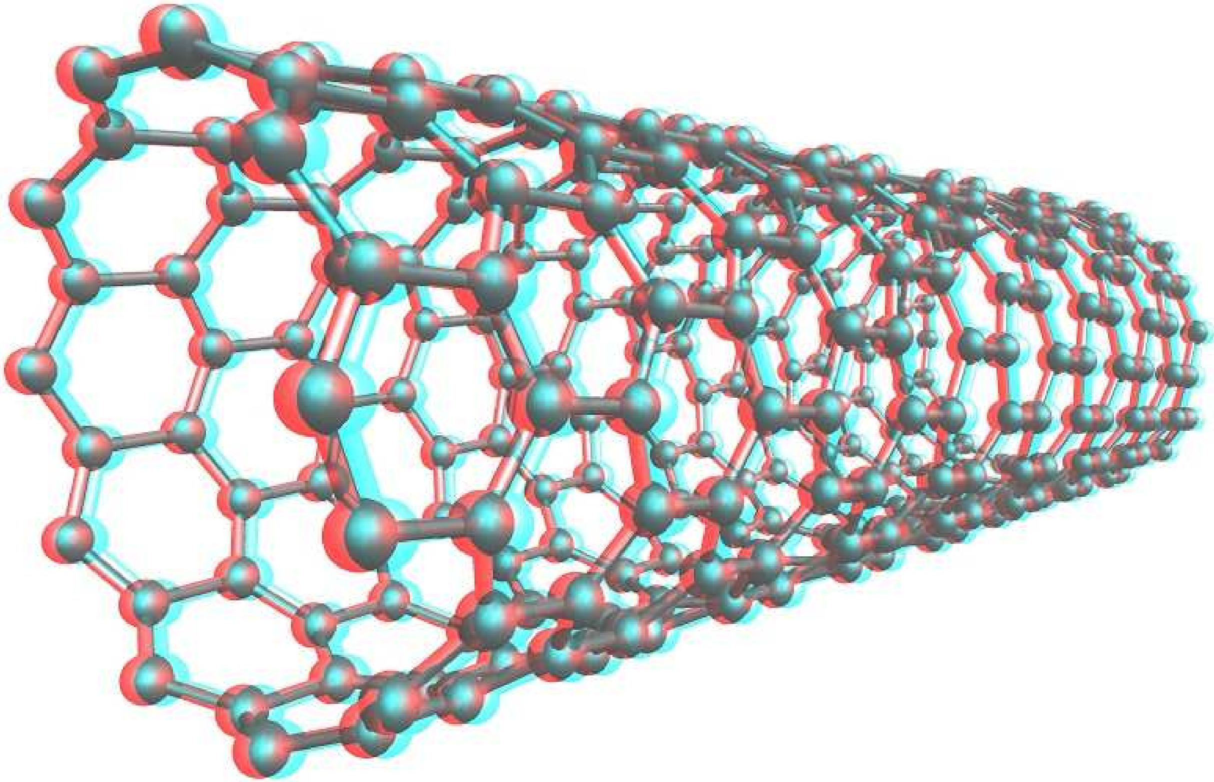


Quantum dot conclusion

- Quantum dots have many applications, some of which are already realized but many require improved fabrication techniques.
- One possible application is a quantum computer but gate manipulation is difficult.
- Although other materials have been more successful as quantum computing qubits, they also have their limitations.

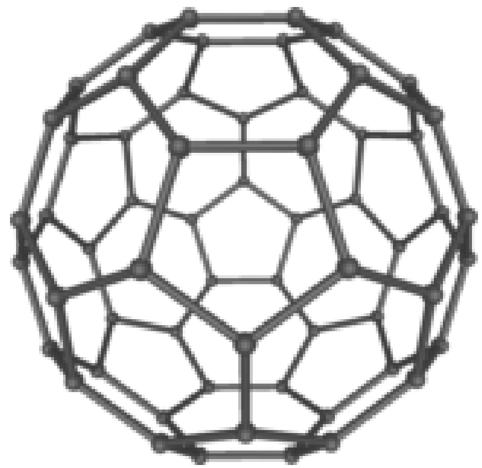
Quantum wires

- Carbon nanotubes
- Nanotube applications
- Some analytic results



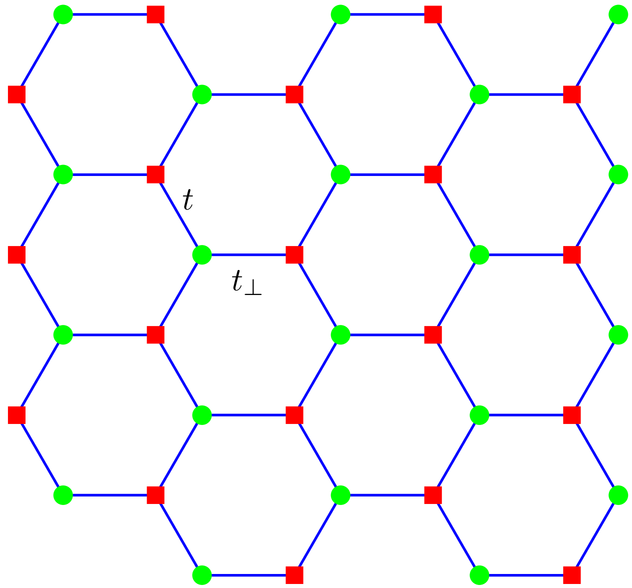
The fullerenes

Spheres, ellipsoids or tubes of carbon



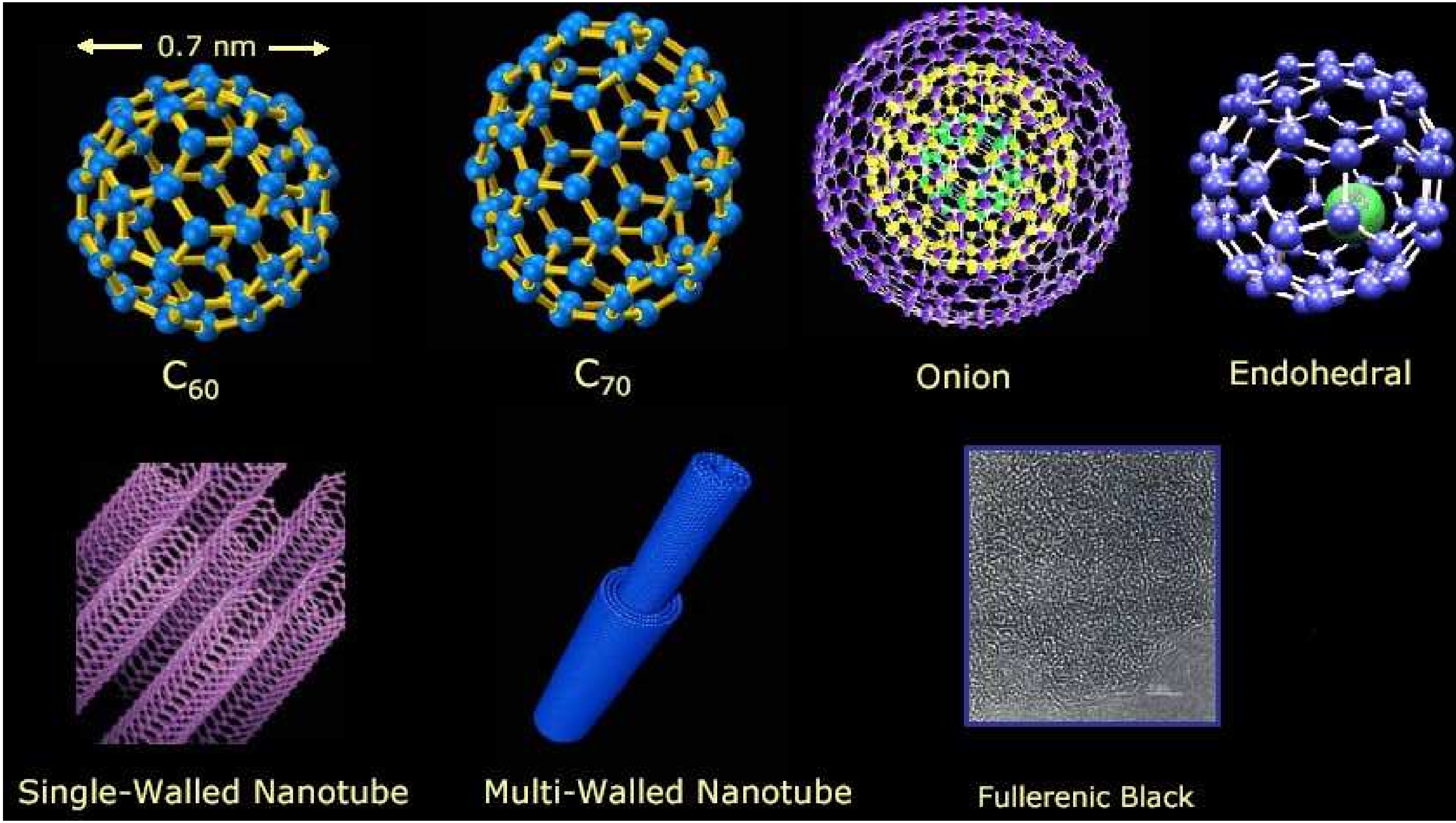
Buckminsterfullerene (C_{60})

