Numerical studies of quantum transport in carbon nanotubes

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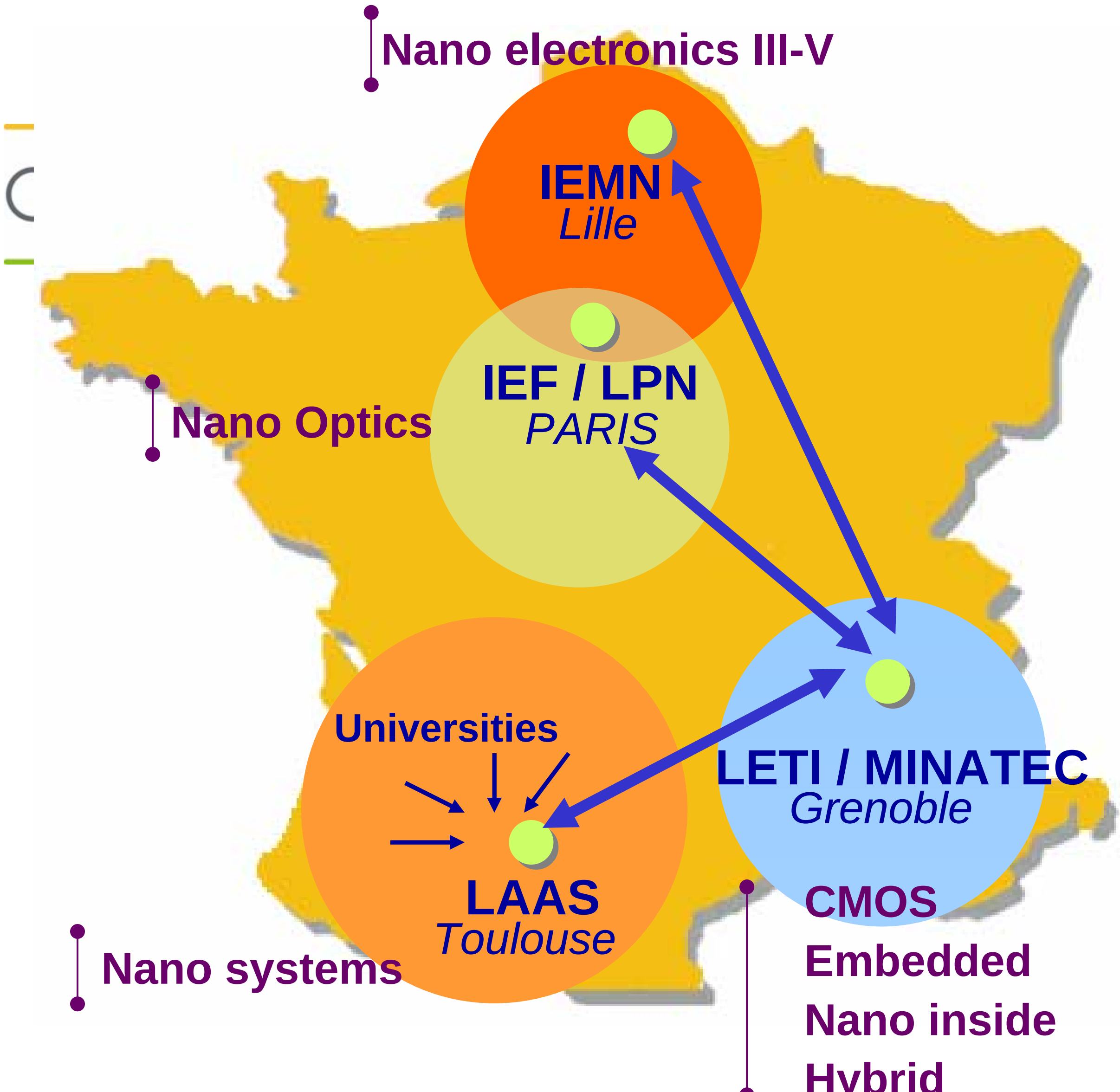
Outline

- Research environment : « RTB » projects
- Intrinsic transport in CNTs : role of disorder
- Magnetotransport : generalities and experiments
- Magnetotransport simulation: combined role of disorder + parallel magnetic field
- Perspectives

Recherche Technologique de Base



nch network of Research Centres in MNT

(2003 – 2006)

Biology/Health

Micro-Nanotechnologies

MEMS and Micro-systems

3D Integration

Photonics

New architectures

and system integration

Our scientific interests

• Quantum simulation of CNT field effect transistors : transmission through metal-nanotube interfaces, gate electrostatics

• Intrinsic transport properties of CNTs : role of disorder and magnetic field

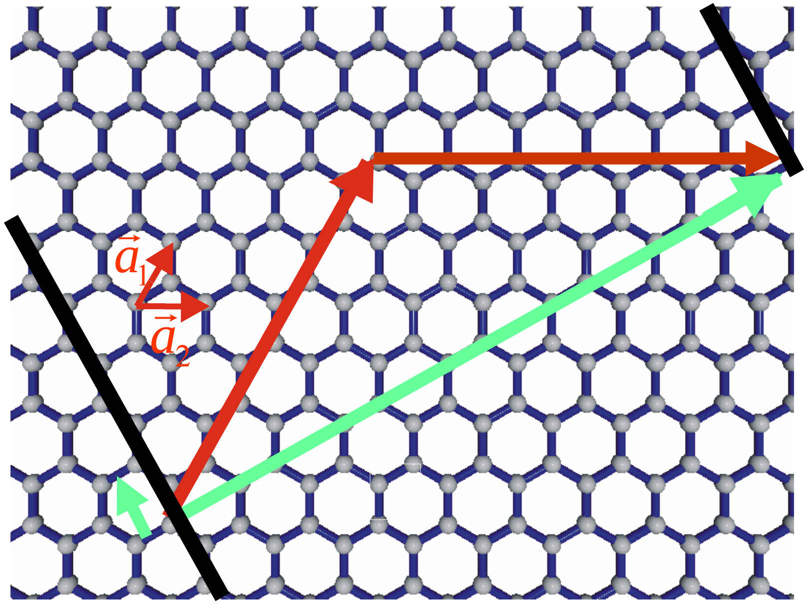
• Generalization to other nano-systems : nanowires, molecules…

<u>Methods</u> :

• tight-binding hamiltonians $\rightarrow$ large systems

• coupling with ab-initio calculations (DFT) to improve tight-binding parameters

Carbon nanotubes



Helicity

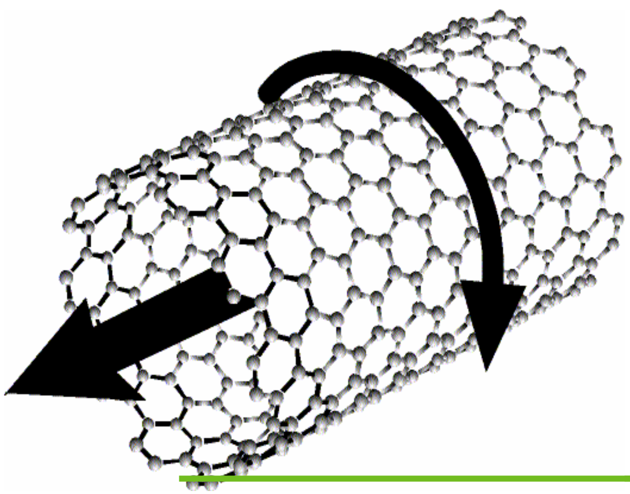
$$\vec{C}_{(l,m)} = l\,\vec{a}_1 + m\,\vec{a}_2$$

