Magnetoconductance in disordered carbon nanotubes

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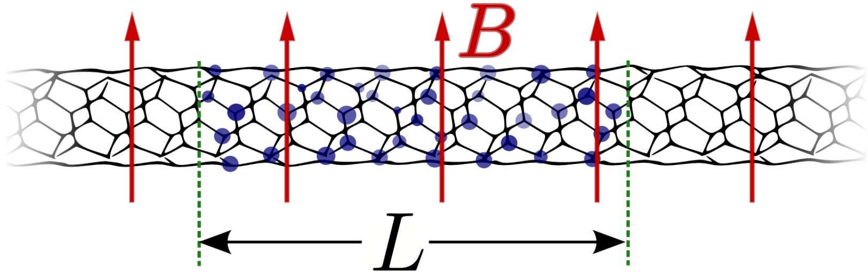
Outline

- Quantum transport in carbon nanotubes (CNT)
- Effects of disorder
- Magnetic field and disorder



Motivation

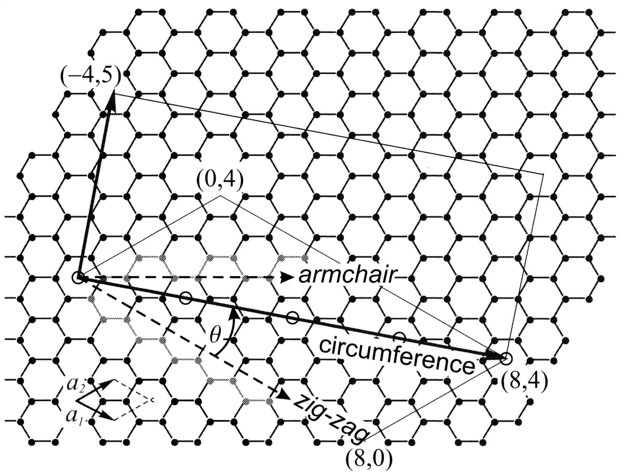
- typically studied: localization effects and simple bandstructure
- experimental evidence for interplay of quasi-1D bandstructure and weak localization in MWCNT.

  (B. Stojetz, 2004)
- strong indications for similarity:

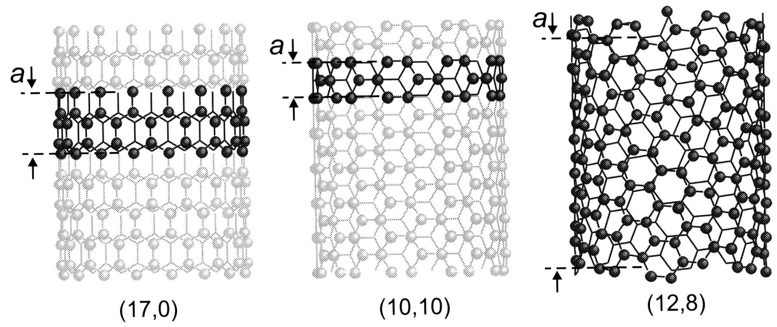
  (incommensurate) MWCNT $\leftrightarrow$ disordered SWCNT

$\rightarrow$ **goal**: study the interplay of nontrivial bandstructure, disorder and magnetic fields in SWCNTs of realistic lengths

Carbon Nanotubes (CNT)



