Magnetoresistance and contact effects in carbon nanotubes

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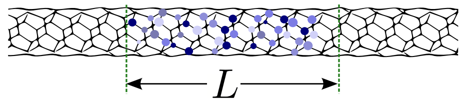
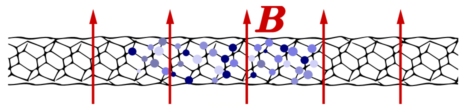
Outline

NT05 posters

- Length scales in disordered CNTs



- Magnetoresistance in CNTs



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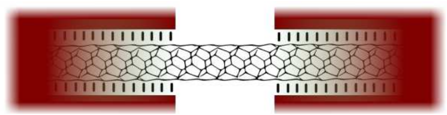
- Effects of extended contacts



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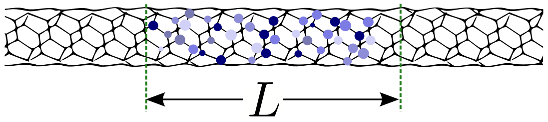
Motivation



- typically studied:
  localization phenomena and *simple bandstructure*

- experimental evidence for interplay of
  quasi-1D bandstructure and weak localization in MWCNT

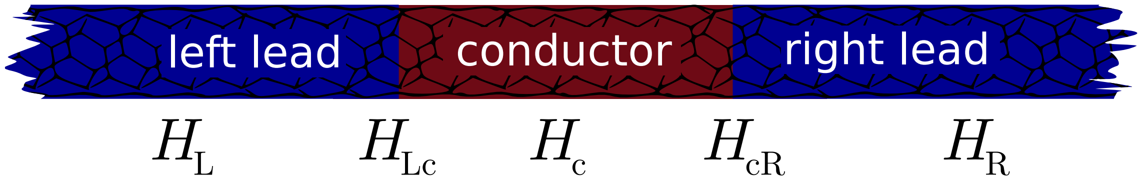
  Stojetz et al., PRL **94***, 186802 (2004)*

- strong indications for similarity:
  (incommensurate) MWCNT $\leftrightarrow$ disordered SWCNT

$\Rightarrow$ **our goal:**

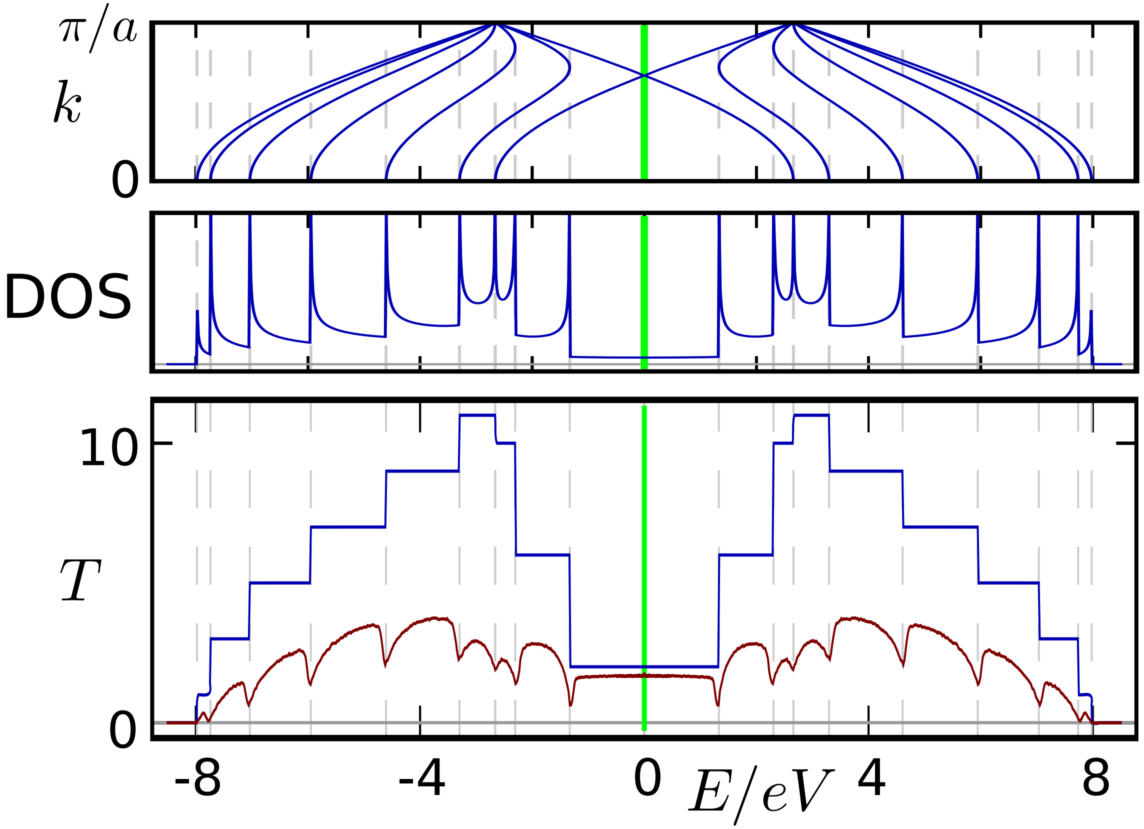
study the interplay of nontrivial bandstructure, disorder
and magnetic fields in SWCNTs of realistic lengths