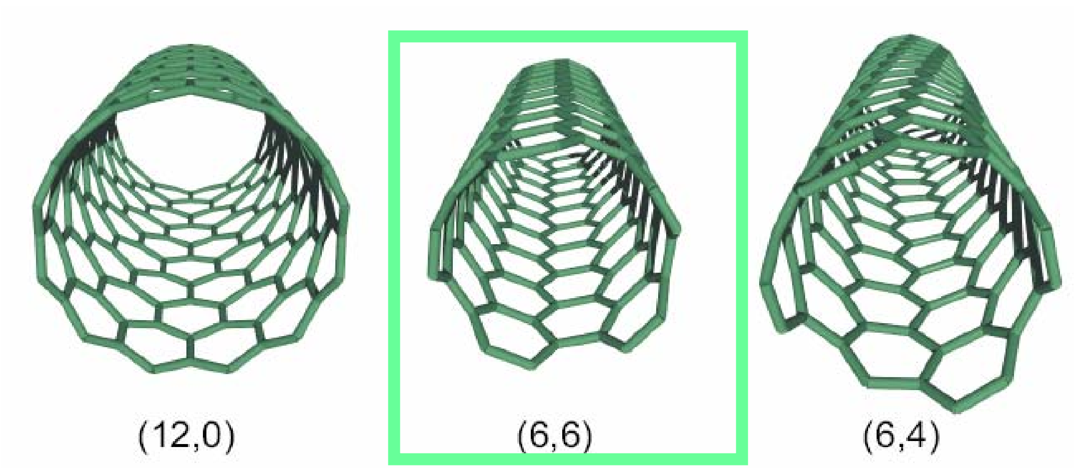
Diameter

$$d_{(l,m)} = \frac{\left|\vec{C}_{(l,m)}\right|}{\pi}$$

Unit-cell length

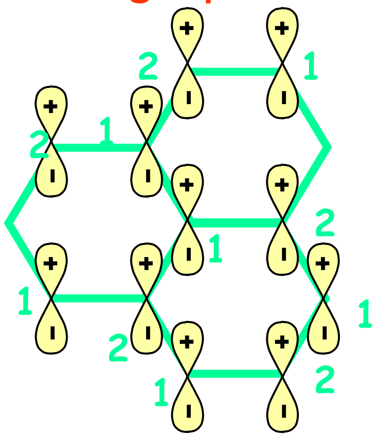
$$\left|\vec{T}_{(l,m)}\right|$$

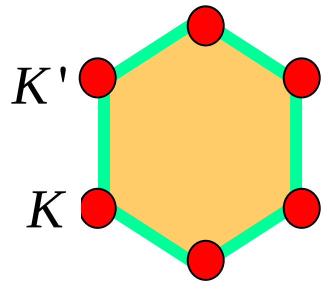




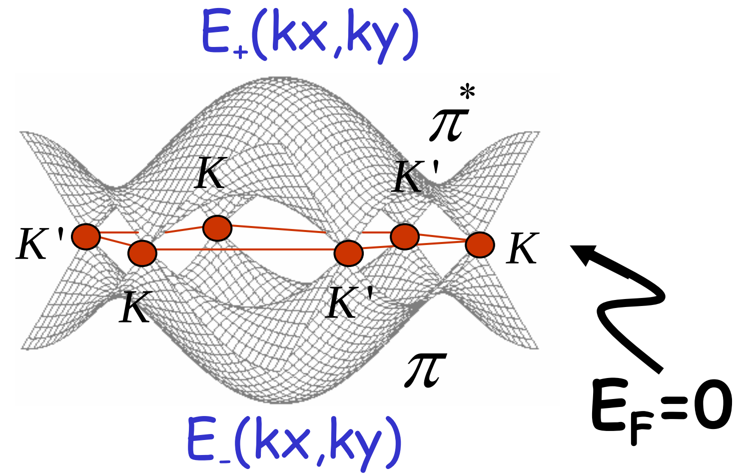
Electronic properties

from graphene :

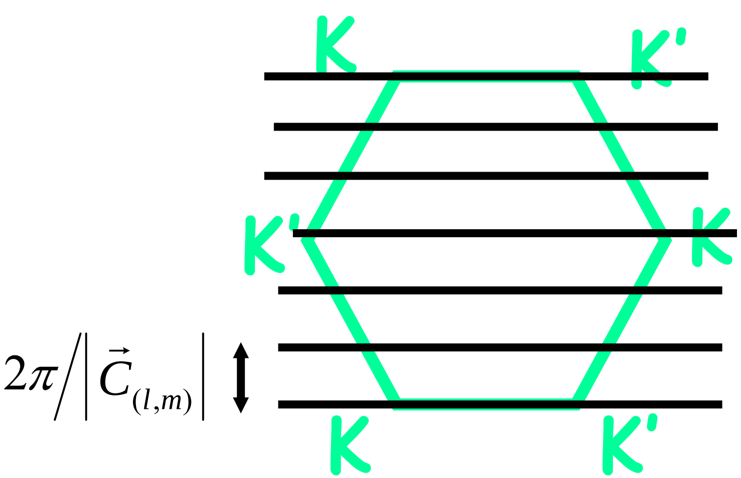




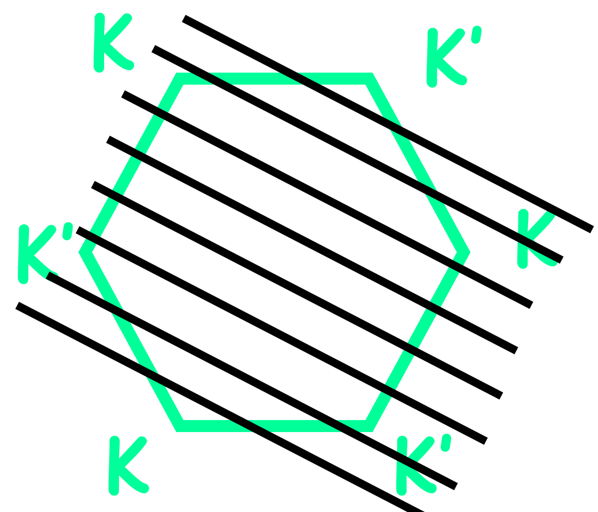
1st Brillouin zone



to nanotubes :