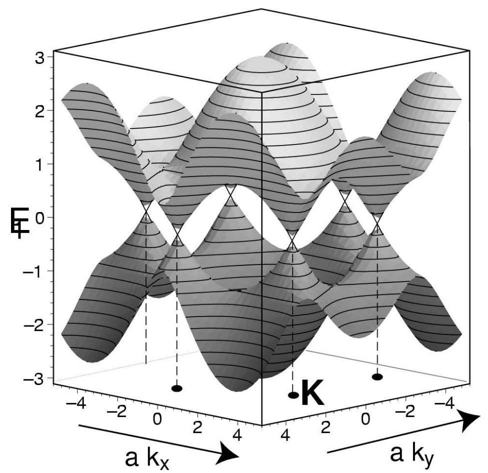
$\longrightarrow$ roll up



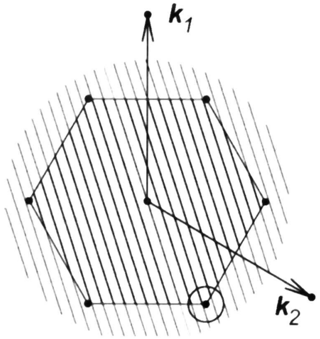
zig-zag armchair chiral

real space

reciprocal space

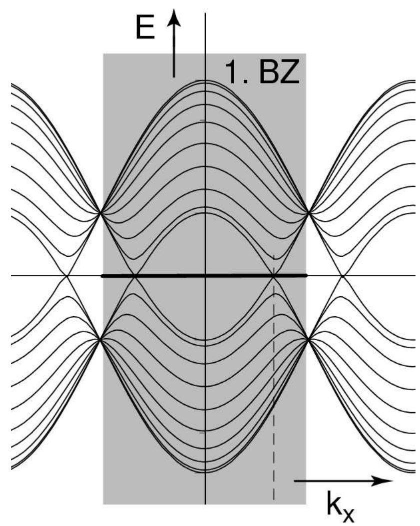


$\rightarrow$

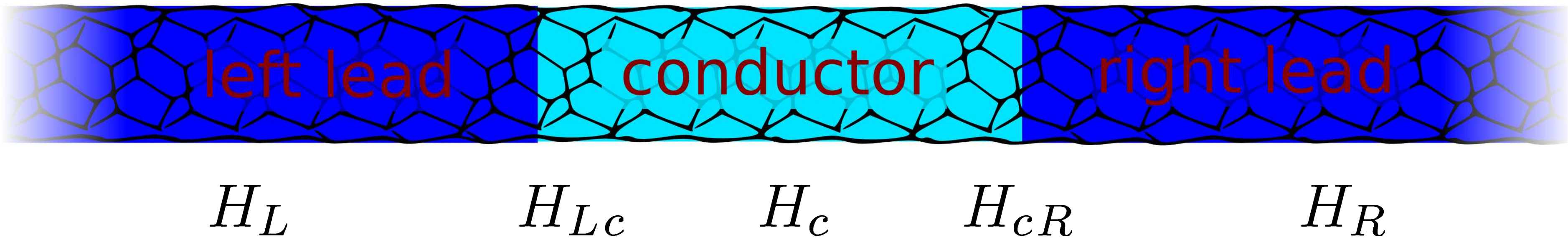


zone-folding

$\rightarrow$



Quantum-transport in two-probe systems



Conductance as scattering process (Landauer formula):

$$G = \frac{2e^2}{h} T(E_F)$$

Transmission coefficient:

$$T(E) = \mathrm{tr}\,\{\Gamma_L \mathcal{G}_c^a \Gamma_R \mathcal{G}_c^r\}$$

$$\Gamma_{L/R} = \mathrm{i}(\Sigma_{L/R}^r - \Sigma_{L/R}^a)$$
$$\mathcal{G}_c = (E + \mathrm{i}0^+ - H_c - \Sigma_L - \Sigma_R)^{-1}$$

*Fisher, Lee, PRB **23**, 6851 (1981)*

The model

π-orbital tight-binding model:

$$H = \sum_i \varepsilon_0 c_i^\dagger c_i + \sum_{\langle i,j \rangle} \gamma_0 c_i^\dagger c_j$$

