Nanoscience – quantum transport in carbon-based devices

Janine Splettstößer

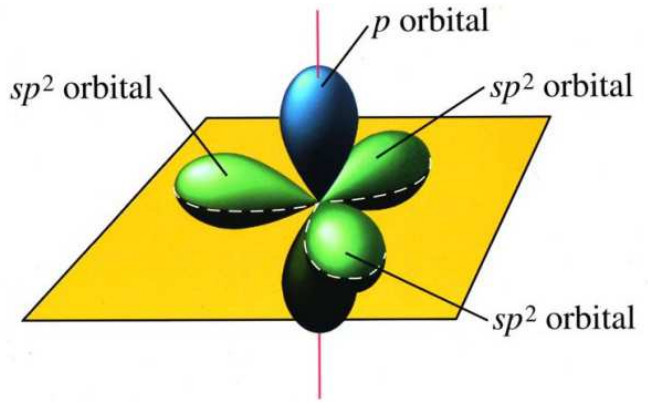
Applied Quantum Physics, MC2, Chalmers University of Technology

Chalmers, November 16, 2018

A different 2d-system: Graphene

Graphene: monolayer of carbon (ideal, stable 2d-material)

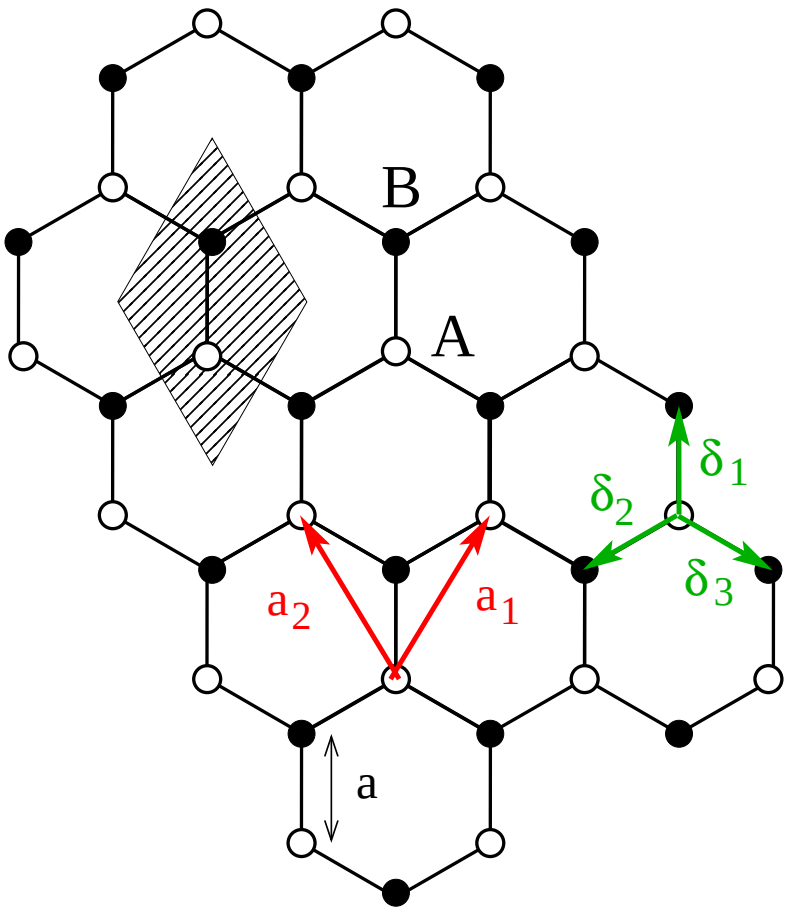
Hybridization of carbon atoms in a graphene sheet:



- Graphene made of mainly ^{12}C atoms (with nuclear spin 0)
- Carbon has 6 electrons occupying the orbitals $1s^2$, $2s^2$, and $2p^2$
- sp^2 hybridization (see figure) $\Rightarrow$ hexagonal graphene structure
- angle $2\pi/3$ between sp^2 orbitals; form covalent bonds with neighbouring orbitals
- Electrons in p_z shell occupy a π or π^* band...

Lattice in real space

Triangular Bravais-lattice with 2-atom basis:



Wigner-Seitz cell of the honeycomb lattice is rhombic containing two atoms (A and B).

Lattice vectors:

$$\boldsymbol{a}_1 = \frac{a}{2}\begin{pmatrix}\sqrt{3}\\ 3\end{pmatrix}\ ,\ \boldsymbol{a}_2 = \frac{a}{2}\begin{pmatrix}-\sqrt{3}\\ 3\end{pmatrix}$$

with atomic spacing $a = 1.42\text{Å}$.