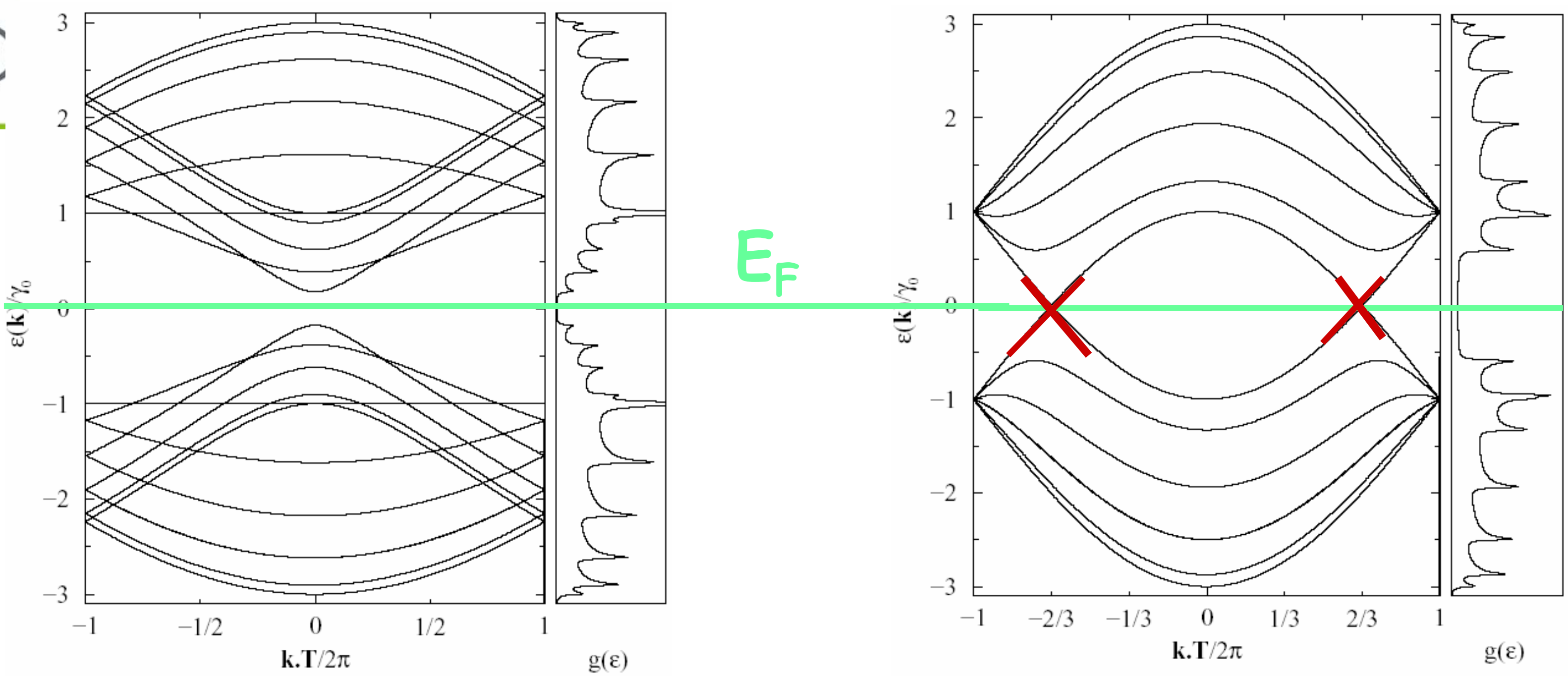
metallic



semiconducting

Band structure and density of states

semiconducting (10,0)　　　　　　metallic (5,5)

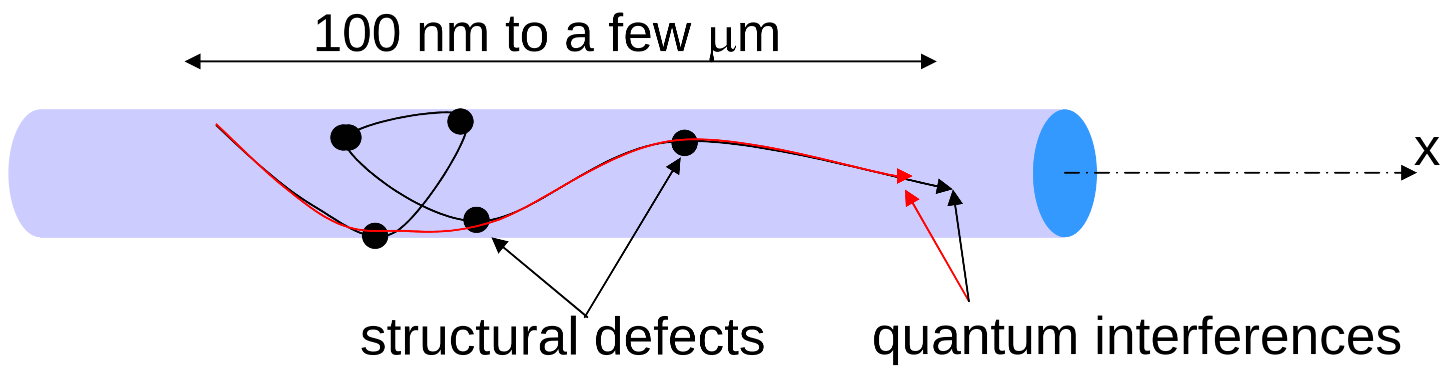


$$E_+(k=0) - E_-(k=0) \equiv \frac{2\pi\, a\, \gamma_0}{\sqrt{3}\,\|\vec{C}_h\|}$$

$$E_\pm(\delta k) \equiv \pm\frac{\sqrt{3}a}{2}\gamma_0\|\delta\vec{k}\|$$

$d_t = 1.4\text{nm} \rightarrow \Delta_g = 0.6$ eV

Scattering and non-ballistic transport



Key quantity : quadratic spreading of wave-packets

$$\Delta X^2(E,t) = \frac{1}{\rho(E)} Tr[\delta(E-\hat{H})(\hat{X}(t)-\hat{X}(0))^2]$$

$\neq$ regimes :

$$\begin{cases} \Delta X^2(E,t) = v^2(E)\times t^2 & \text{ballistic} \\ \Delta X^2(E,t) = D(E)\times t & \text{diffusive} \\ \ldots\ldots\ldots\ldots\ldots & \end{cases}$$

Numerical simulation :
- tight-binding models
- single or multi-wall CNTs

(Coll. : D. Mayou, S. Latil)

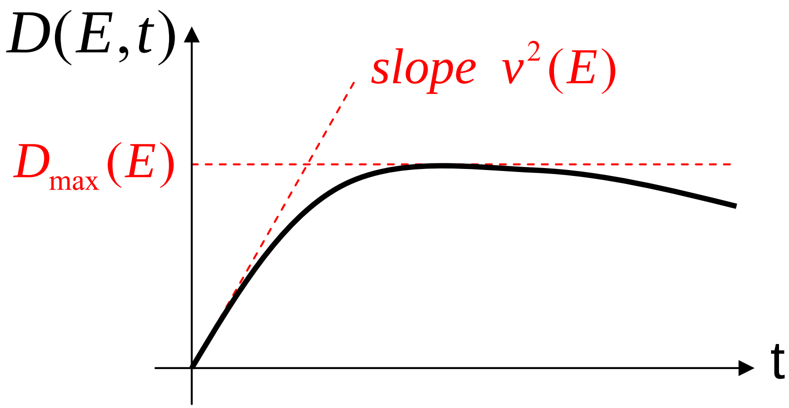
disordered CNTs : mean free path

Hamiltonian : Anderson disorder, no e-e interaction

$$\hat{H} = \gamma_0 \sum_{<i,j>} |j\rangle\langle i| + \sum_i \varepsilon_i |i\rangle\langle i|$$