$$\varepsilon_0 = eV_{\mathrm{g}}$$
$$\gamma_0 = -2.66\,\mathrm{eV}$$

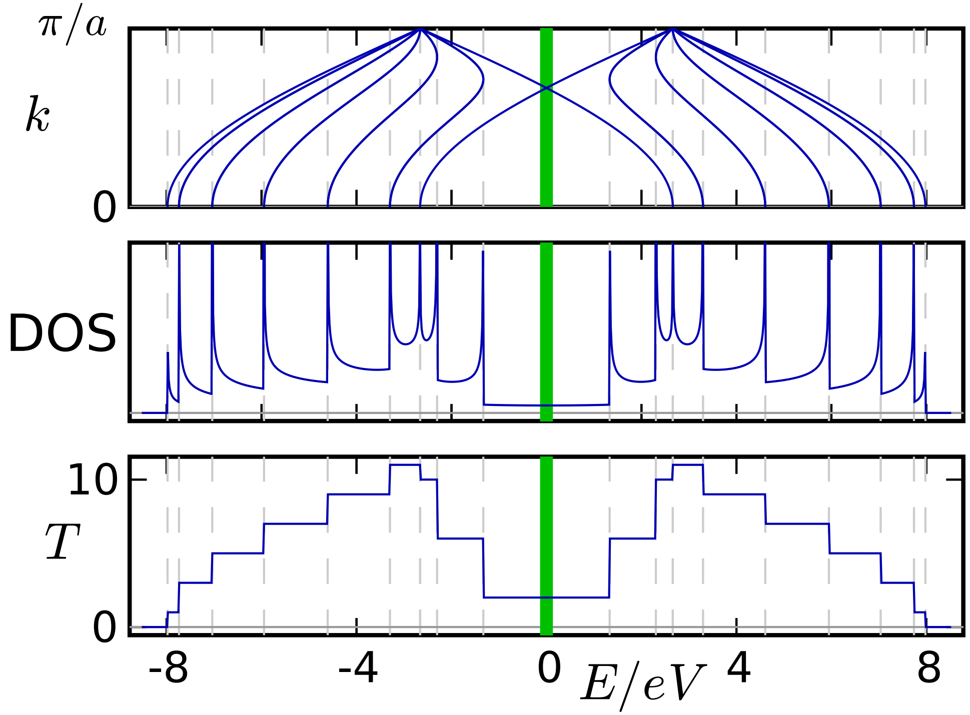
Calculation of an infinite (6,6)-CNT

$E = 0 \rightarrow$ "CNP"

