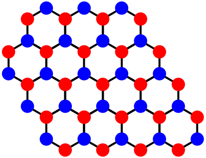
Zener tunneling, Defects and transport in Quasi-metallic carbon nanotubes

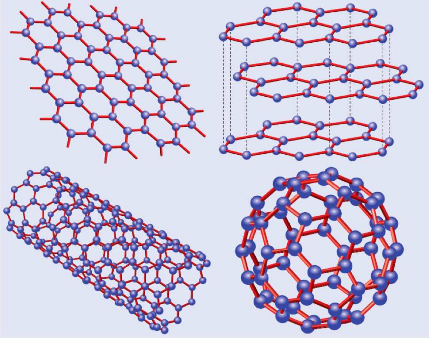
Gaston KANE
LSI, École Polytechnique, Palaiseau, FRANCE

Michele LAZZERI and Francesco MAURI
IMPMC, Université Pierre et Marie Curie, Paris, FRANCE



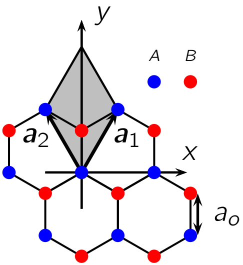
Carbon allotropes

- Graphene ⟹
- Graphite ⟸

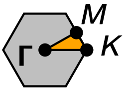


- Nanotubes ⟹
- Fullerene ⟸

Graphene properties



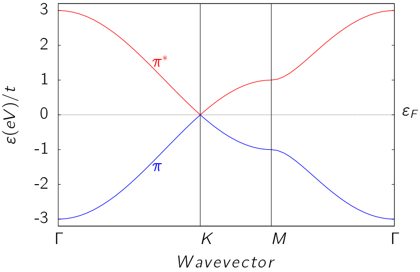
(a) Lattice



(b) Brillouin zone (BZ)

p_z orbitals $\Rightarrow \pi$ and π^* bands

Band Structure: π and π^*



$\varepsilon(\boldsymbol{K}) = 0$

$\Rightarrow$ Graphene is a semi-metal

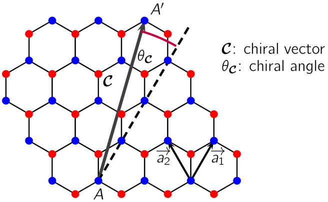
Energy dispersion Near $\boldsymbol{K}$:

$$\varepsilon(\boldsymbol{k}) = \pm\hbar v_F \sqrt{k_x^2 + k_y^2}$$

$v_F \equiv$ Fermi velocity

Carbon Nanotubes properties

Lattice



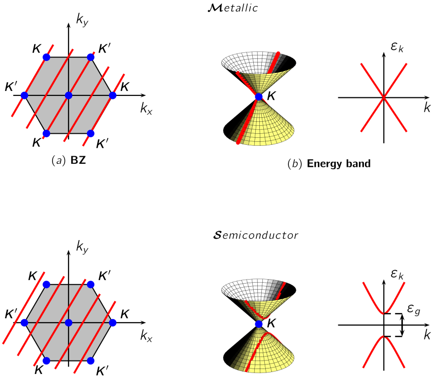
Quasi-metallic nanotubes (QM):

$$\varepsilon(k) = \pm\hbar v_F \sqrt{k^2 + k_o^2}$$

with $k_o = constant$

$$\varepsilon_g = 2\hbar v_F k_o \sim 10 - 100\text{meV}$$

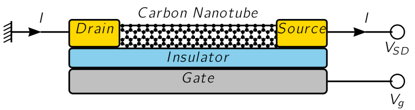
Zone-folding scheme



(a) **BZ**
(b) **Energy band**
(c) **BZ**
(d) **Energy band**

Some transport properties

Experimental device



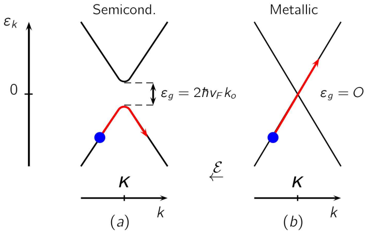
Carbon nanotubes:

- Highest current density 10^9 A$/cm^2$
- Ballistic behavior at room temperature

Applications: interconnects or carbon-based transistor

Zener tunneling in nanotubes:

Boltzmann (BTE)



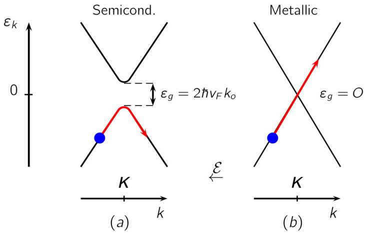
Wavevector time evolution

$$\dot{k} = -e\mathcal{E}/\hbar$$

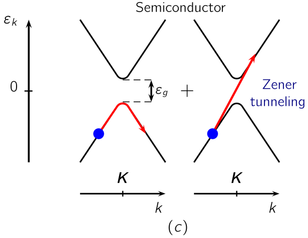
$\mathcal{E}$ source-drain electric field

Zener tunneling in nanotubes:

Boltzmann (BTE)



Quantum



Tunneling Probability

$$T_z = \exp(-\pi\varepsilon_g^2/4\hbar v_F e\mathcal{E})$$

$\mathcal{E}$ source-drain electric field

Andreev PRL 99, 247204 (2007)

Sizable for:

- semiconductor
  $\mathcal{E} = \frac{\pi\varepsilon_g^2}{4\hbar v_F e} \sim 300\ \mathrm{V}/\mu\mathrm{m}\ (\varepsilon_g = 0.5\ \mathrm{eV})$
- Qm nanotubes
  $\mathcal{E} = \frac{\pi\varepsilon_g^2}{4\hbar v_F e} \sim 3\mathrm{V}/\mu\mathrm{m}\ (\varepsilon_g = 0.05\ \mathrm{eV})$

QME in homogeneous system

homogeneous carbon nanotube system under an applied spatially uniform electric field $\boldsymbol{\mathcal{E}} = \mathcal{E}\mathbf{x}$

Boltzmann transport equation (BTE)

$$\frac{\partial f_\alpha(k)}{\partial t} - \frac{e\mathcal{E}}{\hbar}\frac{\partial f_\alpha(k)}{\partial k} = \left.\frac{\partial f(k)}{\partial t}\right]_{\text{coll}}$$

- k // tube axis ($\mathbf{x}$), $\alpha = \pm 1$(band index).
- $f_\alpha \equiv$ population, $\partial f(k)/\partial t]_{\text{coll}} \equiv$ collisions: phonons, defects...

Quantum master equation: Single electron density matrix

- $\alpha = \pm 1$ band index.
- $\rho_{\alpha\alpha} = f_\alpha \equiv$ population
- $\rho_{\alpha\beta}$ $(\alpha \neq \beta) \equiv$ coherent terms

Density matrix: two-bands sytem

$$\rho = \begin{bmatrix} \rho_{-1-1} & \rho_{-11} \\ \rho_{1-1} & \rho_{11} \end{bmatrix}$$

QME in homogeneous system

homogeneous carbon nanotube system under an applied spatially uniform electric field $\boldsymbol{\mathcal{E}} = \mathcal{E}\mathbf{x}$

Boltzmann transport equation (BTE):

$$\frac{\partial \rho_{\alpha\alpha}(k)}{\partial t} - \frac{e\mathcal{E}}{\hbar}\frac{\partial \rho_{\alpha\alpha}(k)}{\partial k} = \left.\frac{\partial \rho(k)}{\partial t}\right]_{\text{coll}}$$

- $\rho_{\alpha\alpha} \equiv f_{\alpha}$

Single-electron quantum master equation (QME)

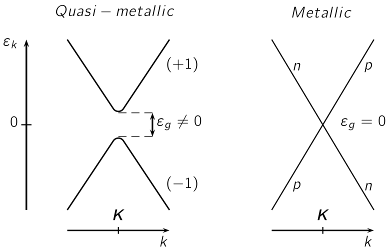
$$\frac{\partial \rho_{\alpha\beta}(k)}{\partial t} - \frac{e\mathcal{E}}{\hbar}\frac{\partial \rho_{\alpha\beta}(k)}{\partial k} = G_{\alpha\beta}(\rho) + \left.\frac{\partial \rho(k)}{\partial t}\right]_{\text{coll}}$$

- $G_{\alpha\beta}(\rho)$ contains the terms responsible for Zener tunneling.
- In Boltzmann model $G_{\alpha\beta}(\rho) = 0$, $\rho_{\alpha\beta} = 0$ $(\alpha \neq \beta)$.