$\gamma_0 = 2.9\, eV$ hopping energy $\varepsilon_i \in [-W/2, W/2]$

We compute the diffusivity $D(E,t) = \dfrac{\Delta X^2(E,t)}{t}$ for each energy E



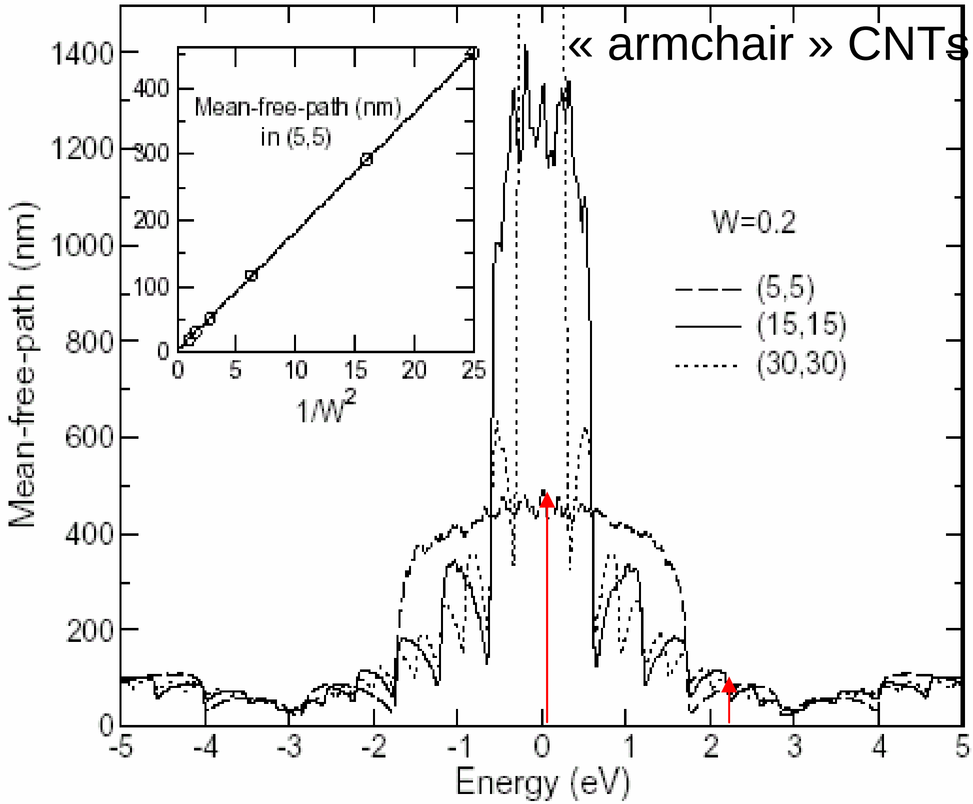
mean free path :

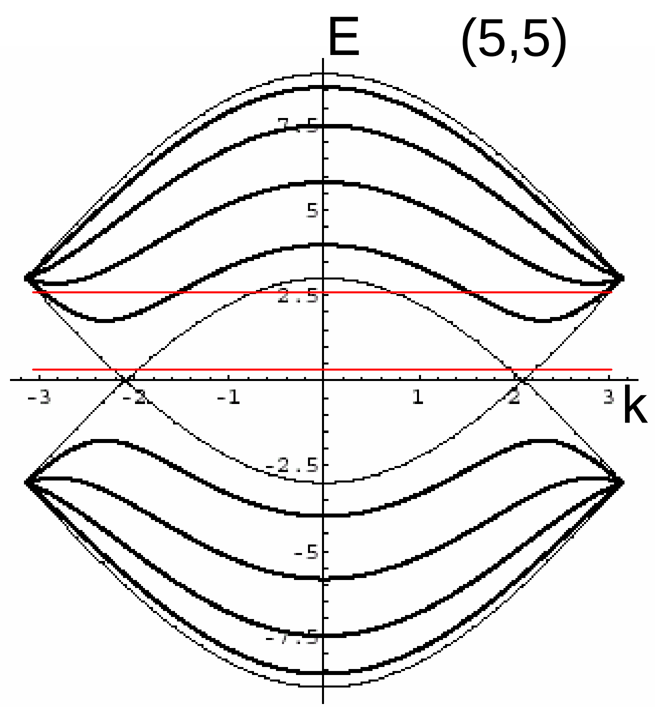
$$l_e(E) \equiv \frac{D_{max}(E)}{v(E)}$$

$l_e(E)$ depends on helicity, disorder W, energy E

Energy dependence

F.T., S. Roche, A. Rubio, D. Mayou, Phys. Rev. B (2004)

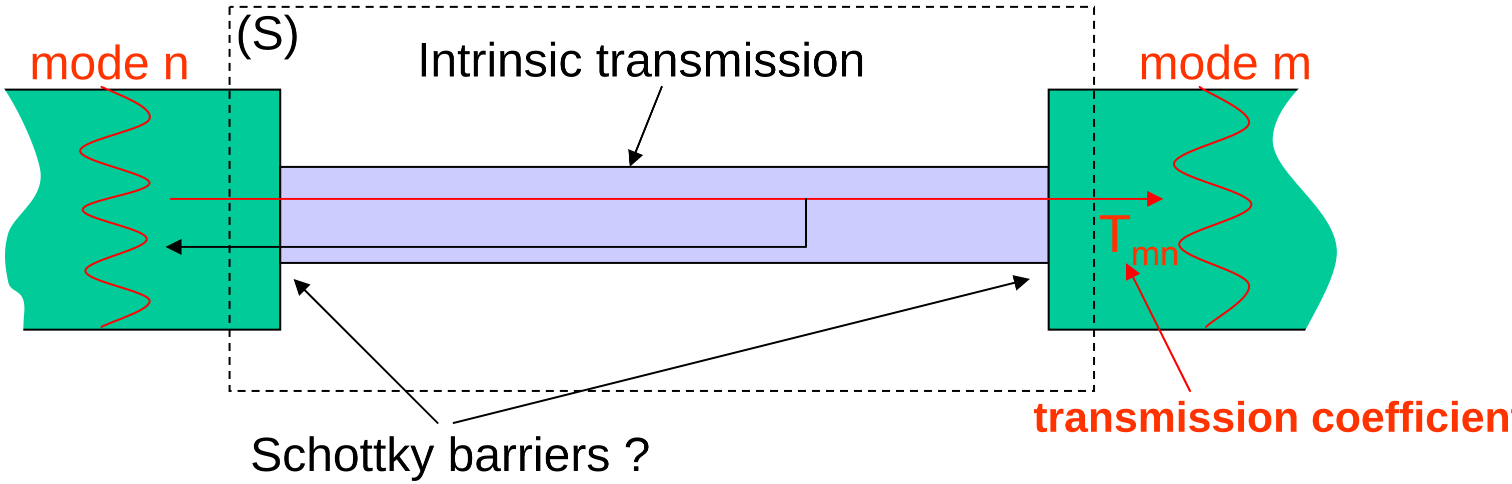




At E = 0 : $\ell_e = \frac{18}{\sqrt{3}}\left(\frac{\gamma_0}{W}\right)^2 \|\vec{C}_h\|$