The model



Minimal model: $H = \sum_i \varepsilon_i c_i^\dagger c_i + \sum_{\langle i,j \rangle} \gamma_{ij} c_i^\dagger c_j$ (π-orbital tight-binding)

Calculation of CNT-(6,6)



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

with $T = \sum_{n=1}^{N_{ch}} T_n$

clean tube: $\varepsilon_i = \varepsilon_0$

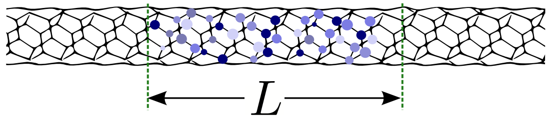
$\Rightarrow$ perfectly periodic system

with Anderson disorder:

$\varepsilon_i = \varepsilon_0 + \delta\varepsilon_i, \ \ \delta\varepsilon_i \in \left[-\frac{W}{2}, +\frac{W}{2} \right]$

in finite region length L

Length scales



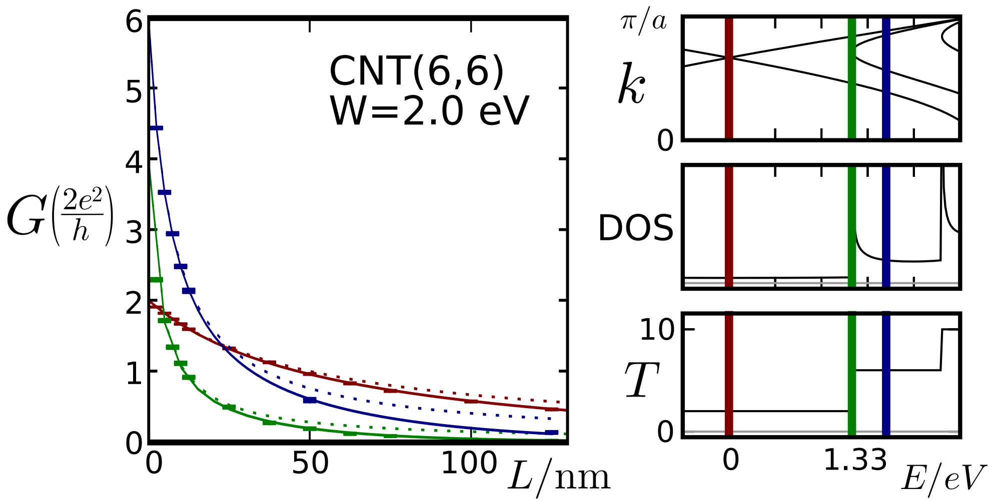
$L \ll \ell_{\rm loc}$: $G_\Omega = \frac{2e^2}{h} N_{\rm ch} \left(1 + \frac{L}{\ell_{\rm el}}\right)^{-1}$ $L \gg \ell_{\rm loc}$: $G_{\rm loc} \propto \exp(-L/\ell_{\rm loc})$