Carbon nanotube

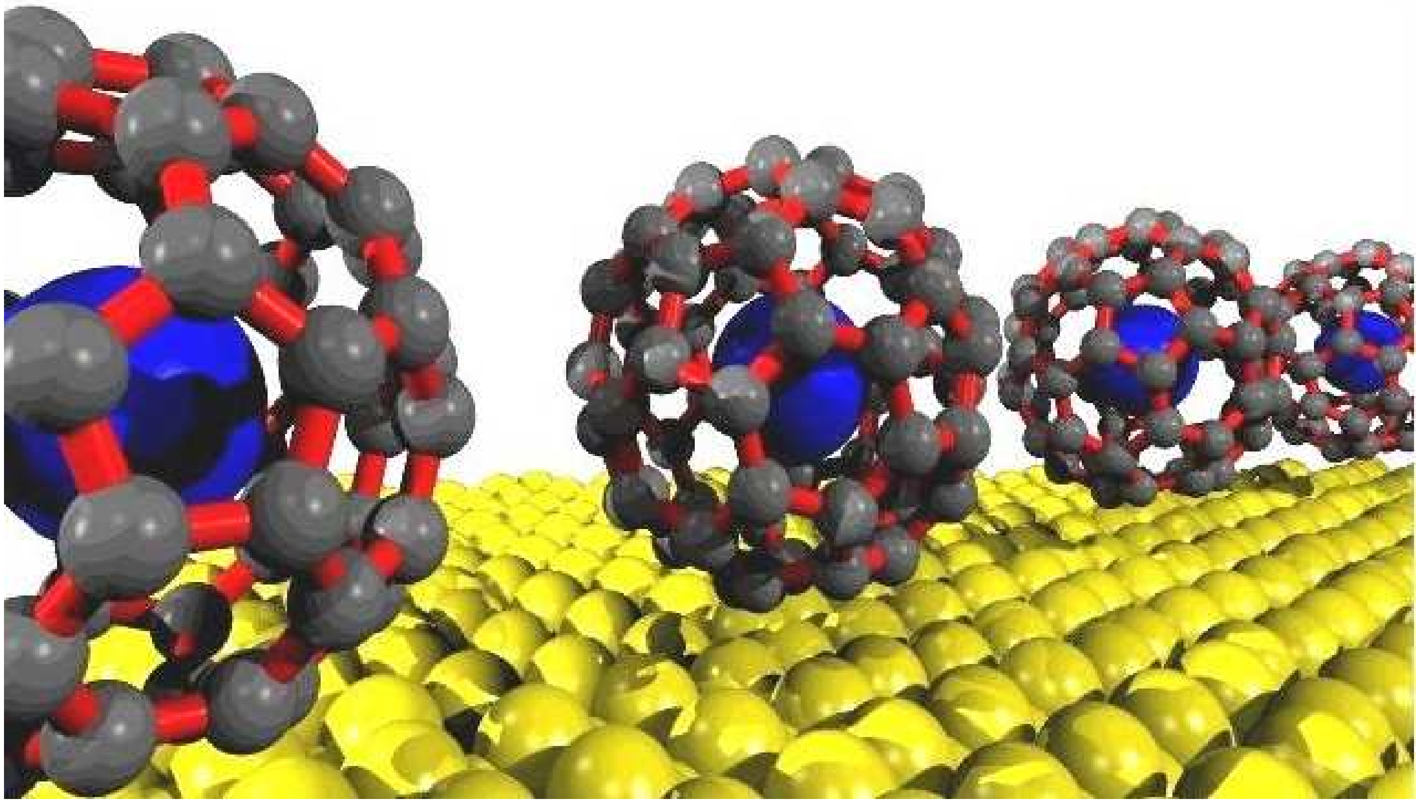


graphene lattice

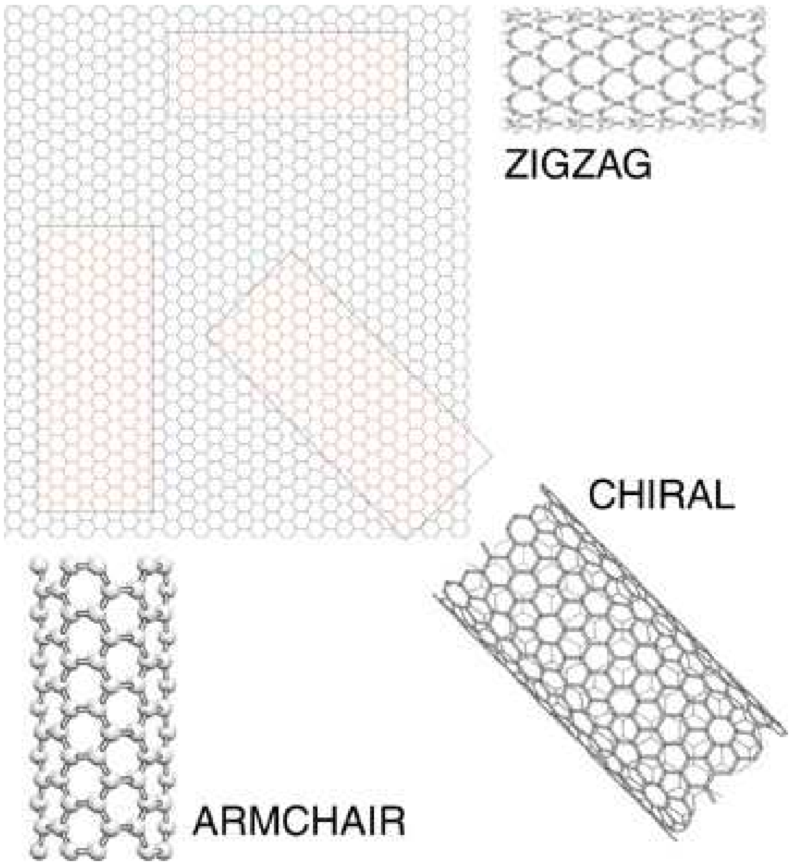
Fullerene examples



Fullerene quantum computer



Quantum wires: carbon nanotubes

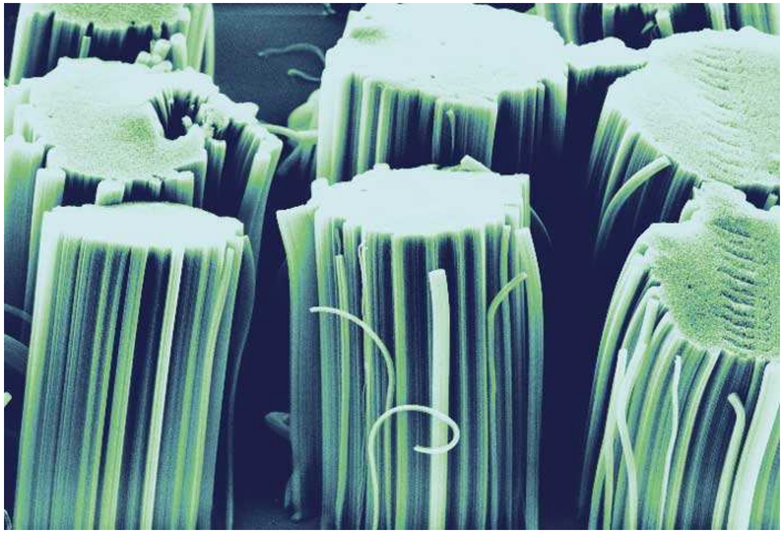


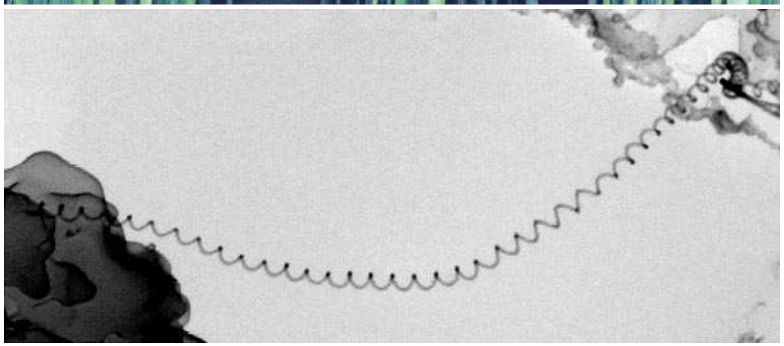
- Impressive strength:
  - tensile strength:

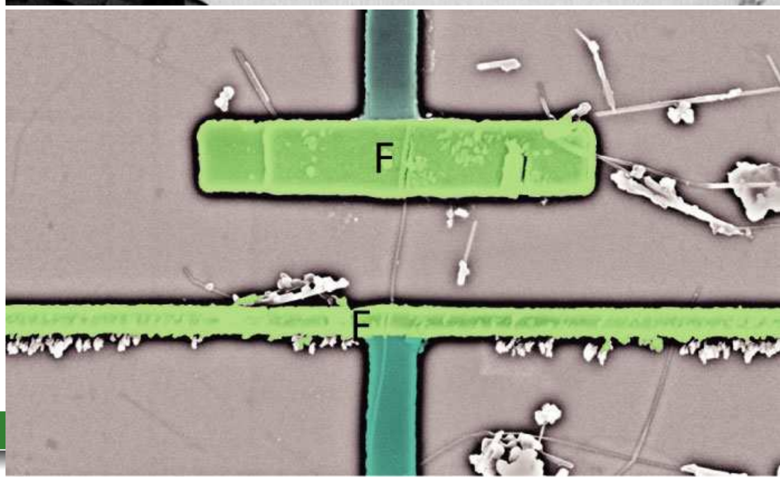
63 GPa (steel: 1.2GPa).
  - Young's modulus:

1000 GPa (steel: 200 GPa).
- Metallic or semiconducting depending on the structure (armchair, zigzag or chiral)
- Occur naturally, but even small defects will seriously affect a nanotube's performance.
- Synthesis is expensive.