C. White and T.N. Todorov, Nature (1998)

Nanotube + metallic contatcs



Landauer-Büttiker formula :

$$G = G_0 \sum_{n,m} T_{mn} = Tr[\hat{\Gamma}_G \hat{G}^r \hat{\Gamma}_D \hat{G}^a]$$

$$\hat{G}^{r,a}(E) = \frac{1}{E - \hat{H} - \hat{\Sigma}_G^{r,a}(E) - \hat{\Sigma}_D^{r,a}(E)}$$

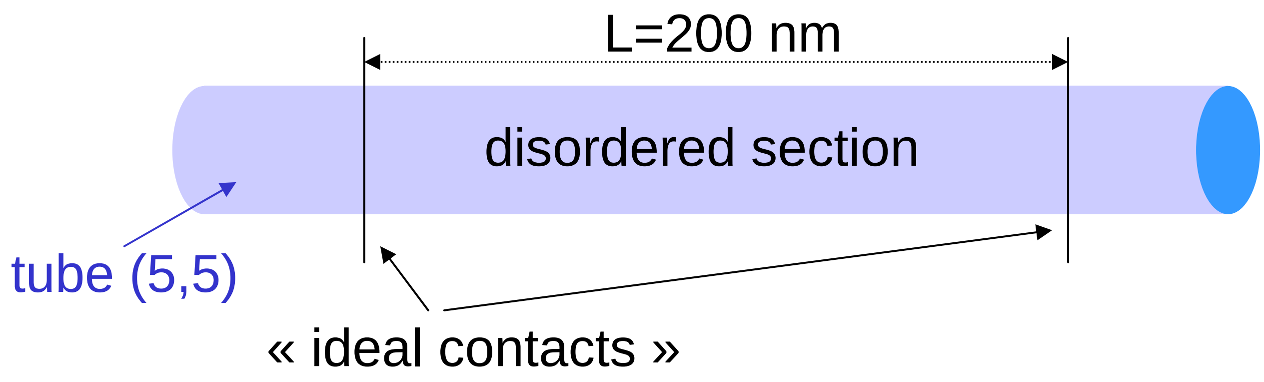
Green functions

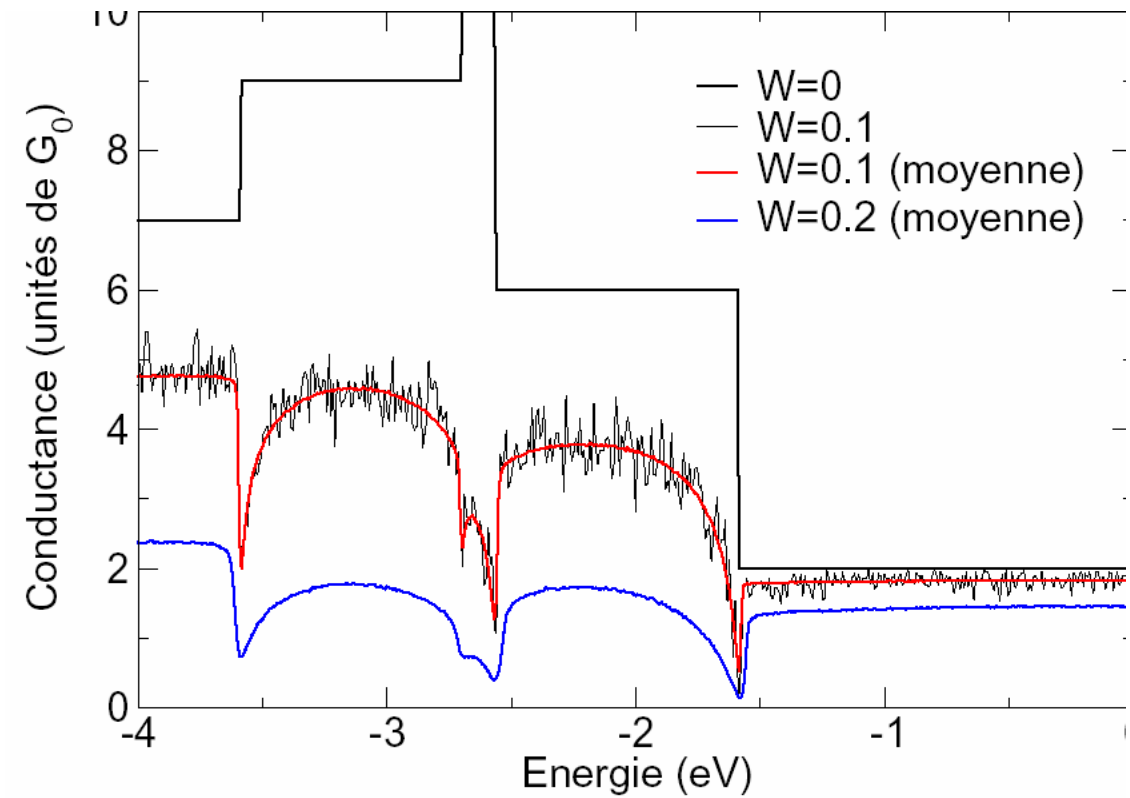
hamiltonien of finite system (S)

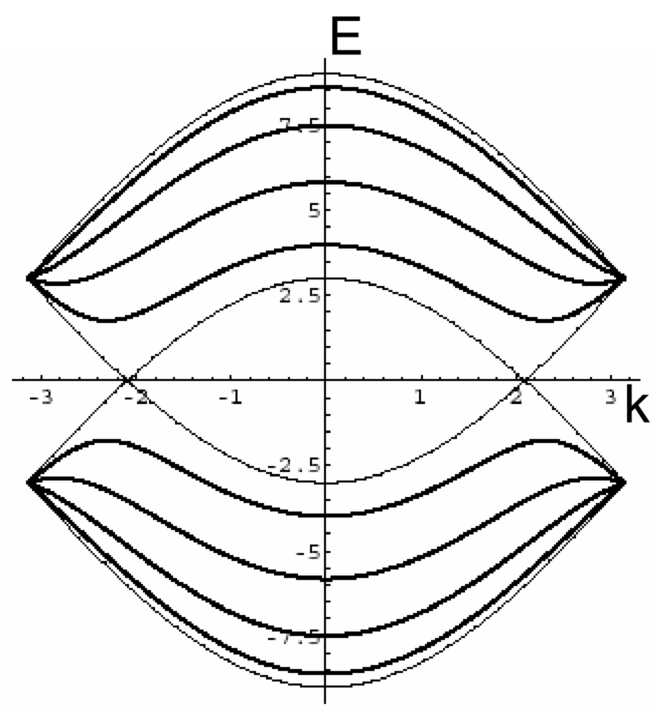
self-energies due to coupling of (S) with electrodes

$$\hat{\Gamma}_{G,D}(E) = i(\hat{\Sigma}^r_{G,D} - \hat{\Sigma}^a_{G,D})$$

Conductance through a disordered section

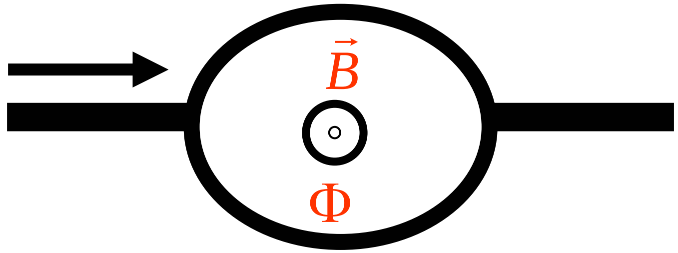






Magnetotransport : Aharonov-Bohm phenomena

Doubly connected systems (rings), cylinders



I- Electronic structure : periodic oscillations of period Φ_0 (=h/e)