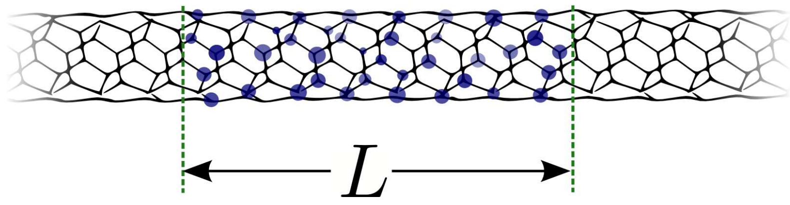
bandstructure

bulk density of states

conductance



Anderson disorder

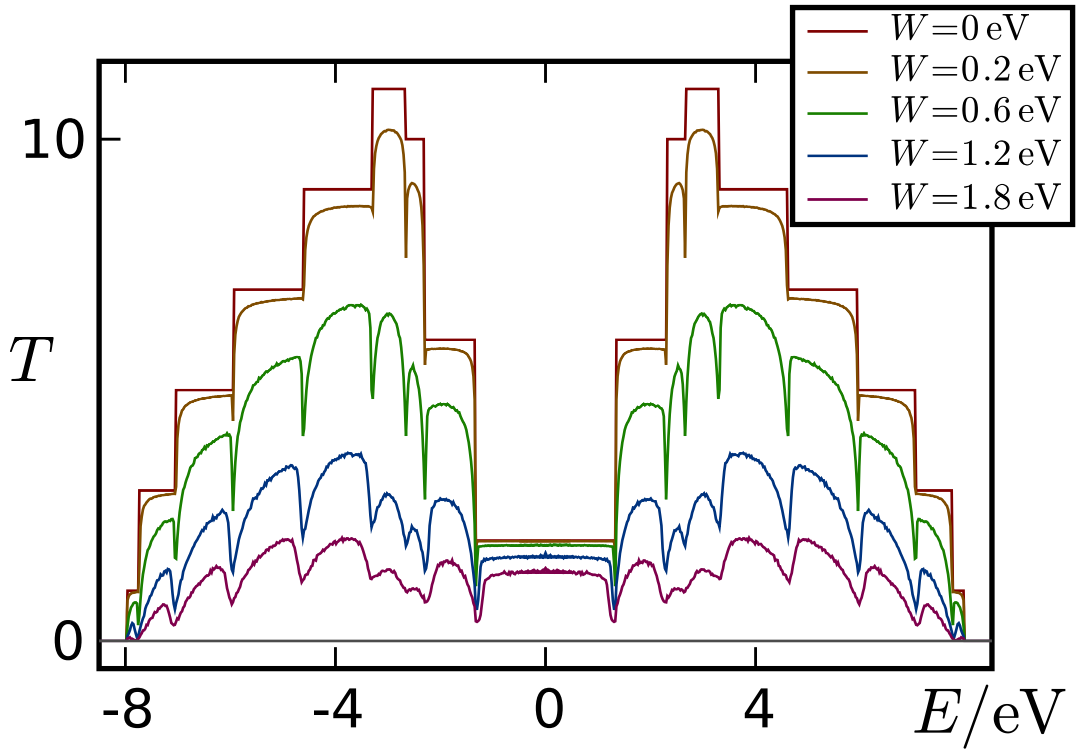


- $\varepsilon_0 \rightarrow \varepsilon_0 + \Delta\varepsilon_i$, uniformly distributed $\Delta\varepsilon_i \in [-W/2; W/2]$
- finite disordered region of length L, semi-infinite leads

CNT-(6,6)

length:
$L \approx 25\,\mathrm{nm}$

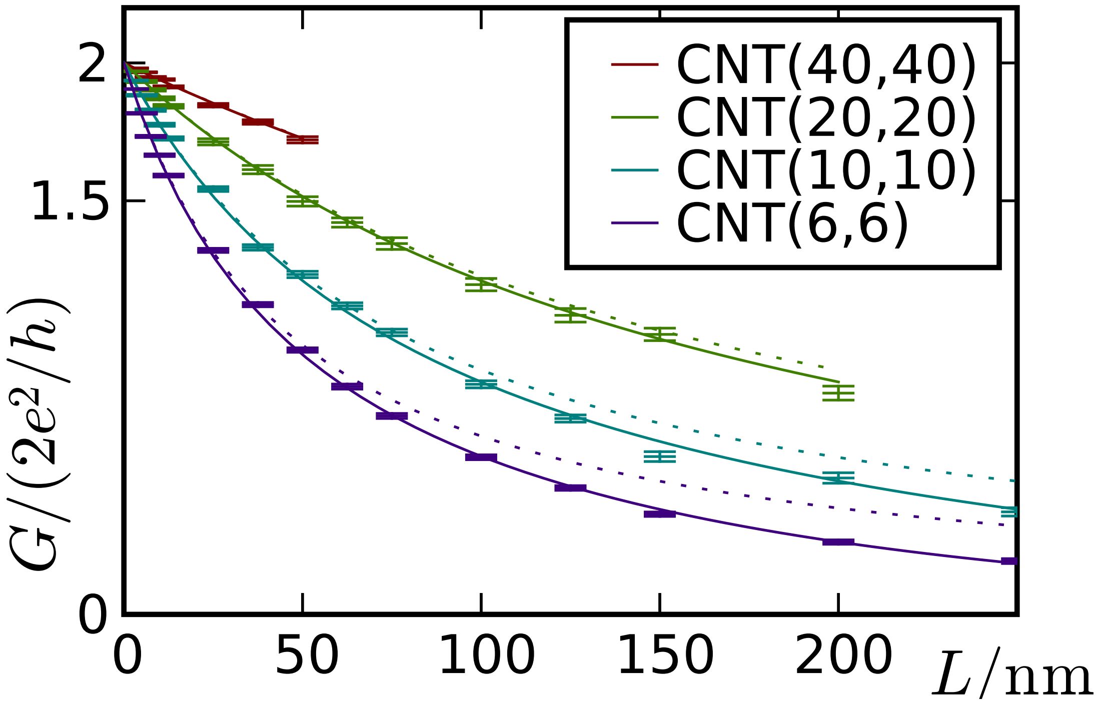
CNP at $E = 0\,\mathrm{eV}$



Strong localization at the CNP

Length dependent conductance *Tartakovski, PRB **52**, 2704 (1995)*

$$G = \frac{2e^2}{h}\left(\frac{1}{N_{\rm ch}}\cosh\frac{L}{\ell_{\rm loc}} + c\sinh\frac{L}{\ell_{\rm loc}}\right)^{-1}$$



$W = 2.0\mathrm{eV}$
$E = 0\mathrm{eV}$ (CNP)