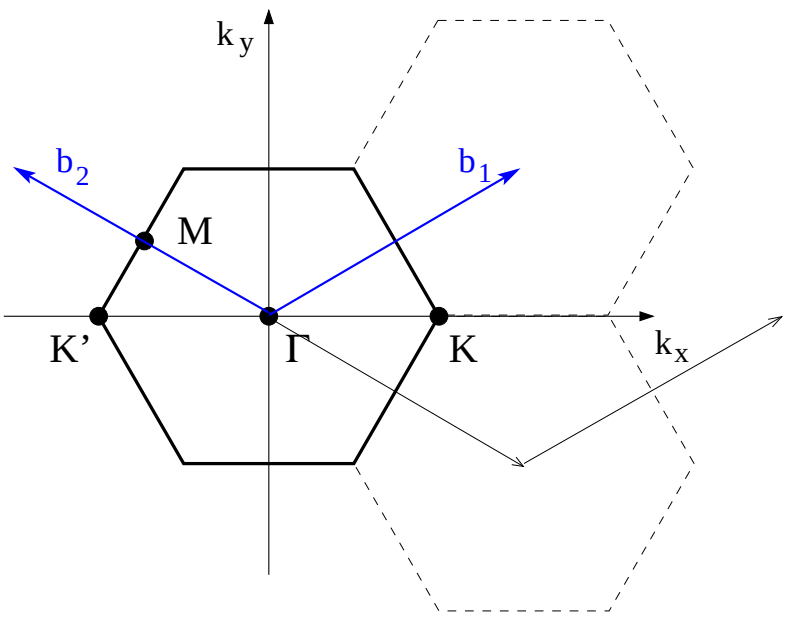
Vectors connecting next neighbours:

$$\boldsymbol{\delta}_1 = a\begin{pmatrix}0\\ 1\end{pmatrix}\ ,\ \boldsymbol{\delta}_2 = \frac{a}{2}\begin{pmatrix}-\sqrt{3}\\ -1\end{pmatrix}\ ,$$

$$\boldsymbol{\delta}_3 = \frac{a}{2}\begin{pmatrix}\sqrt{3}\\ -1\end{pmatrix}$$

Lattice in momentum space (reciprocal lattice)

Reciprocal hexagonal lattice with two inequivalent "Dirac-points" $\boldsymbol{K}$ and $\boldsymbol{K}'$



Obtain lattice vectors of the reciprocal lattice from $\boldsymbol{a}_i \cdot \boldsymbol{b}_j = 2\pi\delta_{ij}$:

$$\boldsymbol{b}_1 = \frac{2\pi}{3a}\begin{pmatrix}\sqrt{3}\\1\end{pmatrix}\ ,\ \boldsymbol{b}_2 = \frac{2\pi}{3a}\begin{pmatrix}-\sqrt{3}\\1\end{pmatrix}$$

Γ-point: center of Brillouin zone.

Coordinates with respect to it:

$$\boldsymbol{K} = \frac{4\pi}{3\sqrt{3}a}\begin{pmatrix}1\\0\end{pmatrix}$$

$$\boldsymbol{K}' = \frac{4\pi}{3\sqrt{3}a}\begin{pmatrix}-1\\0\end{pmatrix}$$

$$\boldsymbol{M} = \frac{\pi}{3a}\begin{pmatrix}-\sqrt{3}\\1\end{pmatrix} = \frac{1}{2}\boldsymbol{b}_2$$

Energy spectrum

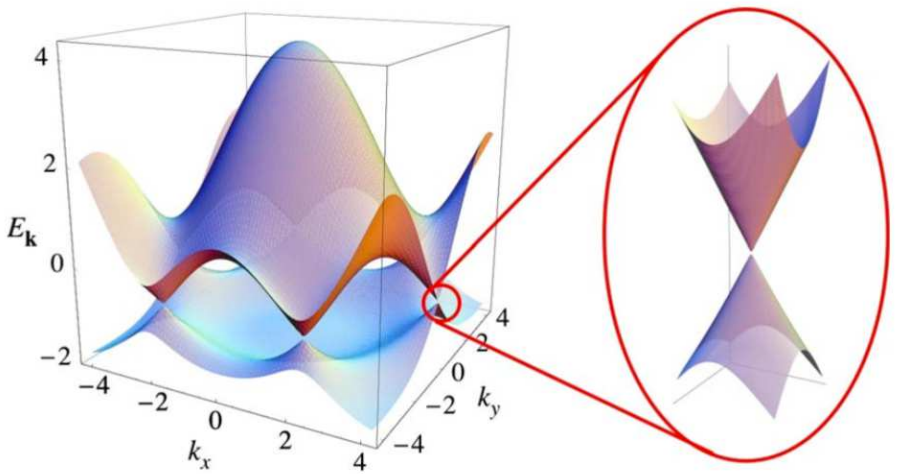
Bandstructure calculation within a tight-binding approximation yields:

$$E_\pm = t' g(\boldsymbol{k}) \pm |t\, f(\boldsymbol{k})|$$

with transfer integrals t and t' between nearest and next nearest neighbours

and $g(\boldsymbol{k})$ and $f(\boldsymbol{k})$ given by

$$\begin{aligned} g(\boldsymbol{k}) &= 4\cos\left[\frac{3a}{2}k_y\right]\cos\left[\frac{\sqrt{3}a}{2}k_x\right] + 2\cos\left[\sqrt{3}ak_x\right] \\ f(\boldsymbol{k}) &= 2\cos\left[\frac{\sqrt{3}a}{2}k_x\right]e^{-i\frac{k_y a}{2}} + e^{ik_y a} \end{aligned}$$



Linearized spectrum in the vicinity of the $\boldsymbol{K}$-points (valleys):

$$E_\pm = \pm v_\mathrm{F}|\boldsymbol{k}|$$

with Fermi ($\simeq$light!) velocity

$$v_\mathrm{F} = 3at/2$$

A. H. Castro Neto et al.: Rev. Mod. Phys. **81**, 109 (2009)

Graphene: massless, relativistic electrons

Low-energy approximation... **Dirac equations!**

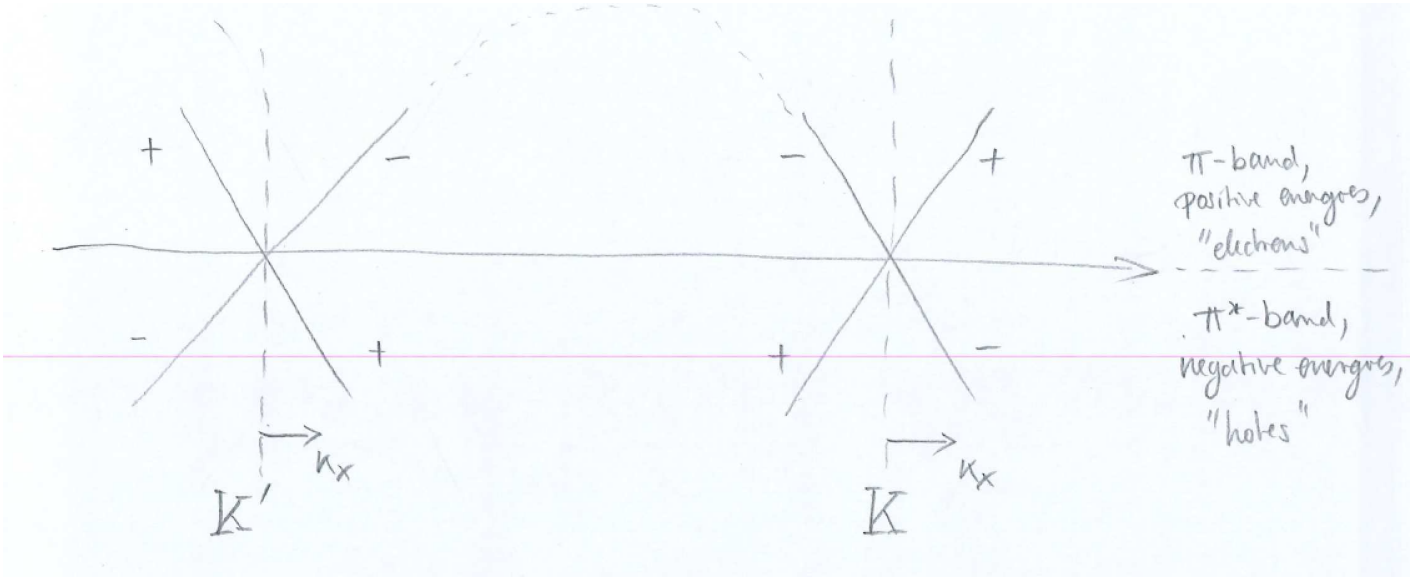
In the vicinity of the ***K***-point:

$$-iv_F\vec{\sigma}\vec{\nabla}\Psi(\vec{r}) \quad = \quad E\Psi(\vec{r})$$

in the vicinity of the ***K***$'$-point:

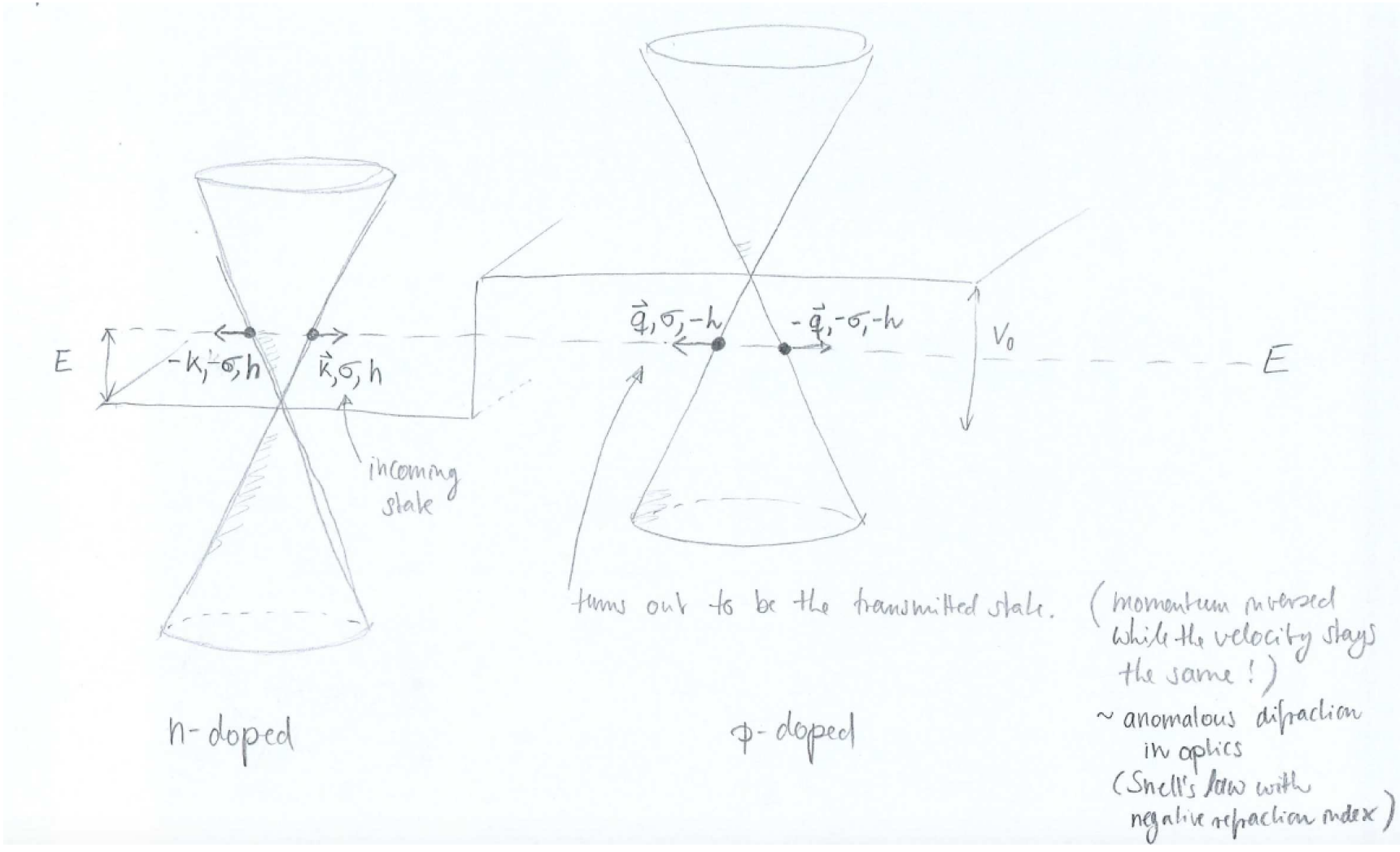
$$iv_F\vec{\sigma}^*\vec{\nabla}\Psi(\vec{r}) \quad = \quad E\Psi(\vec{r})$$

with vectors in A,B-space $\Psi(\vec{r})$. Eigenvectors are symmetric/antisymmetric superpositions of A,B components.