II- Weak localization :
$\Phi_0/2$-periodic oscillations

III- Persistent currents : Φ_0-periodic oscillations

Nanotube in parallel field

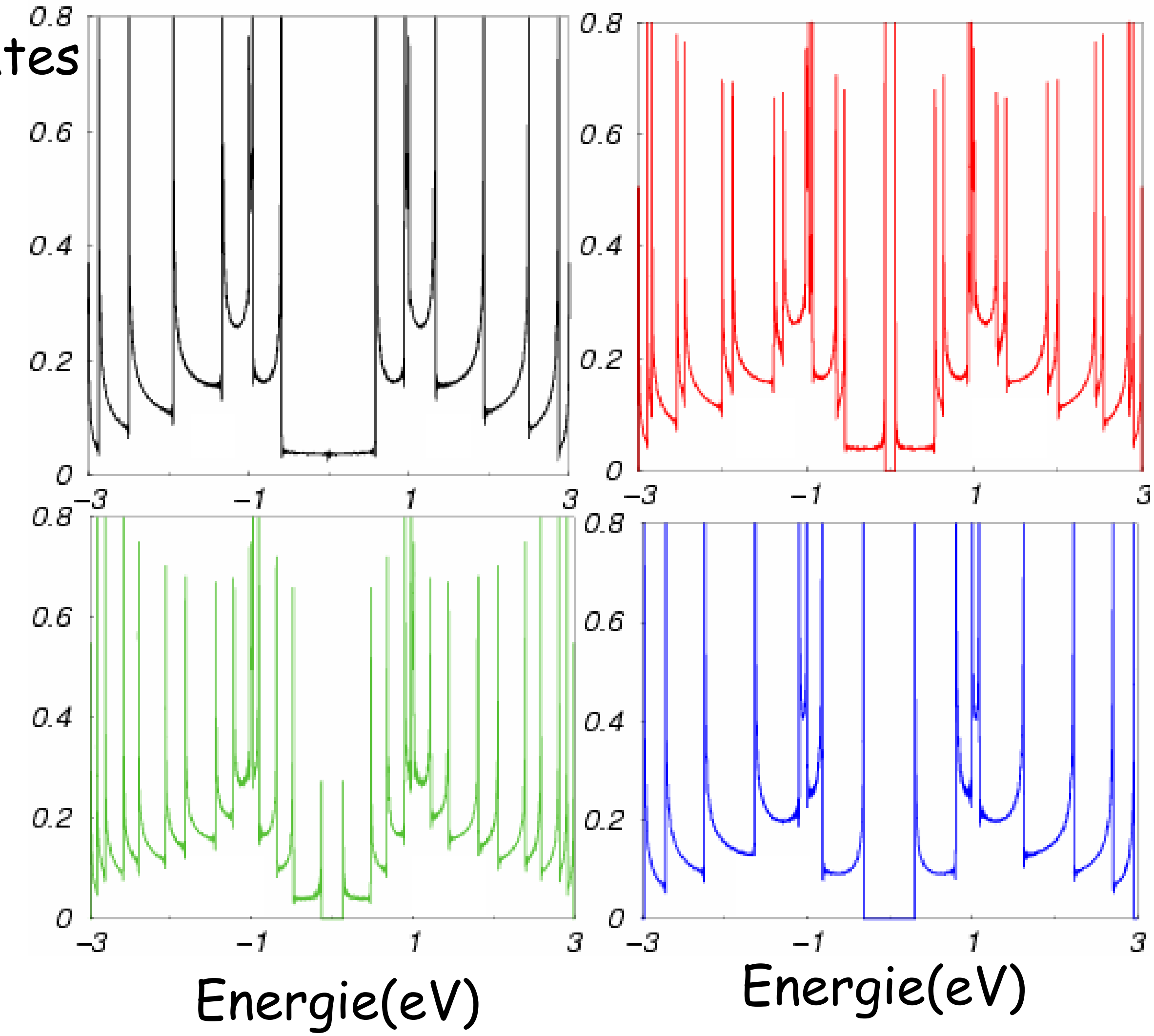
Density of states

$\Phi = 0.0$
$= \Phi_0$

$\Phi = 0.1\Phi_0$
$= 0.9\Phi_0$

$\Phi = 0.2\ \Phi_0$
$= 0.8\ \Phi_0$

$\Phi = \Phi_0/2$



S. R., G. Dresselhaus, M. Dresselhaus & R. Saito, Phys. Rev. B 62, 16092 (2000)

Nanotube in perpendicular field

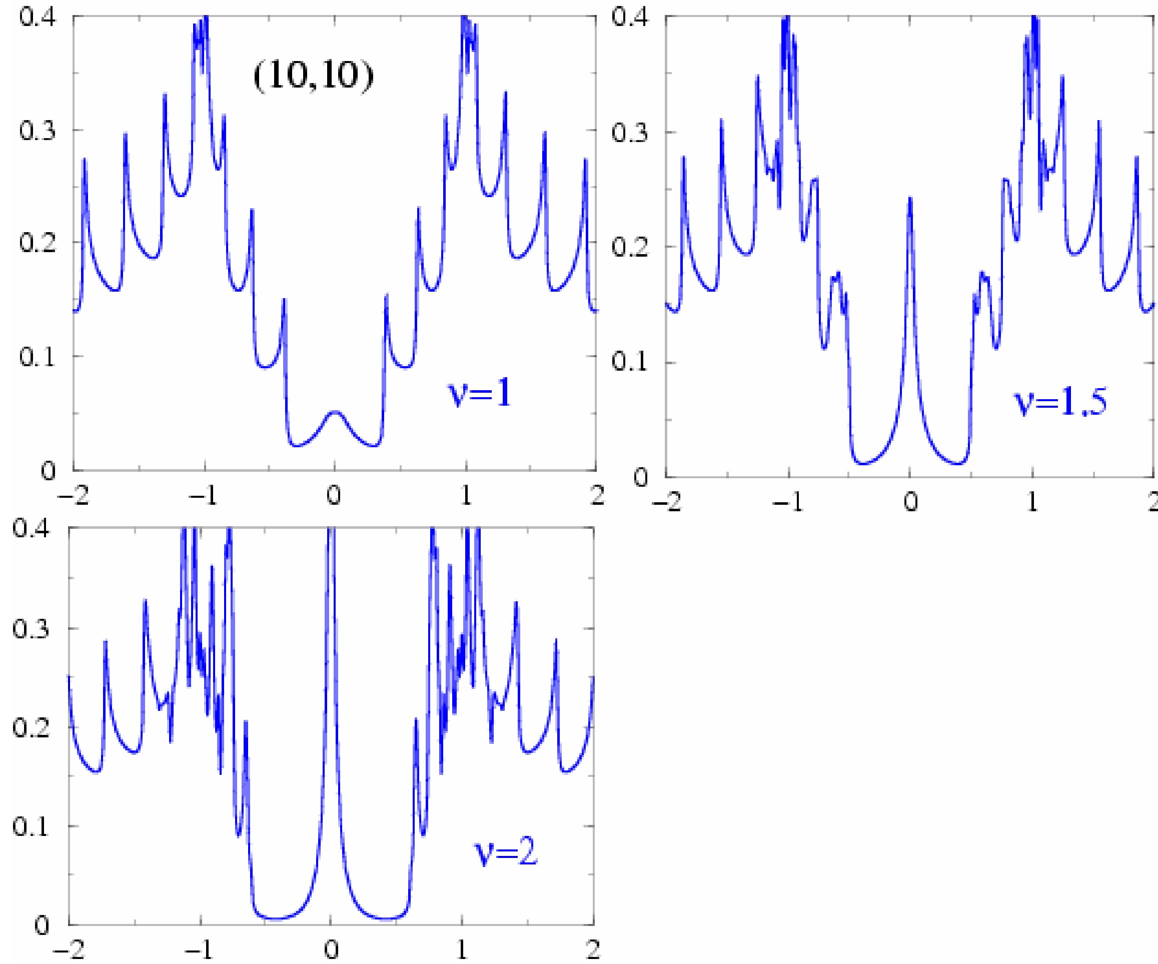