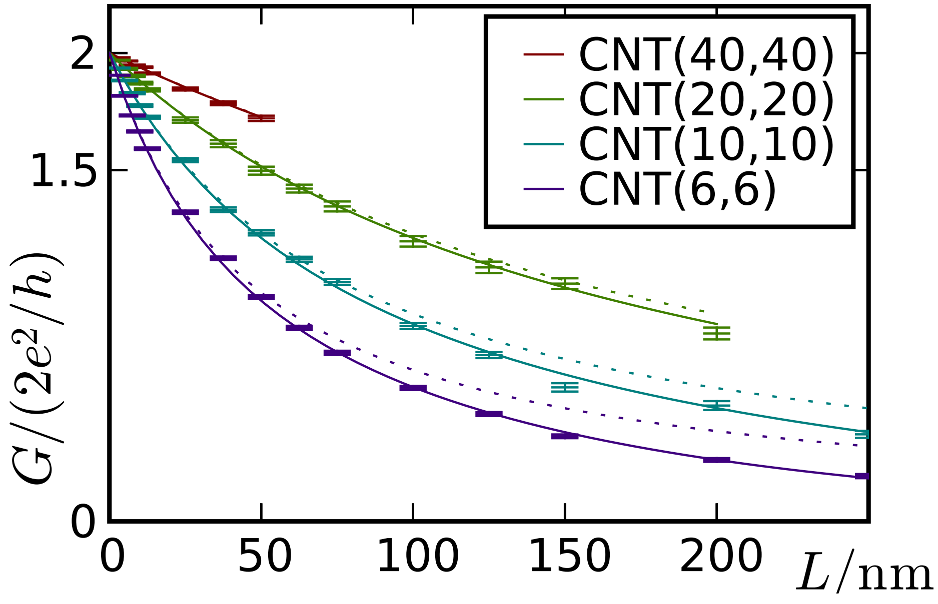
numerical fit:
$c \approx 1.56$
$\ell_{\rm loc} \approx 8\mathrm{nm}\,\frac{\gamma_0^2}{W^2} \times N$

Ohmic regime

For $L \ll \ell_{\rm loc}$:

$$G_\Omega = \frac{2e^2}{h} N_{\rm ch} \left(1 + \frac{L}{\ell_{\rm el}}\right)^{-1}$$

$$\Rightarrow \quad \ell_{\rm loc} = c\, N_{\rm ch} \ell_{\rm el}$$



*consistent with general arguments by Thouless, PRB **39**, 1167 (1977)*

Known analytically for armchair CNT in CNP:

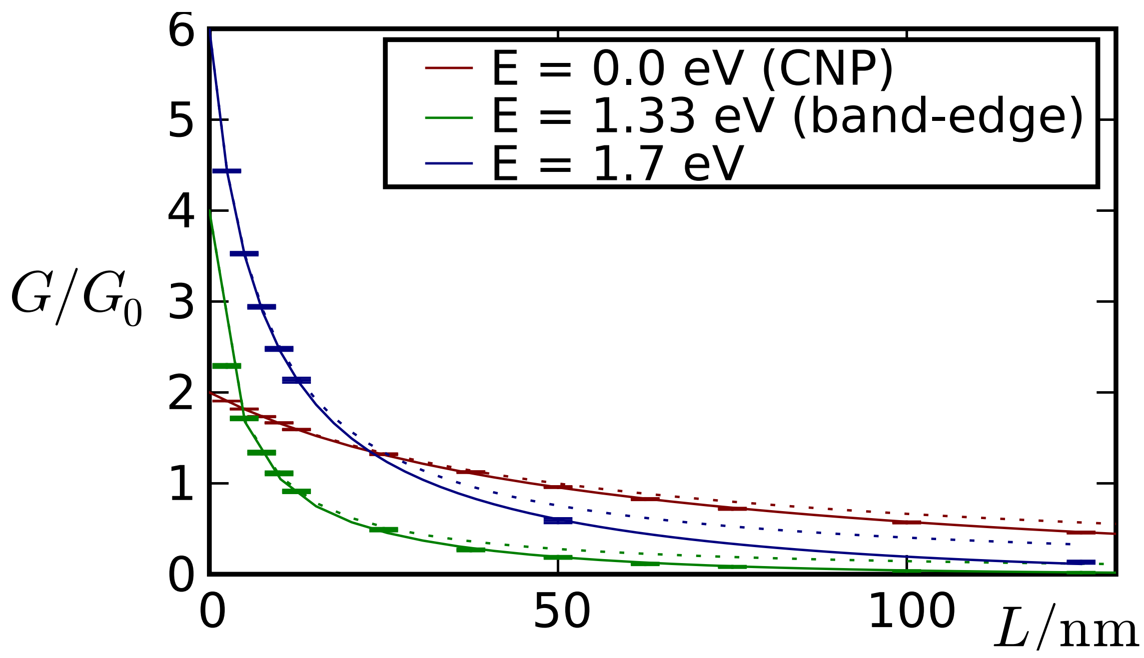
$$l_{\rm el} = \frac{6\sqrt{3}\pi\gamma_0^2}{W^2} D$$