Nanotube applications

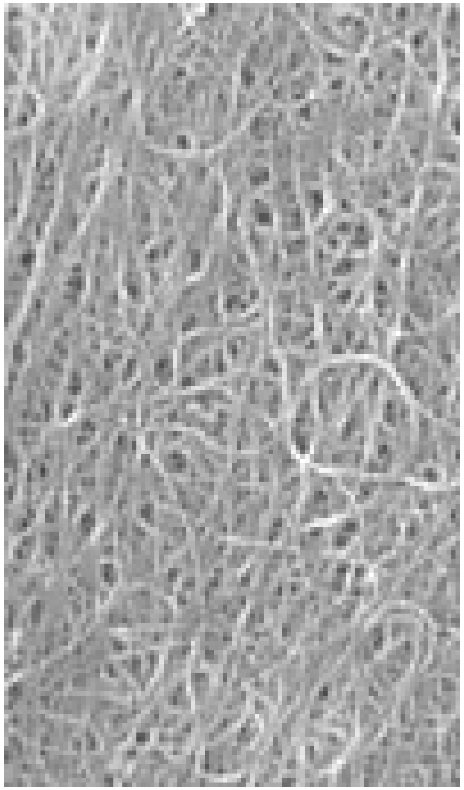






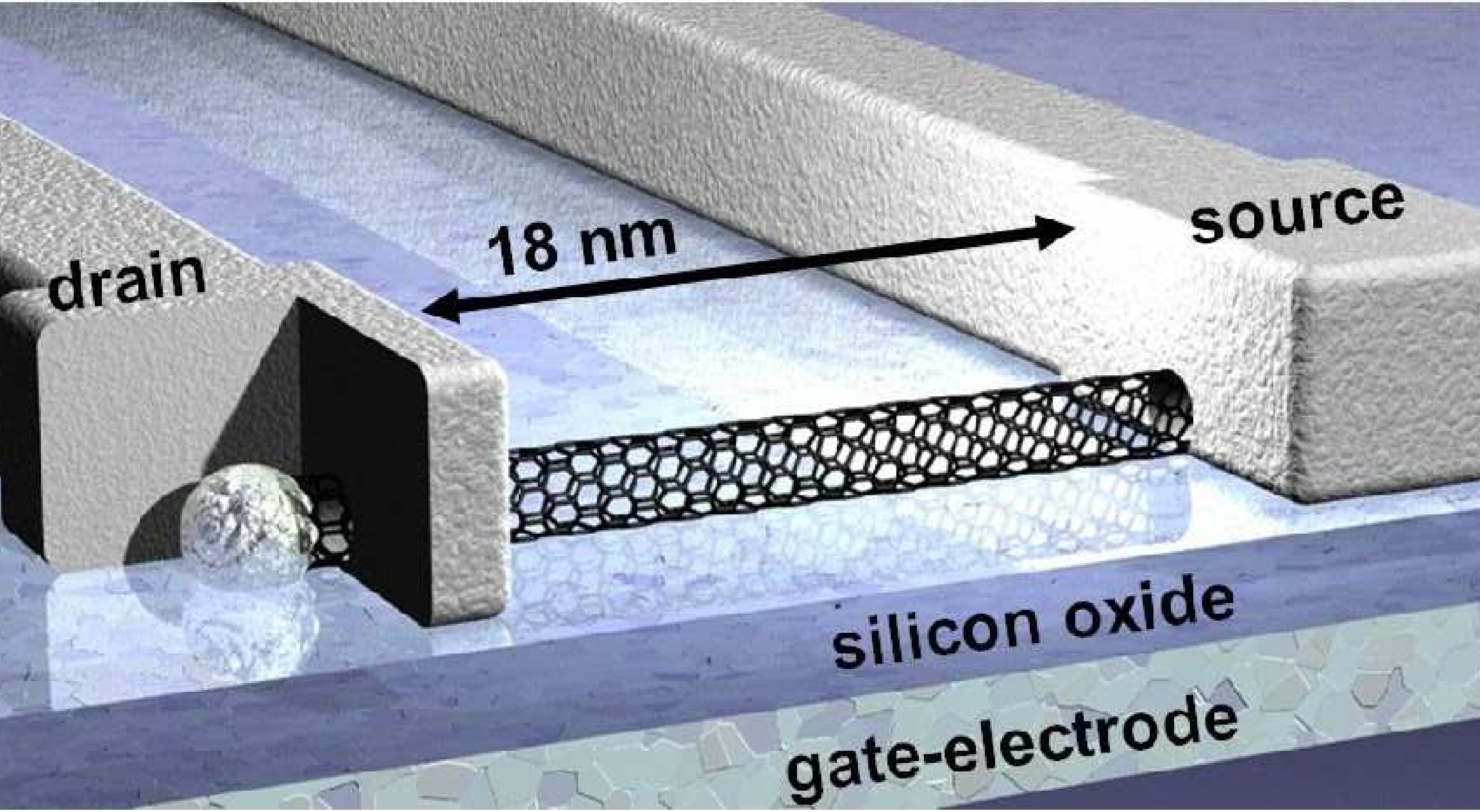
- Most applications use multi-walled carbon nanotubes as they are easier and cheeper to produce.
- Cables, sports gear, clothes, body armor
- Nanoelectronics
- Medical applications
- Fuel cells
- Field emission display (FED) TV

Carbon nanotube fabric

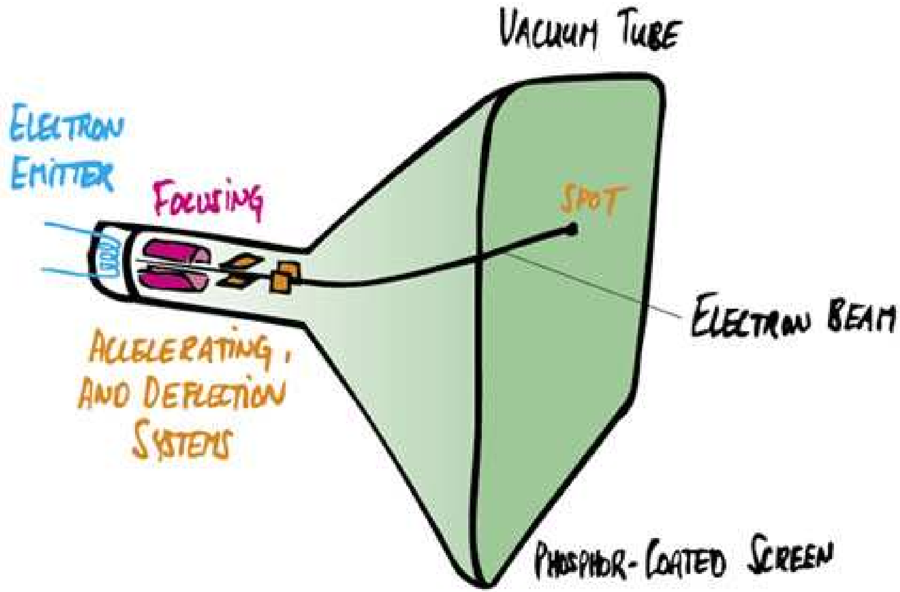


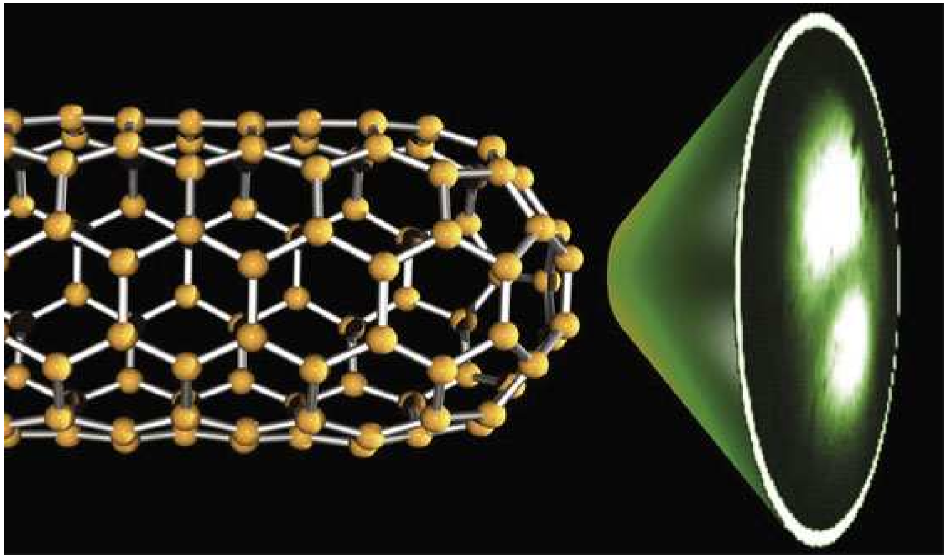
Carbon nanotube bicycle

Carbon nanotube transistor



Field emission display (FED) TV



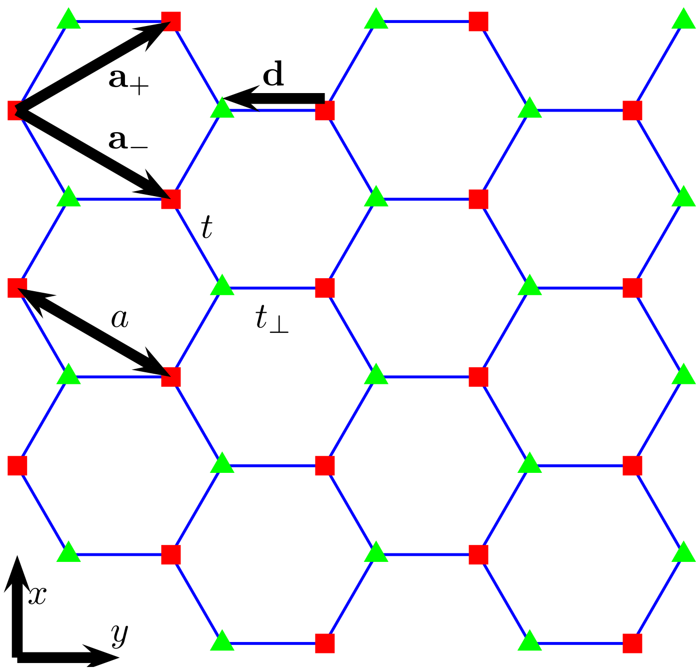


Graphene Hamiltonian

Hubbard model Hamiltonian:

$$H_0 = -\,t \sum_{\mathbf{r}\in\mathbf{R},\alpha} [c^\dagger_{1\alpha}(\mathbf{r})c_{2\alpha}(\mathbf{r}+\mathbf{a}_+ +\mathbf{d}) + c^\dagger_{1\alpha}(\mathbf{r})c_{2\alpha}(\mathbf{r}+\mathbf{a}_- +\mathbf{d})]$$

$$-\,t_\perp \sum_{\mathbf{r}\in\mathbf{R},\alpha} [c^\dagger_{1\alpha}(\mathbf{r})c_{2\alpha}(\mathbf{r}+\mathbf{d})] + h.c$$



$\mathbf{a}_\pm = a(\pm 1/2, \sqrt{3}/2),\ \mathbf{d} = a(0, -1/\sqrt{3})$

Where $\mathbf{R} = n_+\mathbf{a}_+ + n_-\mathbf{a}_-$.