Formation of Landau levels

$$\nu = \frac{C_h}{2\pi l_m}$$

$$l_m = \sqrt{\frac{\hbar}{eB}}$$

$$\mathrm{DoS}(\varepsilon = 0) \approx \frac{e^{2\nu^2}}{\sqrt{4\pi\nu^2}}$$

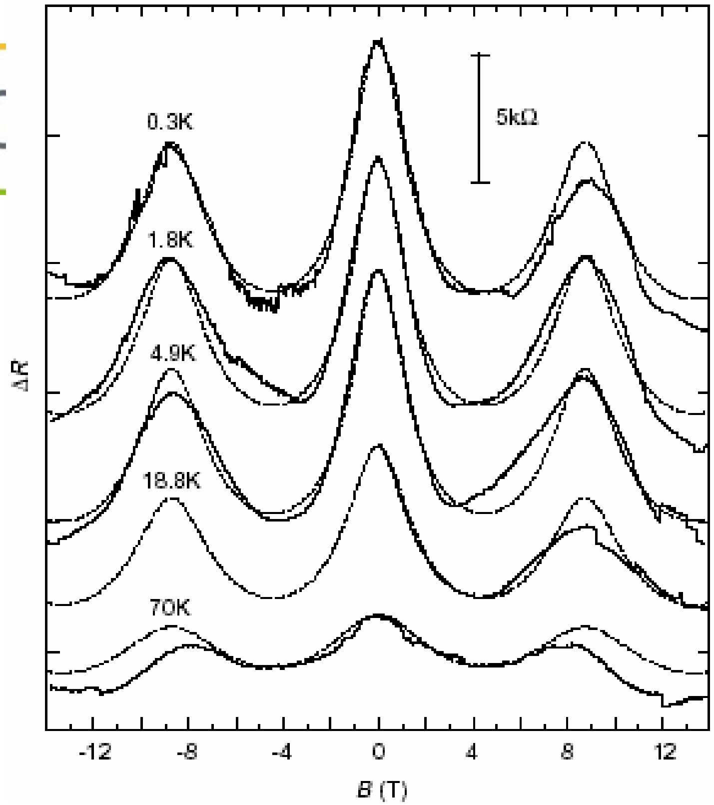
H. Ajiki & T. Ando,
J. Phys. Soc. Jpn 62, 1255 (1993)



S. R., G. Dresselhaus, M. Dresselhaus & R. Saito,
Phys. Rev. B 62, 16092 (2000)

Period of AB oscillation in parallel field ?

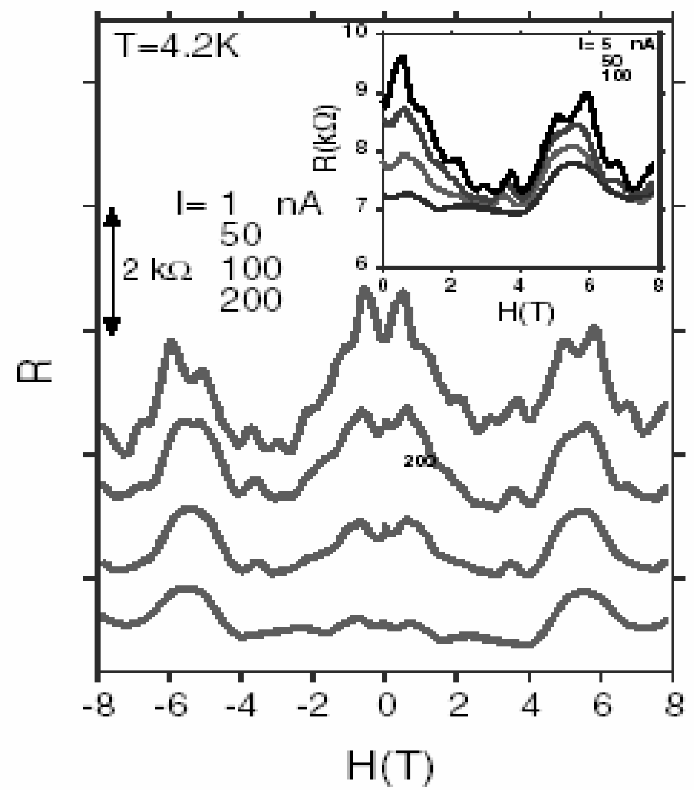
A. Bachtold et al, Nature 397, 673 (1999)