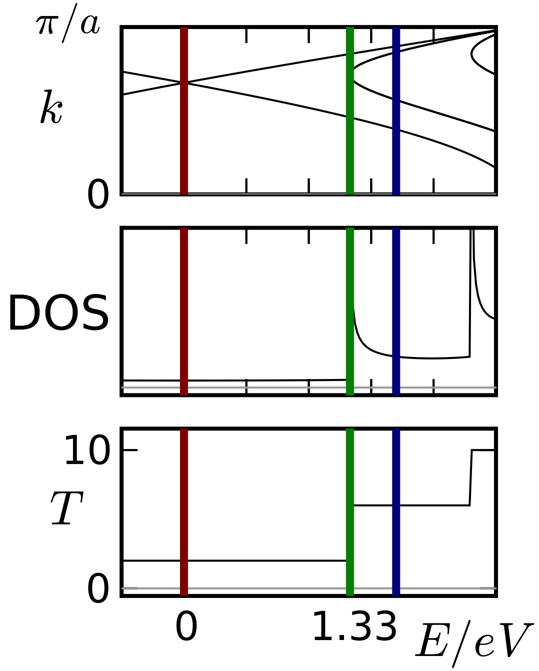
*White, Todorov, Nature **393**, 240 (1998)*

$\rightarrow$ fully consistent with our numerical results

At the band-edge

CNT(6,6), $W = 2.0\mathrm{eV}$



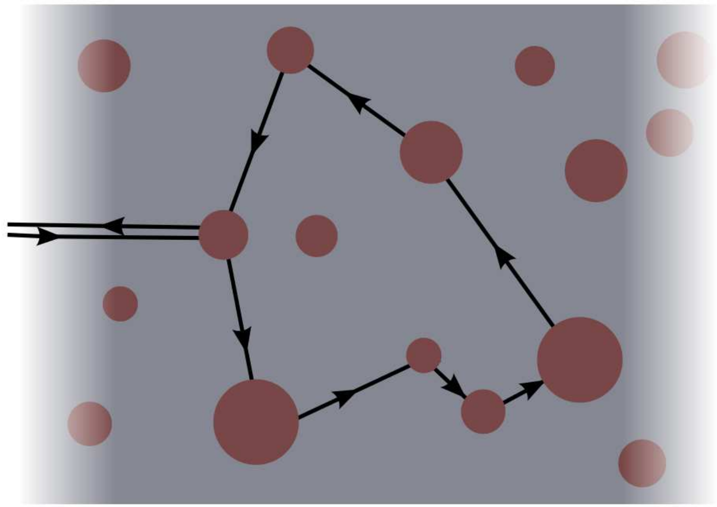


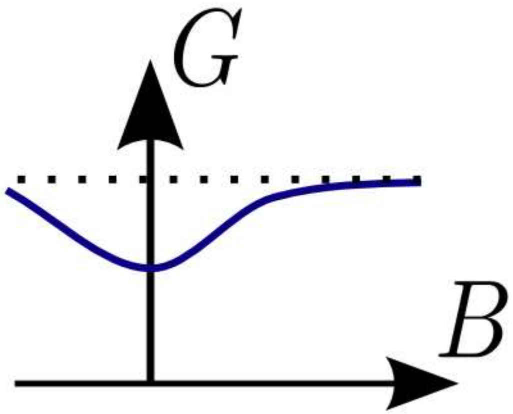
	E	N_{ch}	ℓ_{el}	ℓ_{loc}	ℓ_{loc}/ℓ_{el}
CNP:	$0\mathrm{eV}$	2	$125\,\mathrm{nm}$	$377\,\mathrm{nm}$	3.0
band-edge:	$1.33\,\mathrm{eV}$	≈ 4	**$9.2\,\mathrm{nm}$**	**$85\,\mathrm{nm}$**	**9.2**
beyond:	$1.7\mathrm{eV}$	6	$18\,\mathrm{nm}$	$118\,\mathrm{nm}$	6.5