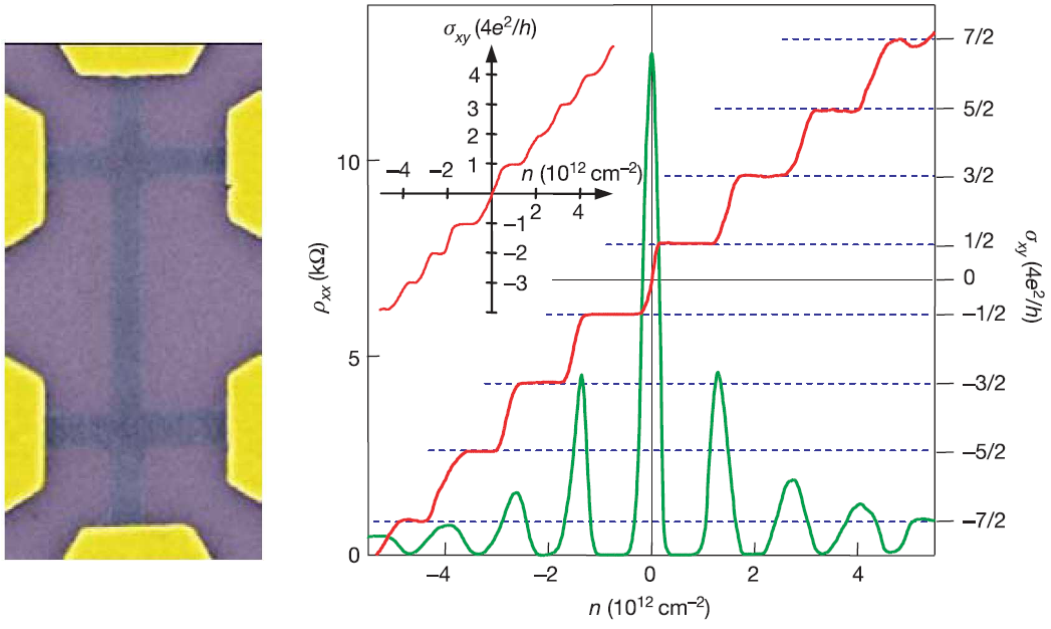
Klein tunneling

Due to missing bandgap AND **pseudospin conservation:**



Confinement via gates is not possible in single-layer graphene!

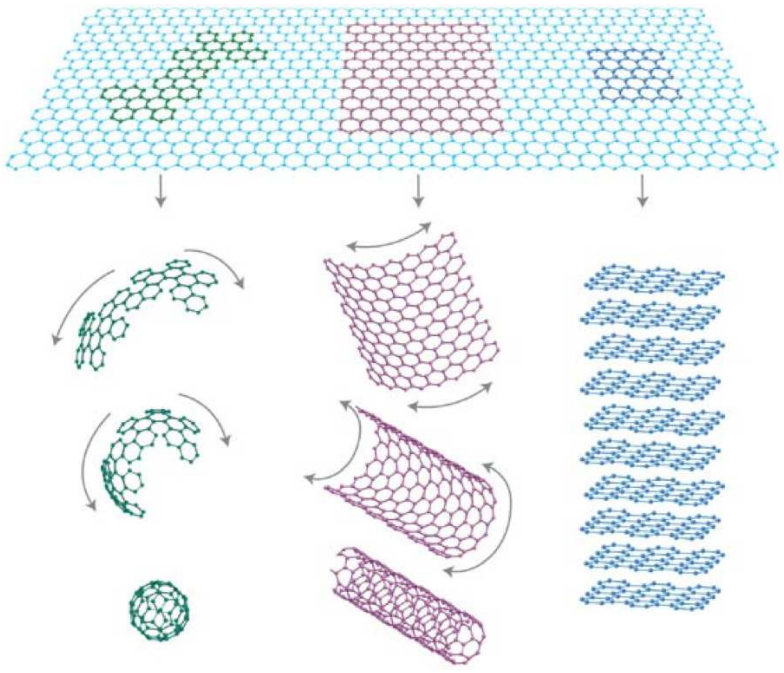
Quantum Hall effect in graphene



K. Novoselov et al., Nature **438**, 197 (2005).

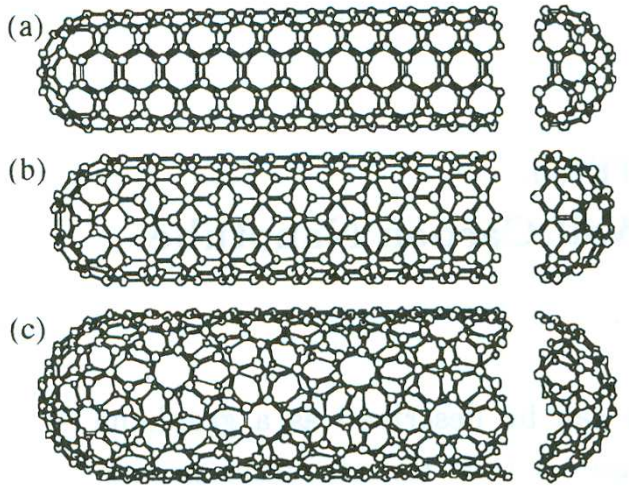
- Hall plateaus for electrons and holes
- Steps of height $4\frac{e^2}{h}$ due to spin+pseudospin degree of freedom
- Special feature of **single-layer** graphene: steps at half-integer multiples of $\frac{4e^2}{h}$

Carbon nanotubes - 1D carbon-based systems



3 different classes of nanotubes:

- zigzag
- armchair
- chiral



Lattice structure of a carbon nanotube

Define the chiral vector

$$\vec{C}_h = n \cdot \vec{a}_1 + m \cdot \vec{a}_2$$

The nanotube is

- **armchair** if $(n, m) = (n, n)$
- **zigzag** if $(n, m) = (n, 0)$
- **chiral** otherwise