Energy spectrum

We can diagonalize the Hamiltonian using the Fourier transform

$$c_{i\alpha}(r) = \frac{1}{\sqrt{N_i}} \sum_k c_{i\alpha}(k) e^{ir.k}$$

$$\Longrightarrow \; H_0 = -\sum_{k,\alpha} \left(c^\dagger_{1\alpha}(k), c^\dagger_{2\alpha}(k) \right) \begin{pmatrix} 0 & h(k) \\ h(k)^* & 0 \end{pmatrix} \begin{pmatrix} c_{1\alpha}(k) \\ c_{2\alpha}(k) \end{pmatrix}$$

with

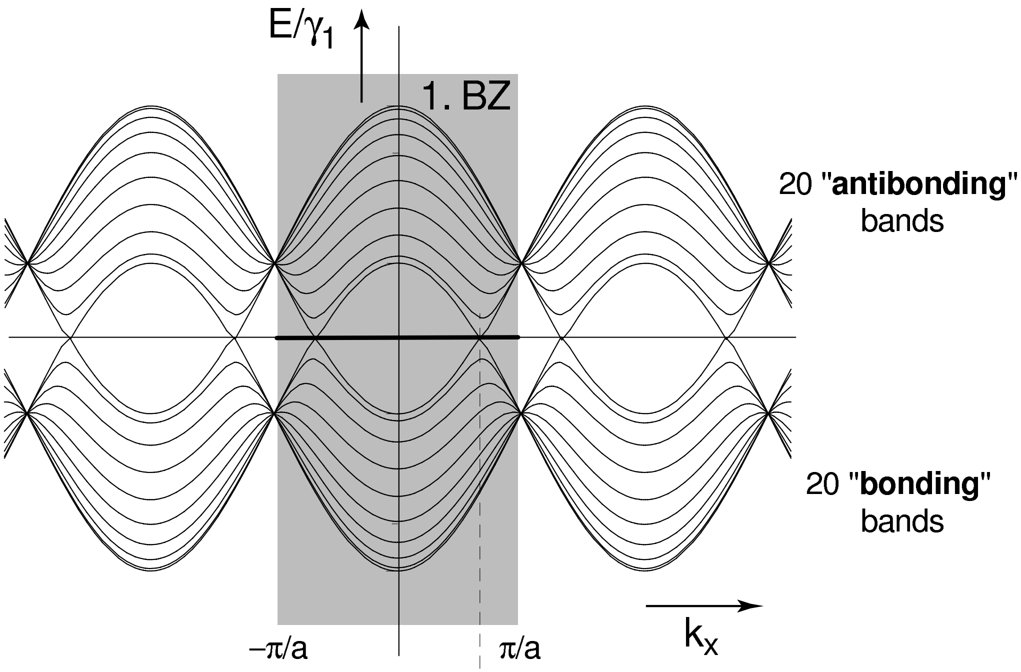
$$h(k) = 2t \cos(ak_x/2) e^{iak_y/2\sqrt{3}} + t_\perp e^{-iak_y/\sqrt{3}}.$$

The energy can be shown to be $\epsilon(k) = \mp |h(k)|$.

Zero energy gap

If $h(k) = 0$ the two bands meet $\Longrightarrow$ a conductor
The lowest momentum for $h(k) = 0$ when $t = t_\perp$:

$$\text{Dirac points}: \mathbf{K} = \left(\pm\frac{4\pi}{3a}, 0\right), \ \mathbf{K} = \left(\pm\frac{2\pi}{3a}, \pm\frac{2\pi}{a\sqrt{3}}\right)$$

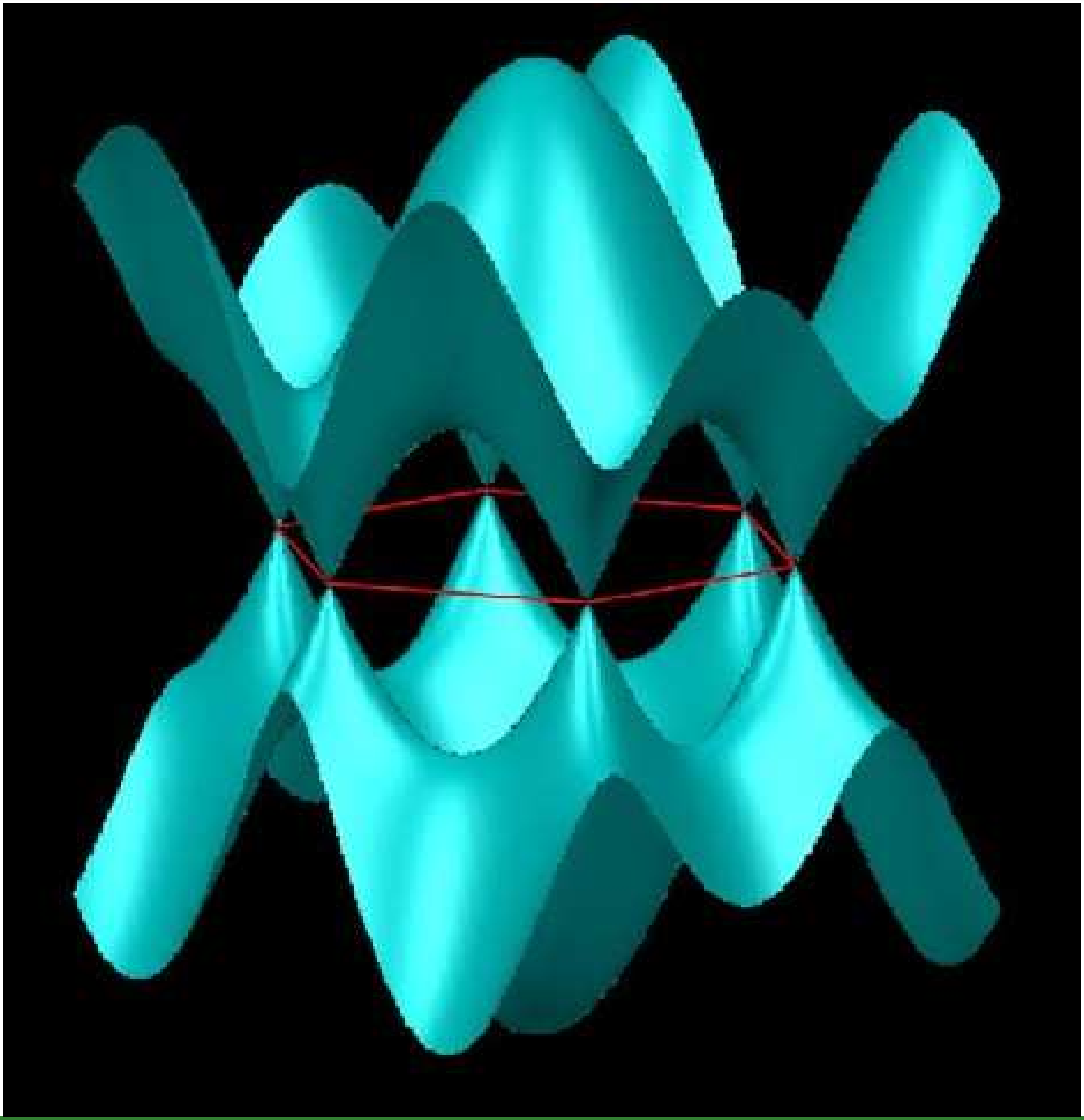


Near Dirac points:

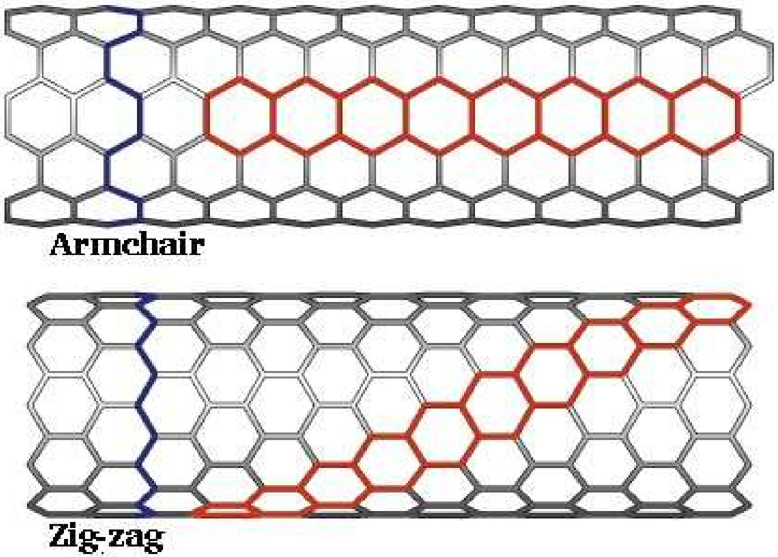
$$\epsilon(k) = \mp v(k)|\mathbf{k} - \mathbf{K}|,$$

$$v(k) = at\sqrt{3}/2$$

Dirac points

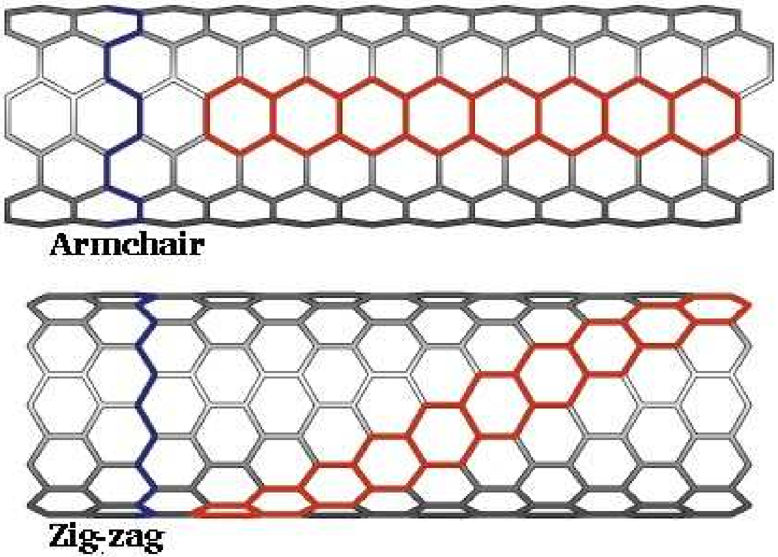


Conducting carbon nanotube



- A carbon nanotube has a finite circumference C which quantizes the momentum around the tube.
- A nanotube
is conducting if the quantized momenta matches a Dirac point.