Weak localization

Enhanced backscattering reduces conductance by

$$\Delta G = -\frac{2e^2}{h}\sqrt{\left(\frac{L}{\ell_\varphi}\right)^2 + \frac{e^2L^2A}{3\hbar^2}B^2}^{\,-1}$$



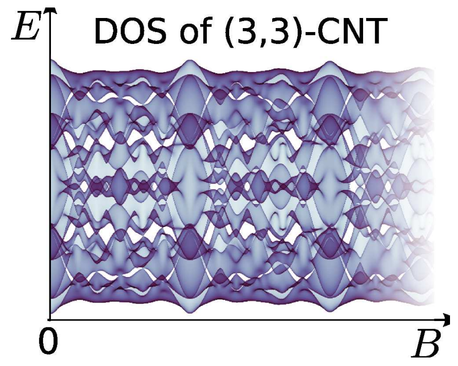


reduction lifted by magnetic fields
($\rightarrow$ *"negative magnetoresistance"*)

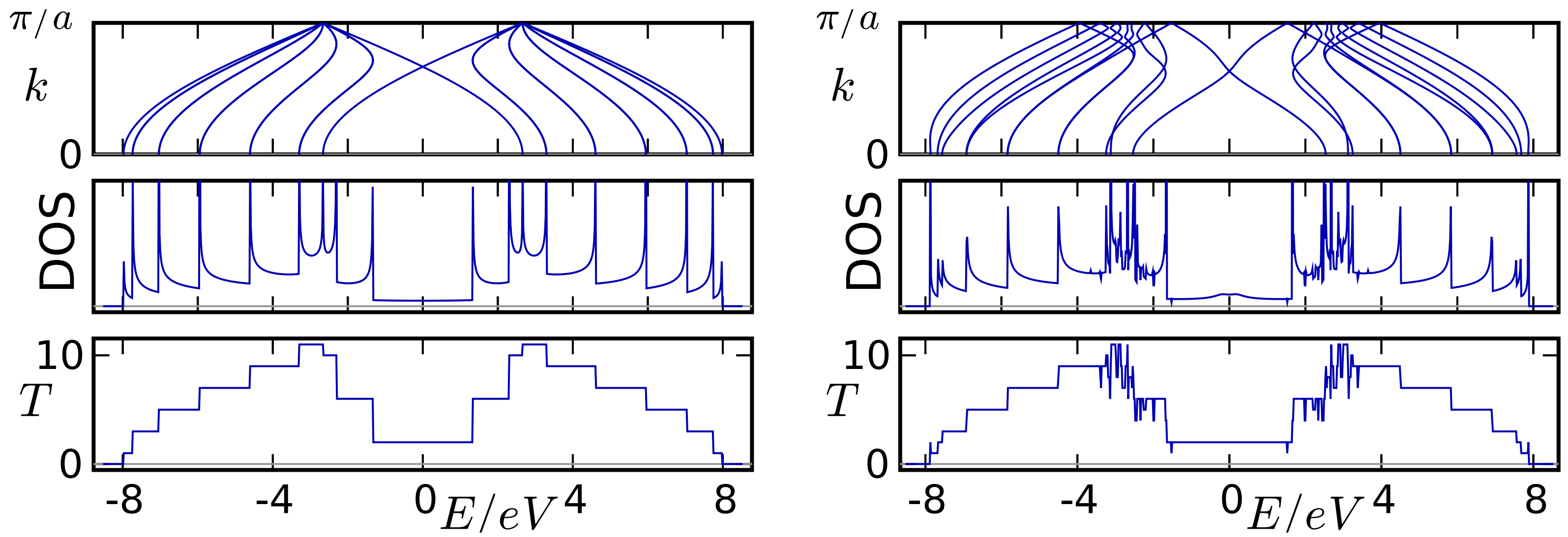
Implementation of magnetic fields

Peierls substitution: $\gamma_0 \rightarrow \gamma_0 \exp\left(\frac{\mathrm{ie}}{\hbar}\int_{x_1}^{x_2} \mathrm{d}\vec{x}\,\vec{A}(x)\right)$