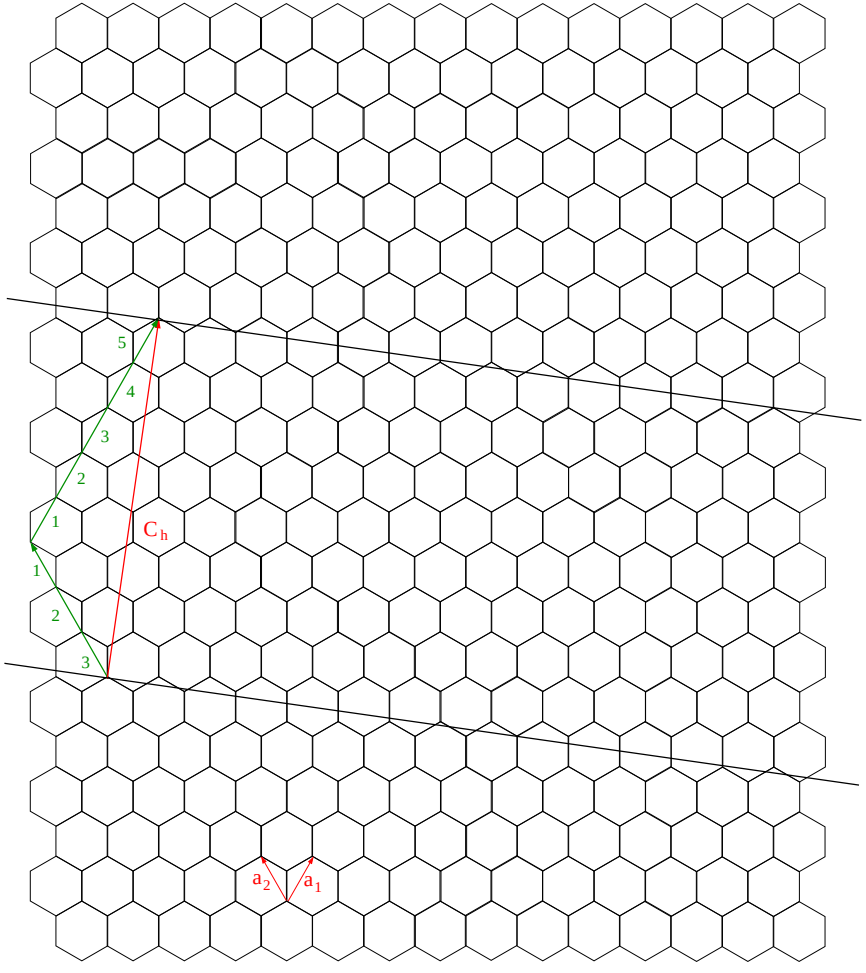
This defines a "unit cell of the CNT

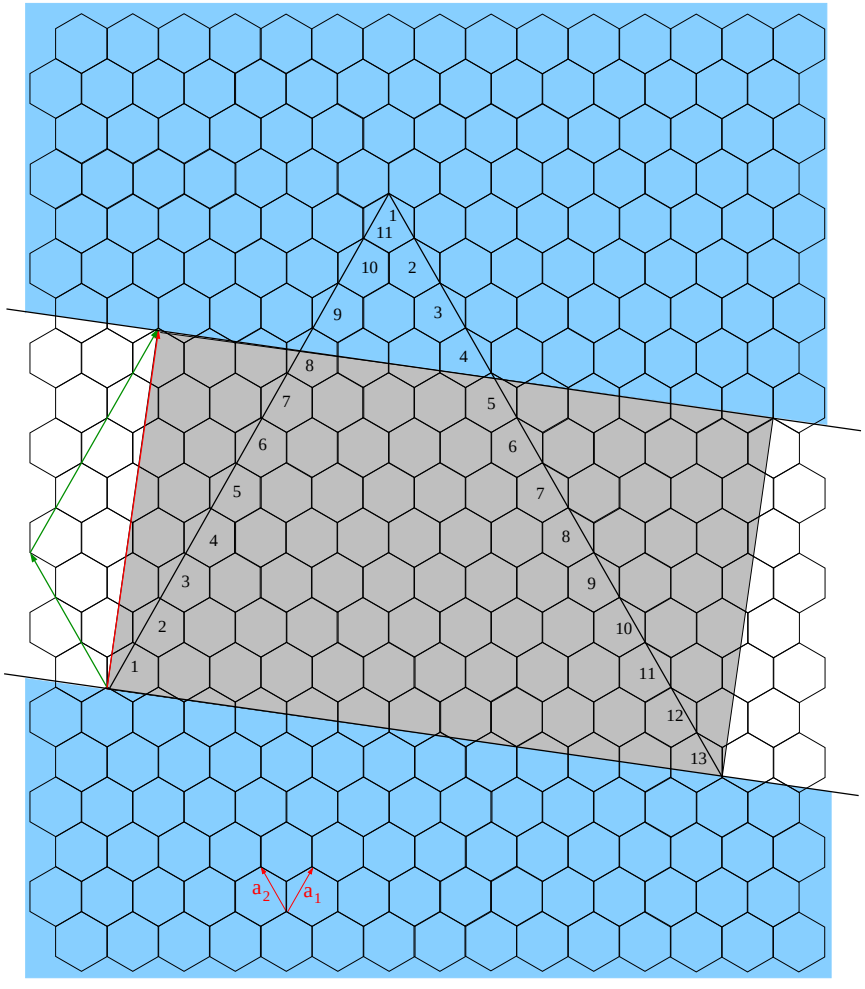
Smallest graphene lattice vector perpendicular to $\vec{C}_h$