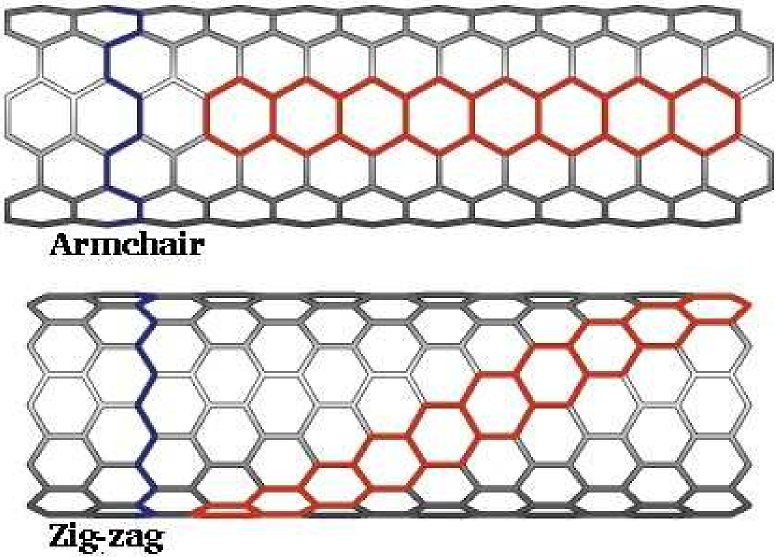
Conducting carbon nanotube



- A carbon nanotube has a finite circumference C which quantizes the momentum around the tube.
- A nanotube is conducting if the quantized momenta matches a Dirac point.
- Armchair: quantized along the y direction, $k_y = 2\pi n/C = 2\pi n/\sqrt{3}aN_y$.

If $n = 0$, $k_y = 0$, Dirac point $\mathbf{K} = \left(\pm\frac{4\pi}{3a}, 0\right)$.

Conducting carbon nanotube



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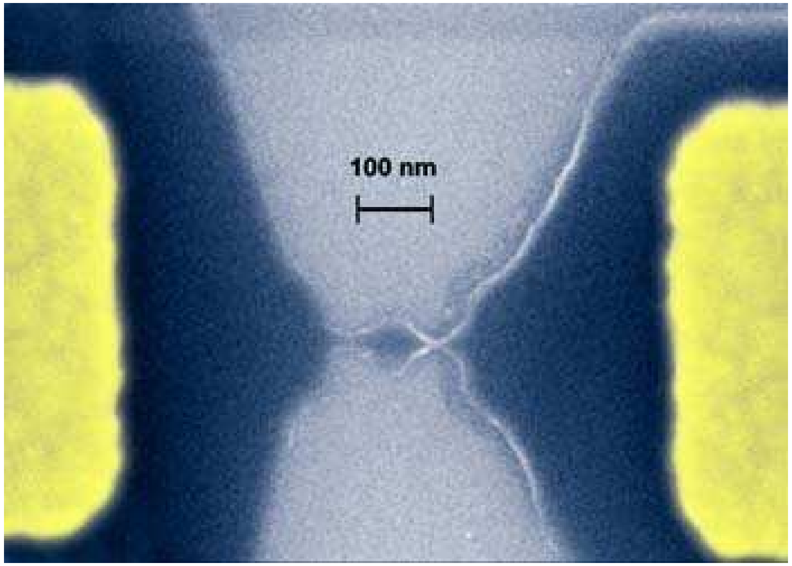
If $n = 0$, $k_y = 0$, Dirac point $\mathbf{K} = \left(\pm\frac{4\pi}{3a}, 0\right)$.

➪ Zigzag: is quantized along the x direction, $k_x = 2\pi n/C = 2\pi n/N_x a$.

If $N_x = 3n$, $k_x = 2\pi/3a$, Dirac point $\mathbf{K} = \left(\pm\frac{2\pi}{3a}, \pm\frac{2\pi}{a\sqrt{3}}\right)$.

Graphene

- Graphene is a single sheet of graphite, one atom thick.
- It can be 2D or cut thin to make a 1D graphene ribbon.
- Strong, thermally conductive, electrically conductive.
- Cheaper and easier to make than carbon nanotubes.
- Easier to integrate into electronic devices than nanotubes.



Graphene transistor

Quantum wire conclusion

- A promising candidate for a practical quantum wire is a carbon nanotube.
- But due to engineering difficulties a graphene ribbon may be better.
- Both these materials have many potential applications, notably in nanoelctronics.
- Limitations at this point are mainly due to difficulties in constructing pure, regular samples of significant size.

2D wells/barriers

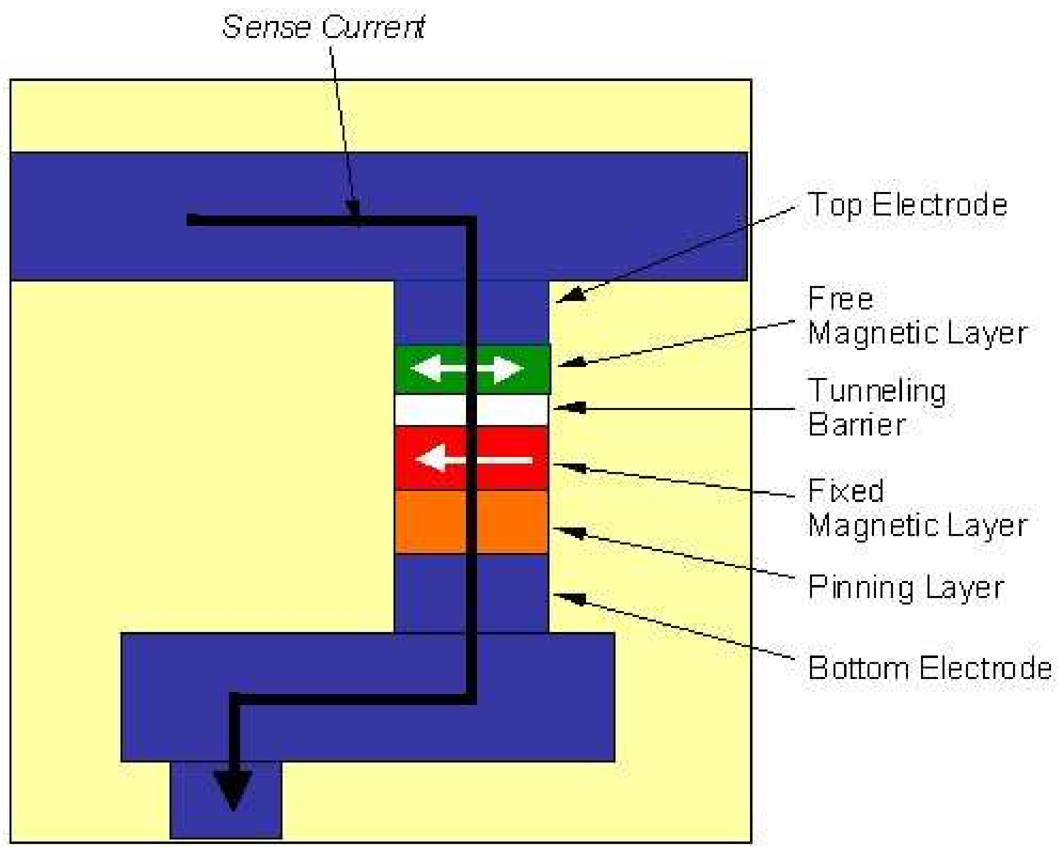
- Layered structures
- Example of a 2D barrier between two magnetic materials (magnetic tunnel junction- MTJ)
  - evaluate the conductance
  - evaluate the tunelling magnetoresistance (TMR)

Layered structures

- A quasi-2D system forms within each thin layer.

Layered structures

- A quasi-2D system forms within each thin layer.
- Magnetic tunnel junction (MTJ): a thin insulator (~ 1nm) separating two magnetic materials.
- The magnetism is pinned in one material while in the other it is free to rotate.



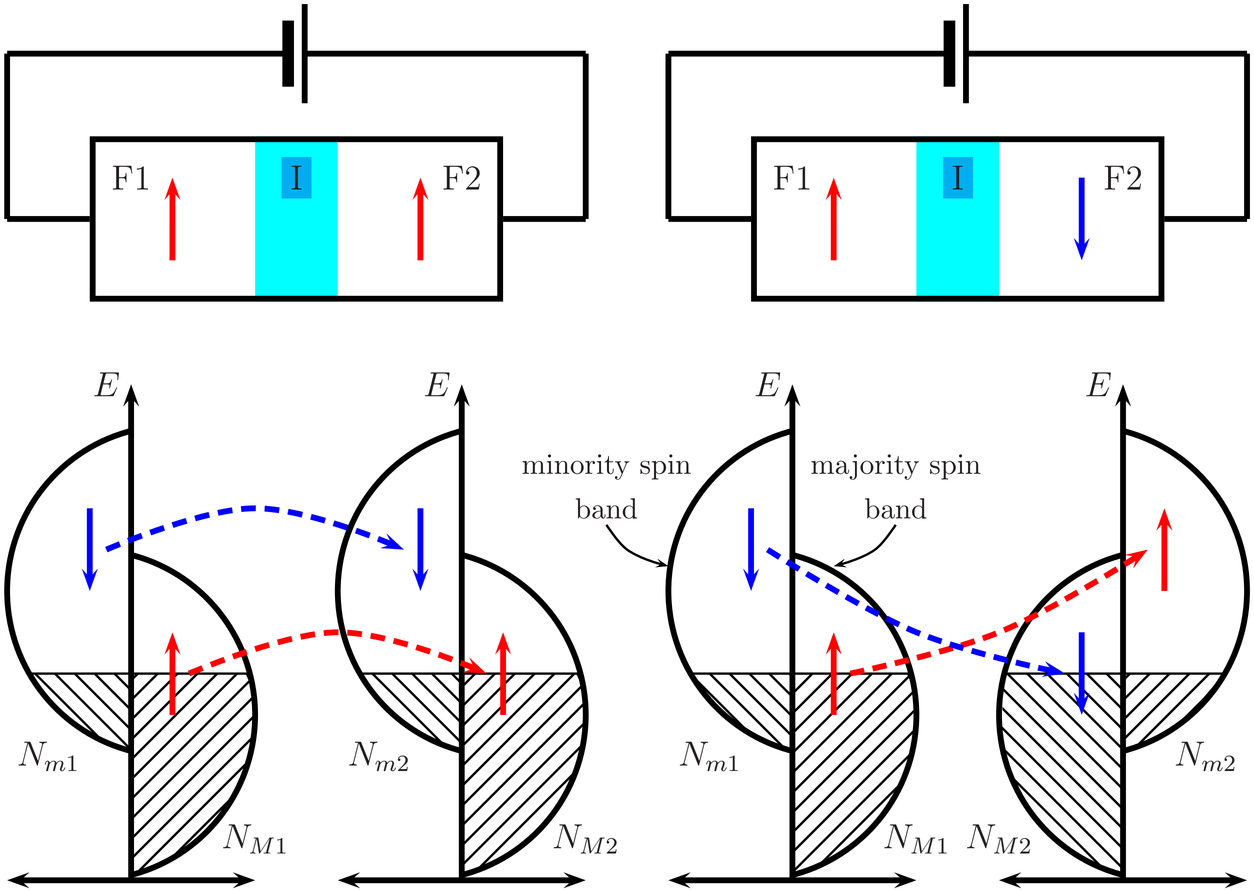
Tunnelling magnetoresistance (TMR)