$\rightarrow$ bandstructure is distorted



CNT(6,6), B-field perpendicular to tube-axis:



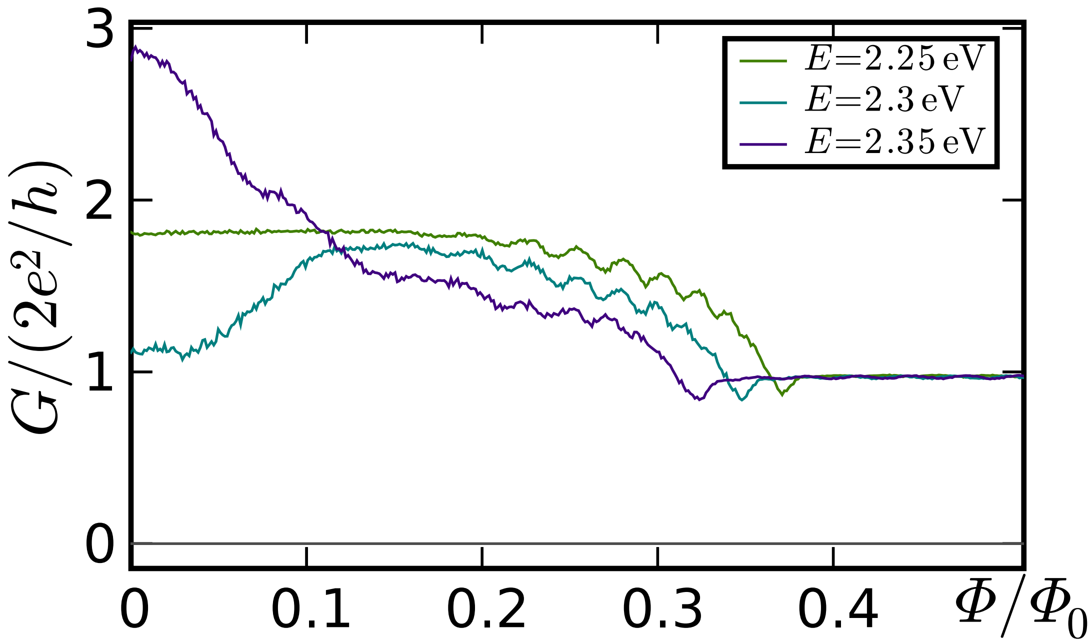
$\Phi = 0$ flux per tube section $\Phi \approx \Phi_0$

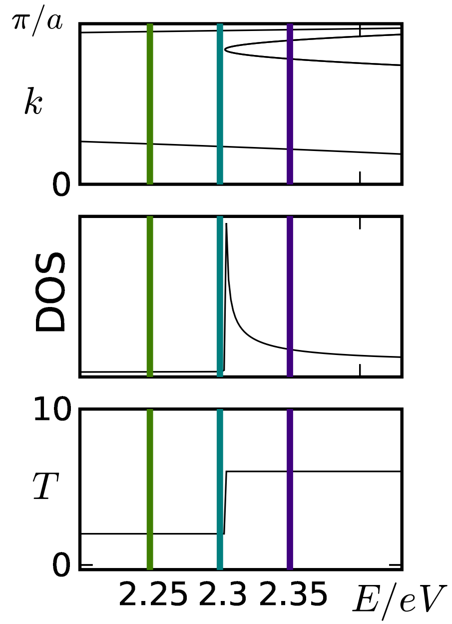
*Saito, Dresselhaus&Dresselhaus, PRB **50**, 14698 (1994)*

Weak localization in CNTs

- strongly dependent on DOS
- competes with bandstructure distortions

CNT(3,3), $W = 0.5\mathrm{eV}$, $L = 15\mathrm{nm}$





Summary

- **at CNP:** previous results could be verified:
  - Ohmic regime $\rightarrow$ mean free path ℓ_{el}
  - strong localization $\rightarrow$ localization length ℓ_{loc}
- **near band-edges:**
  - ℓ_{el} and ℓ_{loc} strongly reduced
  - weak localization: strongly increased

Outlook

- analytics near band-edges
- DWCNT / MWCNT