Systems and Models

Two infinites carbon nanotube with a diameter $d = 2$ nm: a metallic tube and a Qm nanotube with a gap $\varepsilon_g = 60$ meV.

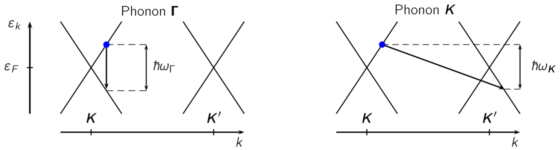
bandstructures



Parameters

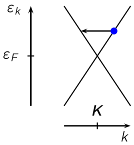
- Optical phonons: only two relevant phonons (Yao et al., PRL, 84 , 2941 (2000))
  - **Γ** and **K**: $\hbar\omega_\Gamma = 200$ meV and $\hbar\omega_K = 150$ meV.

Phonons scattering processes



  - scattering lengths: $L^\Gamma = 451.38$ nm, $L^K = 183.74$ nm
    S. Piscanec et al., PRL, 185503 (2004)/ Lazzeri et al,. PRB 73, 165419 (2006)

Elastic scattering

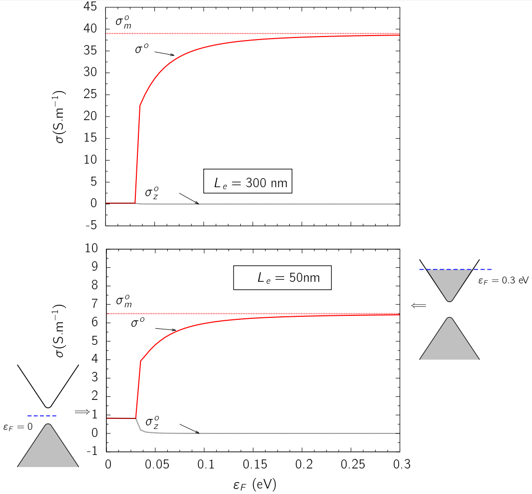


- Short-range impurities (neutral defects, ...)
  - scattering lengths: $L_e = 50$ nm, $L_e = 300$ nm.

Linear regime: Zero-field conductivity σ^o

Zero-field conductivity:
$\mathcal{E}_{SD} \equiv$ source-drain electric field $\rightarrow 0$.

- σ^o can be derived analytically
- $\sigma^o = \sigma^o_b + \sigma^o_z$
- $\sigma^o_b \equiv$ Boltzmann (Semi-classical)
- $\sigma^o_z \equiv$ Zener contribution (Quantum)

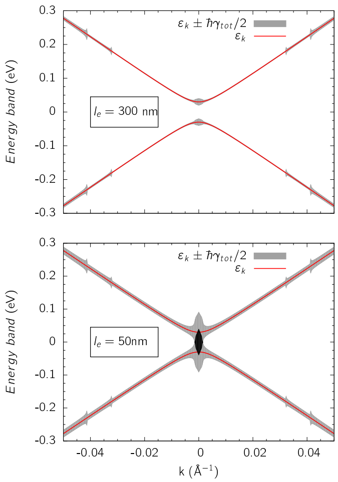


Zener tunneling is made visible by defects.

G. Kané et al., Phys. Rev. B 86, 155433 (2012)

Linear regime: Zero-field conductivity σ^o

Broadening of the electronic bands



- $\varepsilon_k \pm \hbar\gamma_{tot}/2 \rightarrow$ fluctuations of the energy band
- $\gamma_{tot}(k) \equiv$ scattering rate.
  - Elastic.
  - Hole-phonon.
  - Electron-phonon .

Conclusion:

1. Zener tunneling is relevant for small doping, when the Fermi energy lies in or close to the forbidden gap ε_g.
2. Zener tunneling is made visible by defects in Qm tubes.

Thanks for your attention

Minimum conductivity