↘ ↙

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

(Tartakovski, PRB **52***, 2704 (1995))*

with $\ell_{\rm loc} = c N_{\rm ch} \ell_{\rm el}$, $c \sim 1$ *(Thouless, PRL* **39***, 1167 (1977))*



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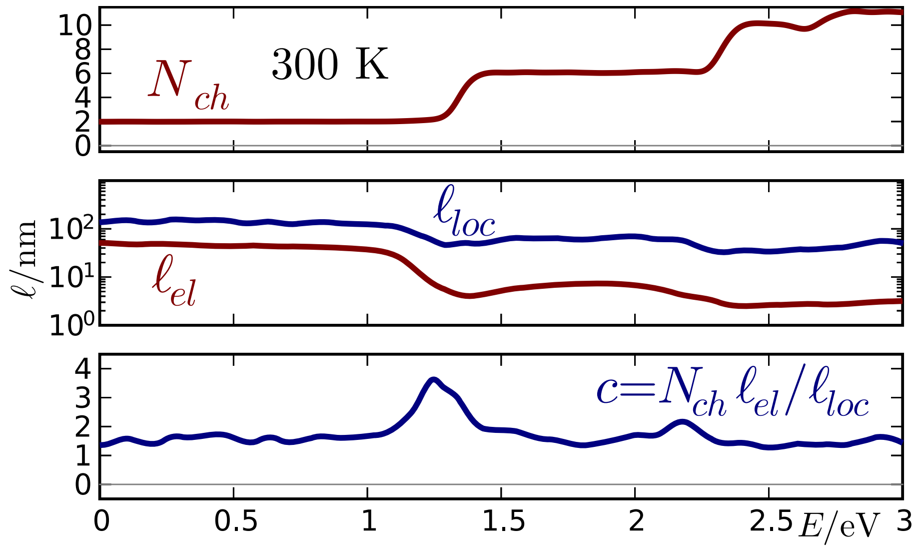


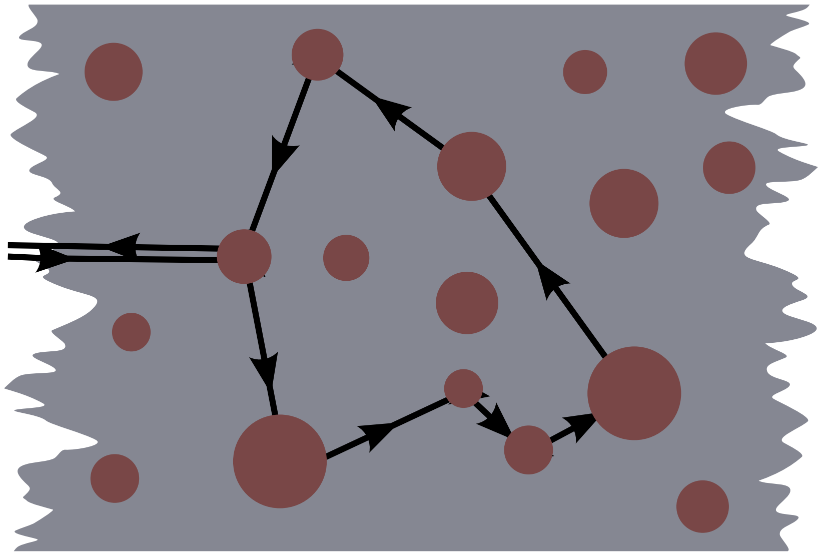
increased $\ell_{\rm loc}/\ell_{\rm el}$-ratio at band-edges