➪ Tunnelling magneto resistance (TMR): when the current through the junction is highly dependent on the orientation of the magnetizations.
➪ Current is maximized when the magnetism in the two materials are parallel and minimized when anti-parallel

$$\mathrm{TMR} = \frac{I_{\uparrow\uparrow} - I_{\uparrow\downarrow}}{I_{\uparrow\downarrow}}$$

➪ TMR can be up to 50% but only at low temperatures when using ferromagnets.

Julliere model of TMR

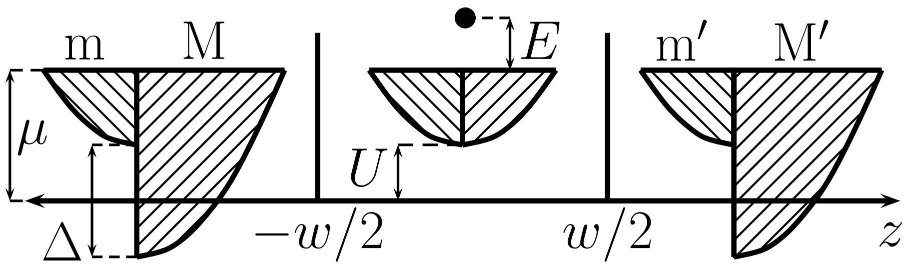


- Current $\sim$ density of states

$$I_{\uparrow\uparrow} \sim N_{m1}N_{m2} + N_{M1}N_{M2} \qquad I_{\uparrow\downarrow} \sim N_{m1}N_{M2} + N_{M1}N_{m2}$$

Hamiltonian and energy

$$H = -\frac{\hbar^2}{2m}\partial_r^2 - \frac{\Delta}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\Theta(w/2 - |z|) + U\Theta(|z| - w/2)$$



- Magnetic materials:
  - majority band: $\hbar k_M/2m = E + \mu + \Delta/2$
  - minority band: $\hbar k_m/2m = E + \mu - \Delta/2$
- Insulator: $\hbar k/2m = E + \mu - U$

Wave functions in magnetic materials

Majority band particle entering LHS:

$$\Psi_L(z) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{ik_M^z z} + C_{MM} \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-ik_M^z z}$$

$$+ C_{Mm} \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{-ik_m^z z}$$

$$\Psi_R(z) = \hat{R} \left[C_{MM'} \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{ik_M^z z} + C_{Mm'} \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{ik_m^z z} \right]$$

Rotation matrix

$$\hat{R} = \begin{pmatrix} \cos(\theta/2) & \sin(\theta/2) \\ -\sin(\theta/2) & \cos(\theta/2) \end{pmatrix}$$

Wave function in insulator

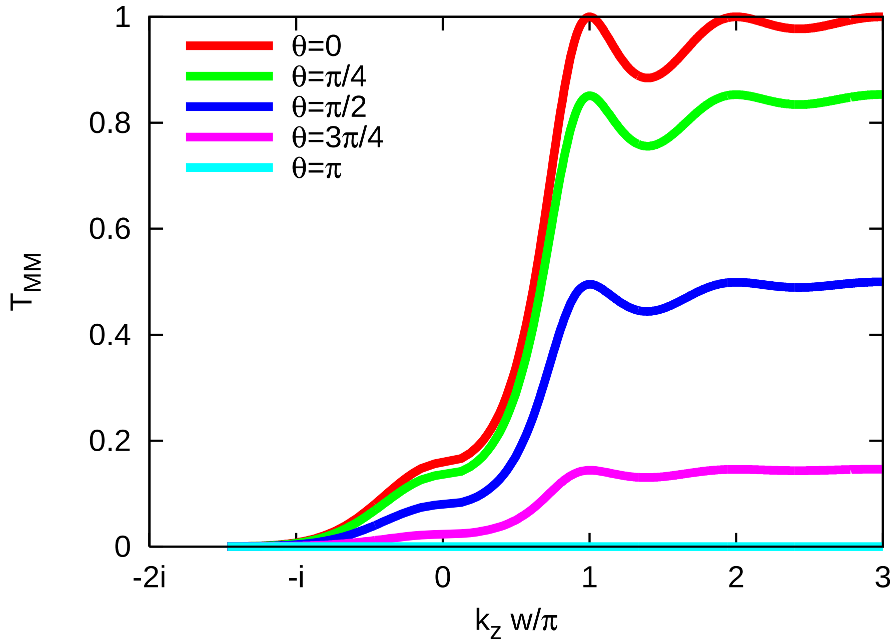
$$\Psi_I(z) = \begin{pmatrix} A_1^+ \\ A_2^+ \end{pmatrix} e^{ik^z z} + \begin{pmatrix} A_1^- \\ A_2^- \end{pmatrix} e^{-ik^z z}.$$

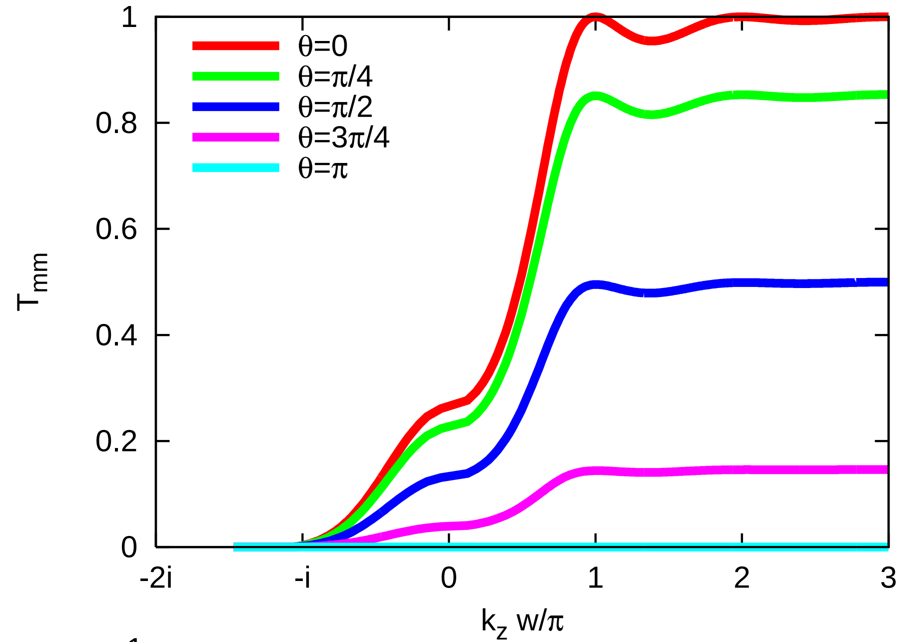
- k^z can be real (quantum well) or imaginary (quantum barrier)
- By matching the wave functions and their derivatives at the boundaries we can evaluate all the coefficients.

$$\psi_L(-w/2) = \psi_I(-w/2), \qquad \psi_R(w/2) = \psi_I(w/2)$$

$$\partial_z\psi_L(-w/2) = \partial_z\psi_I(-w/2), \qquad \partial_z\psi_R(w/2) = \partial_z\psi_I(w/2)$$

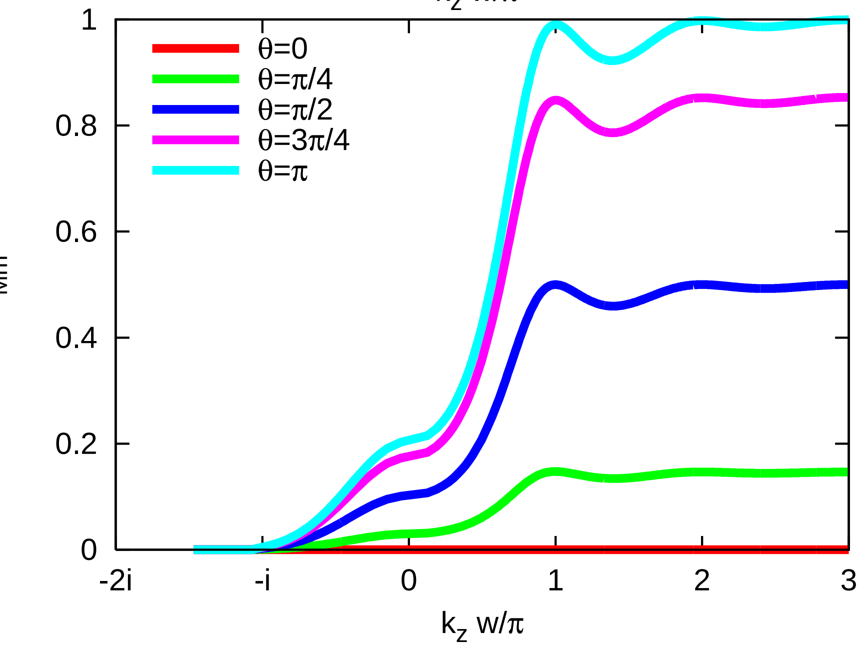
Solutions of the Transmission coefficients





Transmission probability:

$$T_{ab} = \begin{cases} |C_{ab}|^2 k_b^z / k_a^z, & k_b^z, k_a^z > 0 \\ 0, & \text{otherwise} \end{cases}$$