$\frac{\Phi_0}{2}$ $\quad l_e \leq \pi\, d_{tube}$

Diffusive regime and weak localization

J. Lee et al, Sol. St Com 115, 467 (2000)



Φ_0 $\quad l_e \geq L_{tube}$

Ballistic regime DOS effect

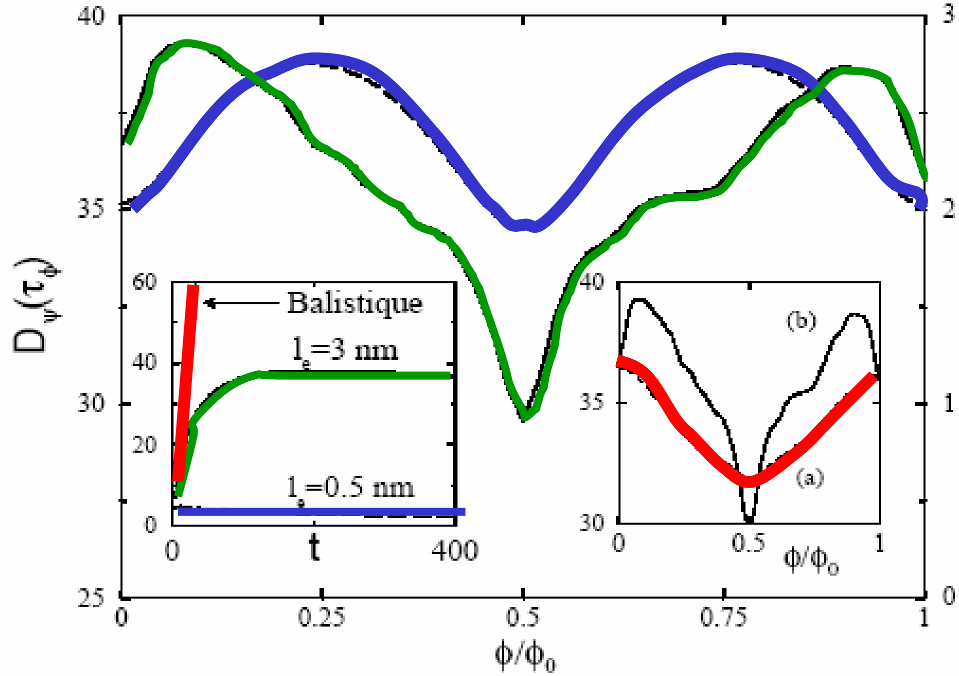
Numerical study of weak localization

Approximation : no DOS effects !

l_e < tube circumference
Negative MR
Oscillations in $\Phi_0/2$

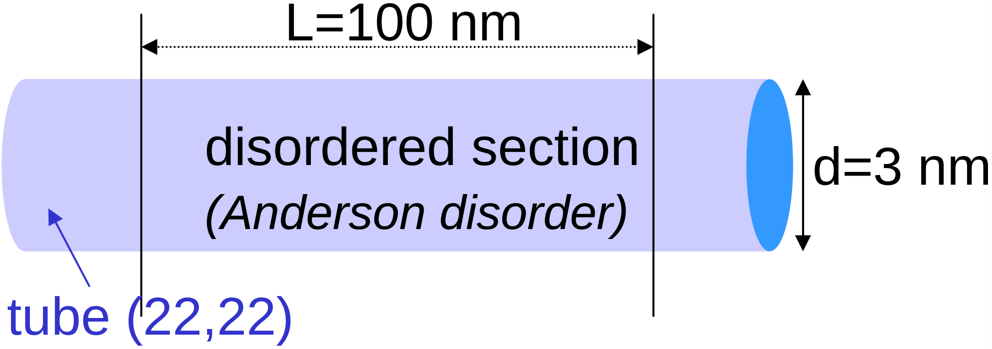
Ltube > l_e > tube circumference
Negative MR
Oscillations in Φ_0

l_e > L_{tube}
Positive MR
Oscillations in Φ_0

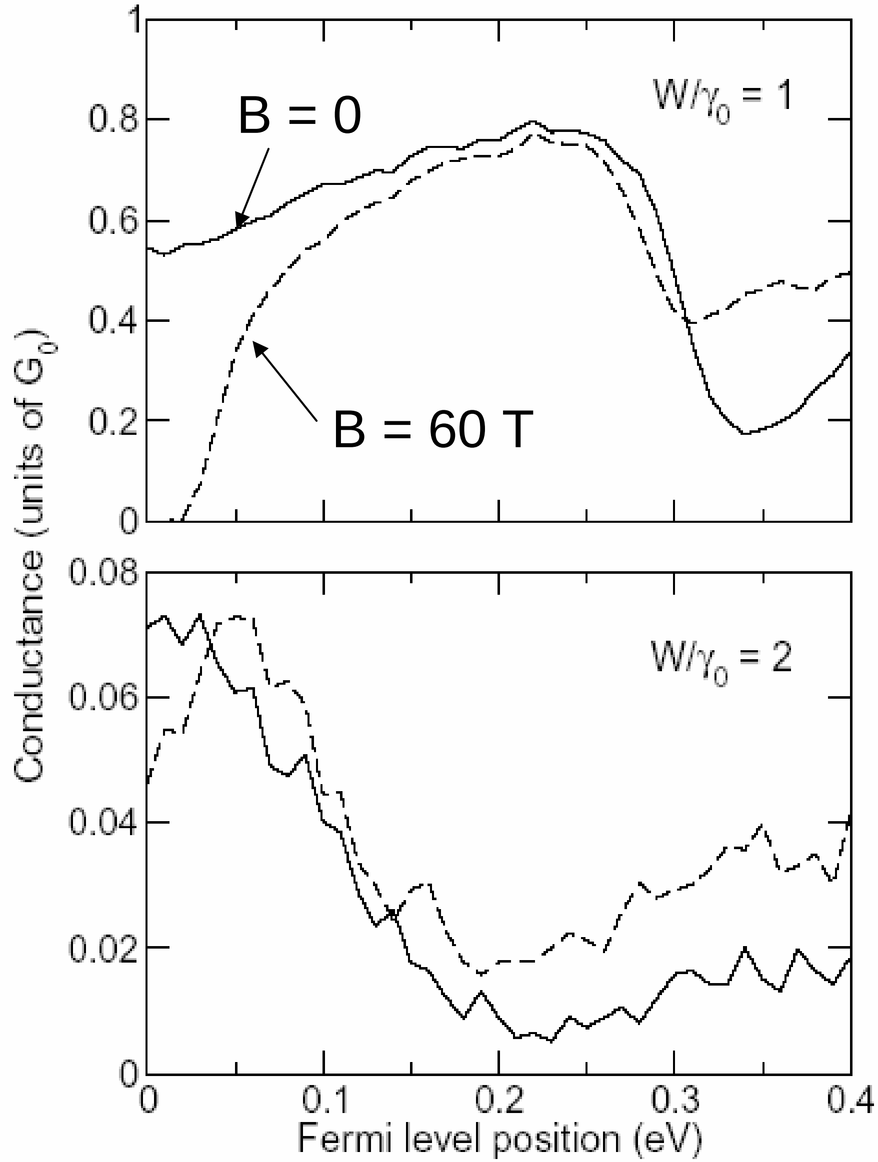


S. R, F. Triozon, A. Rubio, D. Mayou, Phys. Rev. B 64, 121401 (2001)

Simulation in parallel field



$$\Phi(B = 60T) = \Phi_0 / 10$$



Other experiments

h/e oscillation of the gap in parallel field ?

U.C. Coskun et al., Science 304, 1132 (2004)

Regensburg group

Experiments in parallel and perpendicular field,

T=20 mK, tube diameter=20 nm, strong gate coupling

Conclusion and perspectives

- Magnetotransport : DOS effects and localization effects $\rightarrow$ difficult interpretation

- Large diameter nanotubes give more information (several flux quanta) $\rightarrow$ future simulations for d = 10 nm or more

- The nature of disorder (structural or chemical) strongly influences the energy dependence of the mean-free-path $\rightarrow$ go beyond the Anderson model