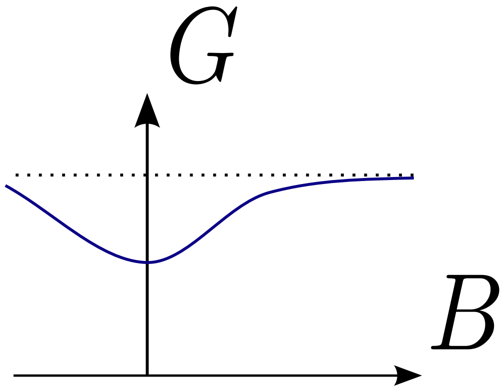
Weak localization:

Enhanced backscattering reduces conductance by

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

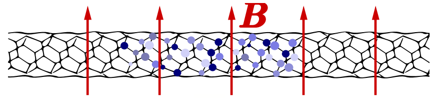
Altshuler et al., PRB **22***, 5142 (1980)*





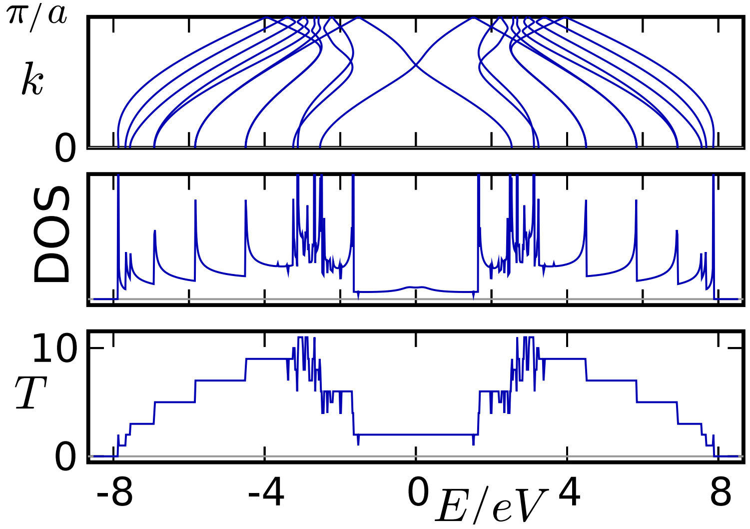
reduction lifted by magnetic fields ($\rightarrow$ "*negative magnetoresistance*")

Implementation of B-fields

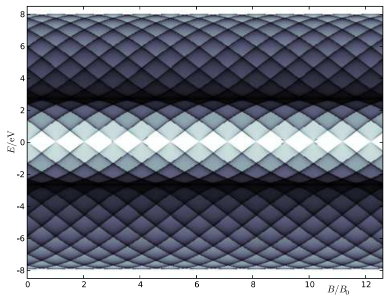


Peierls substitution: $\gamma_0 \rightarrow \gamma_0 \exp\left(\frac{\mathrm{ie}}{\hbar} \int_{x_1}^{x_2} \mathrm{d}\vec{x}\, \vec{A}(x)\right)$