Landauer formula for current density

$$J_{ab} = e \int \frac{d^3 k_a}{(2\pi)^3} [f(E_a) - f(E_a + eV)] T_{ab} v_{za}$$

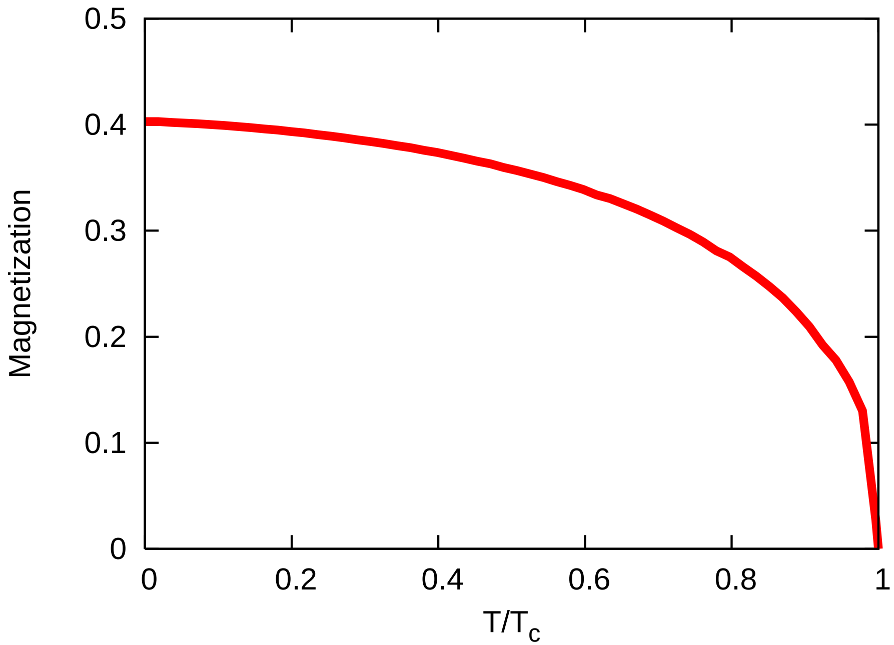
- Fermi-Dirac distribution:

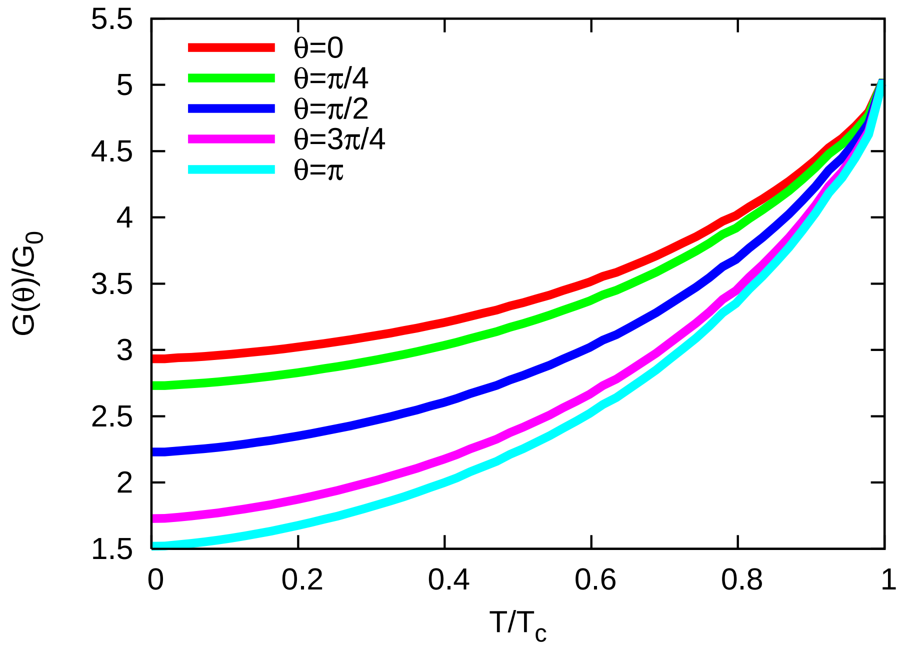
$$f(E_a) = \frac{1}{e^{\beta(E_a - \mu)} + 1}$$

- Voltage across MTJ: V
- Velocity z-component: $v_{za} = \hbar k_a^z / m$
- Conductance