$$\vec{T} = t_1 \cdot \vec{a}_1 + t_2 \cdot \vec{a}_2$$
$$\Rightarrow t_1 = -\frac{2m + n}{2n + m} t_2$$

See also instructions for "assembly" on the following slide....

Construct your own carbon nanotubes





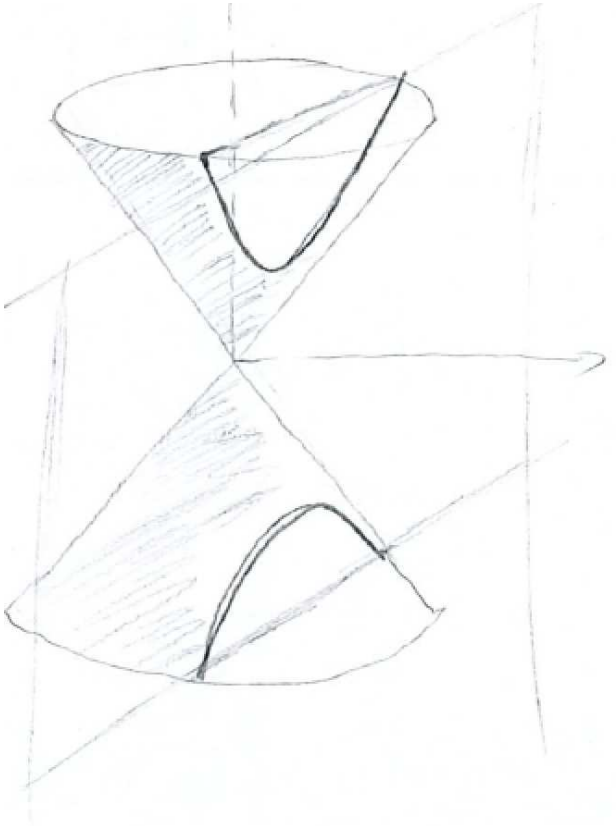
Nanotube spectrum

Additional boundary conditions transversal to the tube direction

ξ : axis parallel to $\vec{C}_h$ $\quad$ k_ξ is quantized

ζ : axis parallel to $\vec{T}$ $\quad$ k_ζ is continuous

Only **cuts** through the graphene spectrum are allowed:



CNTs can be

- metallic, if $\boldsymbol{K}$ and $\boldsymbol{K}'$ are allowed k-values

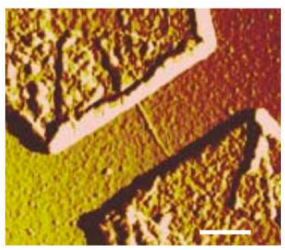
  $$n - m = 3 \cdot N$$

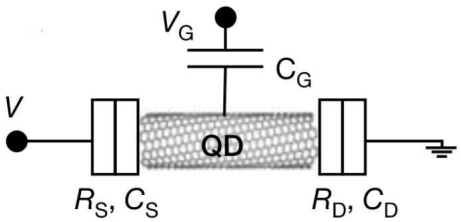
  all armchair and certain zigzag and chiral tubes
- semiconducting, if $\boldsymbol{K}$ and $\boldsymbol{K}'$ are not allowed k-values

  only certain zigzag and chiral tubes

Contacted carbon nanotubes

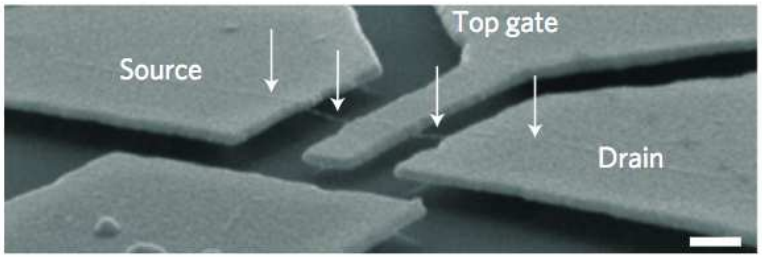
Contacted nanotube on a substrate:

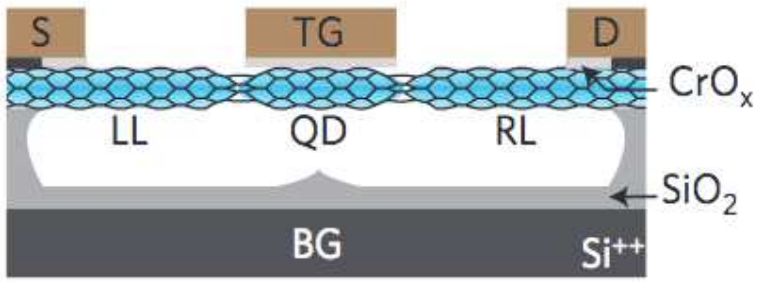




P. Jarillo-Herrero et al.: Nature 429, 389 (2004).

Contacted, suspended nanotube:

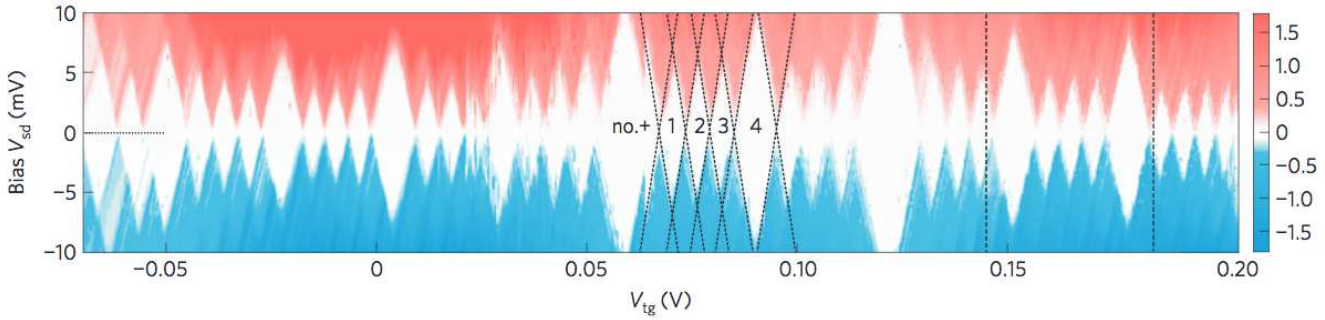




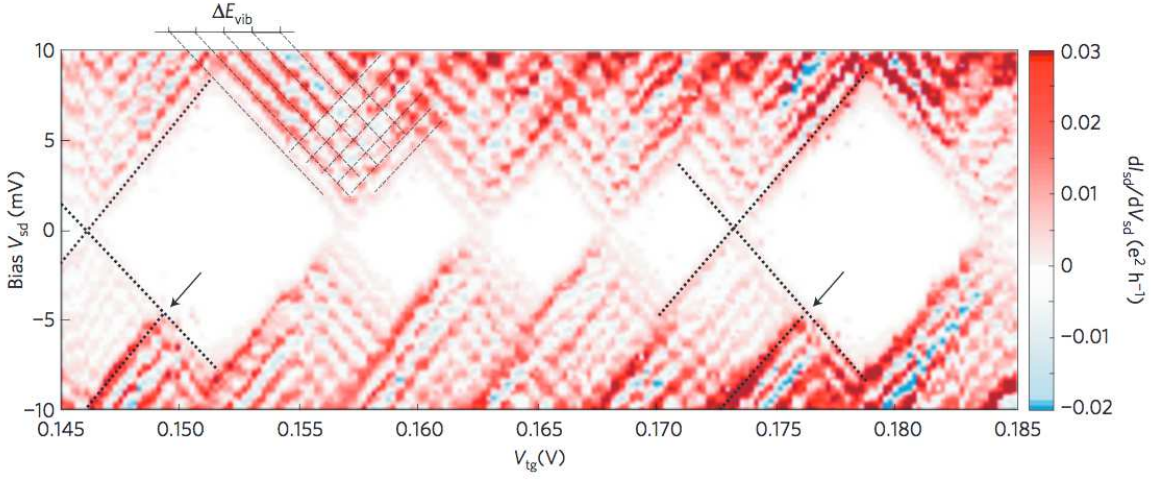
R. Leturcq et al.: Nat. Phys. 5, 327 (2009).

Coulomb diamonds of Carbon nanotubes

Coulomb diamonds displaying four-fold level degeneracy



Excited (vibrational) states and Franck-Condon physics



R. Leturcq et al.: Nat. Phys. 5, 327 (2009).