$$G(\theta) = \frac{1}{V} \sum_{ab} J_{ab}$$

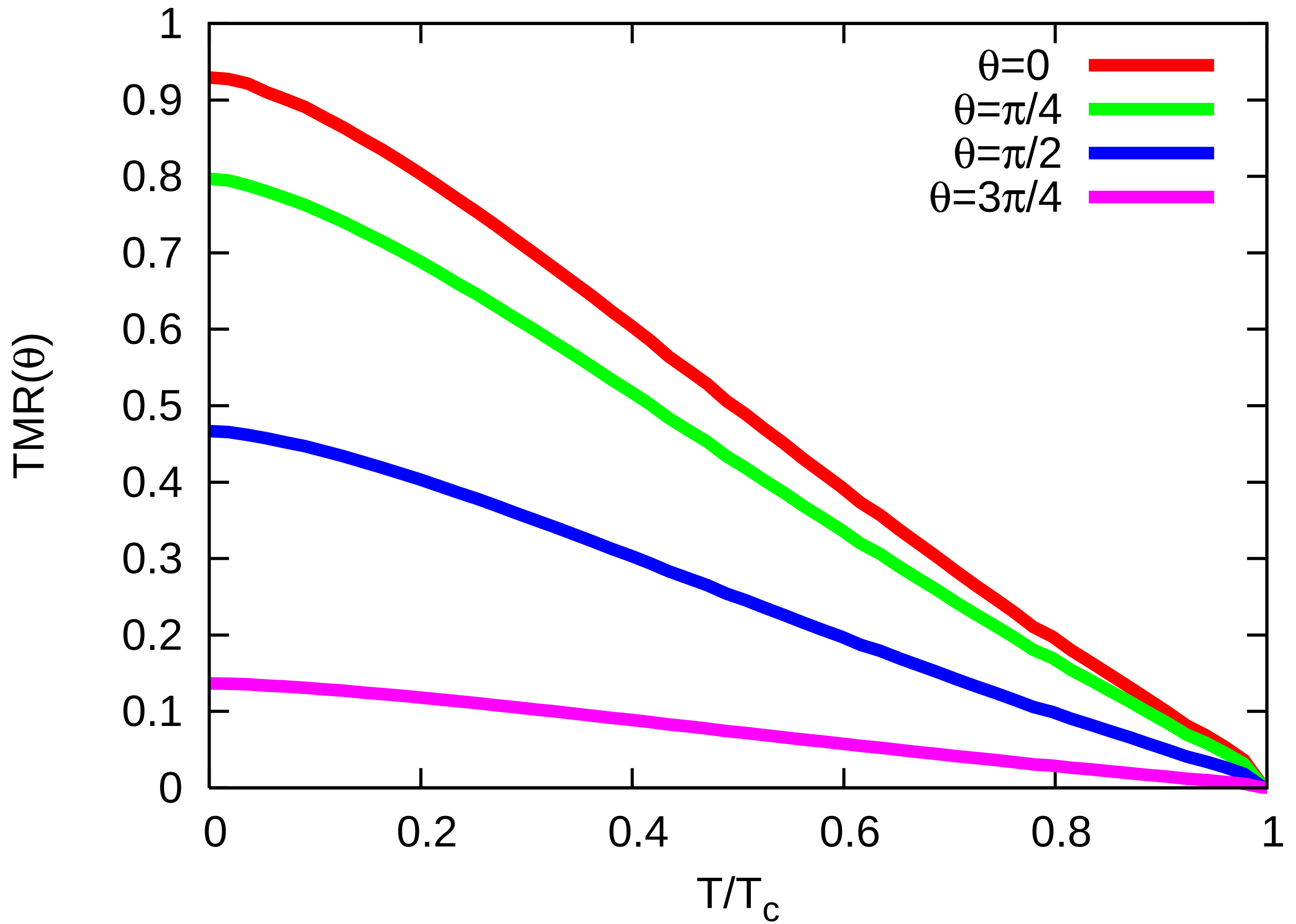
Conductance





width = 1.5 nm
barrier height = 0.55 eV

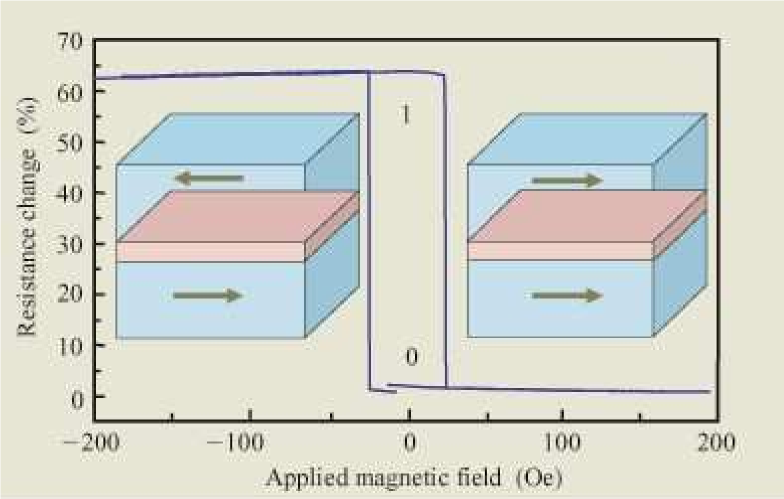
Tunneling magnetoresistance



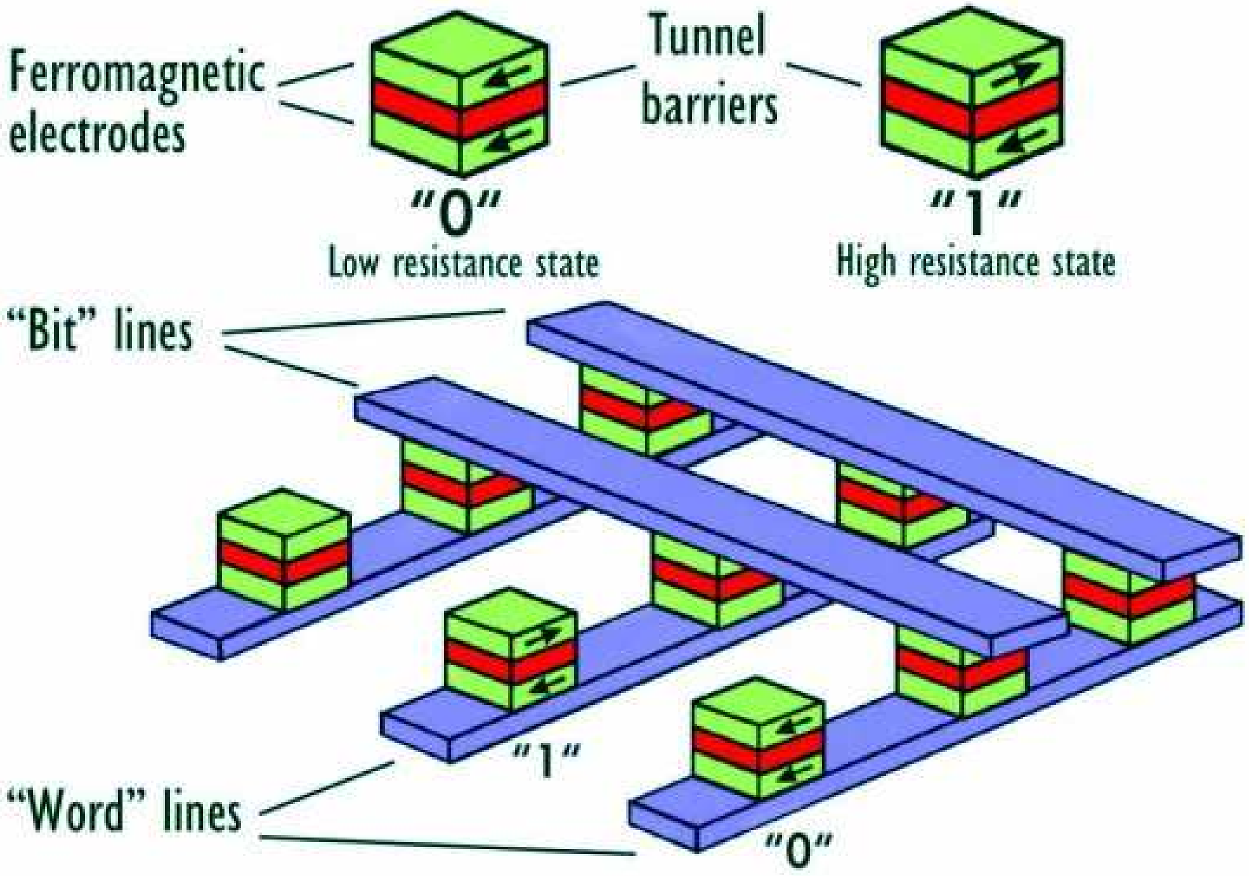
$$\mathrm{TMR} = \frac{I_{\uparrow\uparrow} - I_{\uparrow\downarrow}}{I_{\uparrow\downarrow}} \Longrightarrow \mathrm{TMR}(\theta) = \frac{I(\theta) - I(\pi)}{I(\pi)} = \frac{G(\theta) - G(\pi)}{G(\pi)}$$

Applications of MTJ

- Magnetic read heads in high density HDD and MRAM:
  - data stored by setting the orientation of the variable magnetization
  - data read by measuring the TMR
- The variable magnetization is controlled by a magnetic field.

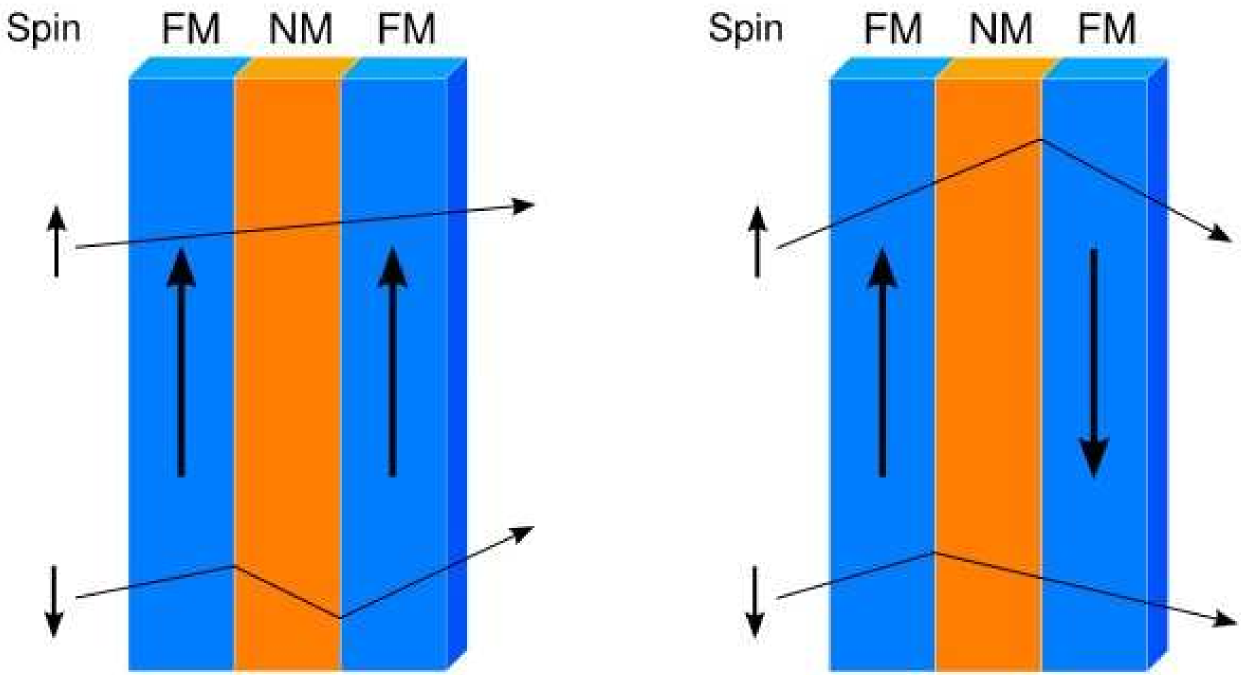


MTJ array

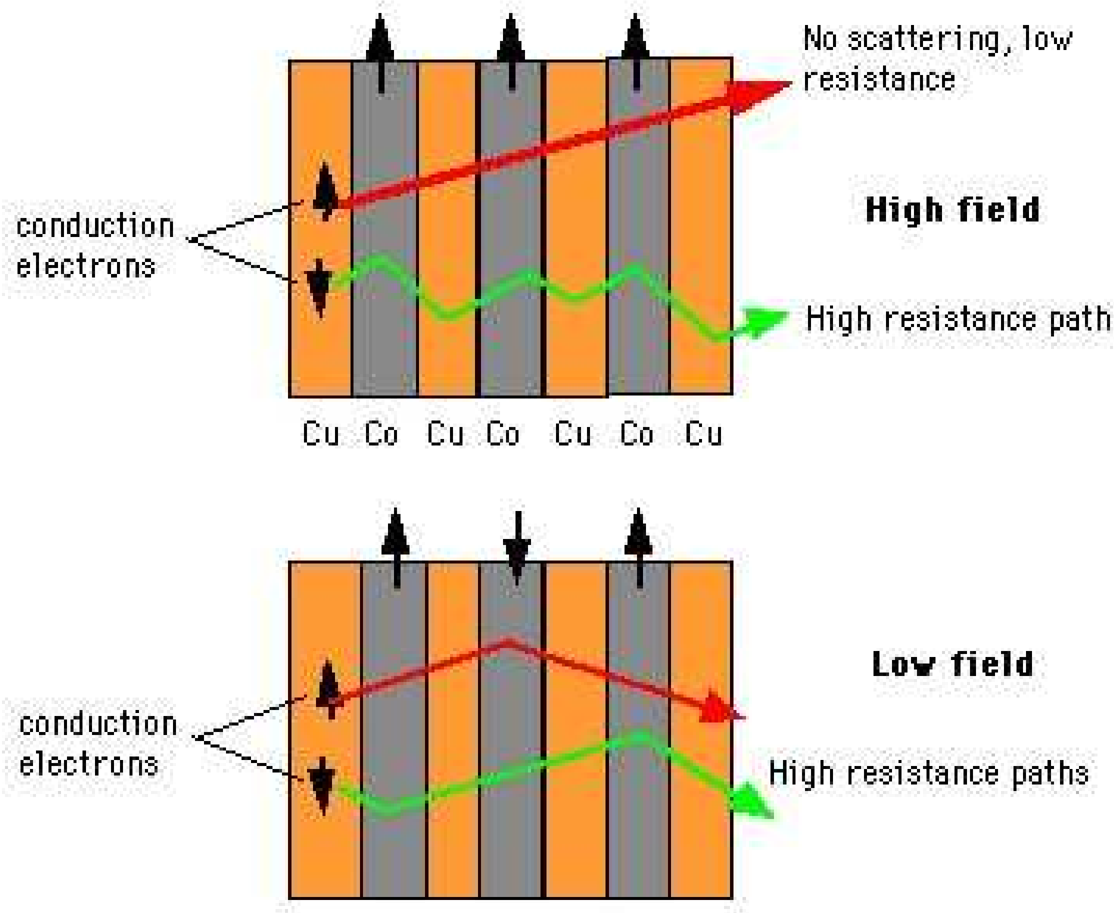

Ferromagnetic electrodes
Tunnel barriers
"0"
Low resistance state
"1"
High resistance state
"Bit" lines
"Word" lines
"1"
"0"

Giant magnetoresistance

- Observed in magnetic-material/metal/magnetic-material junctions
- Like TMR, the resistivity is large when the magnetic materials are antiparallel and small when parallel $\Rightarrow$ GMR
- The GMR is due to scattering.



Enhanced GMR



Quantum well/barrier conclusion

- TMR and GMR are dependant on both the electronic and spin properties of the material $\Rightarrow$ spintronics.
- The main application for layered devices with either TMR or GMR memory storage applications such as MRAM and disk.
- New applications include logic gates (‘Magnetic logic’).