CNT(6,6), $B_\perp \approx 0.5\, B_0$

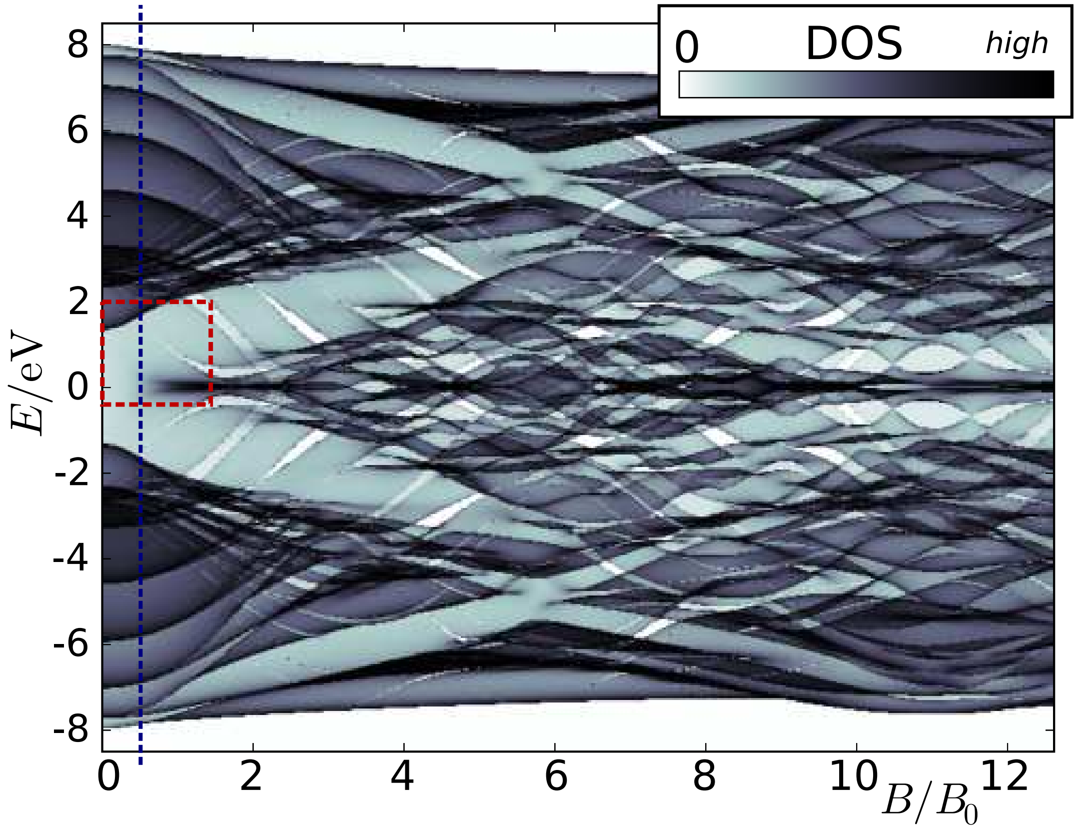


$B_0 = \Phi_0 / \pi r^2_{\text{tube}}$ (→ *for MWCNT:* $B_0 \sim 5T$)



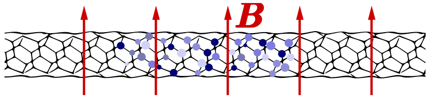
B-field parallel to tube axis

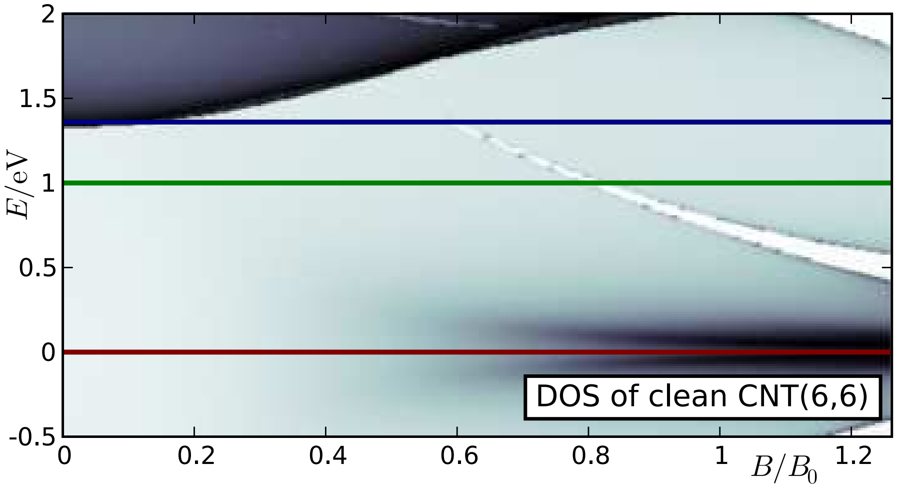
Visualization scheme after the "Hofstadter-Butterfly", PRB **14**, 2239 (1976)



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

Magnetoconductance in CNTs

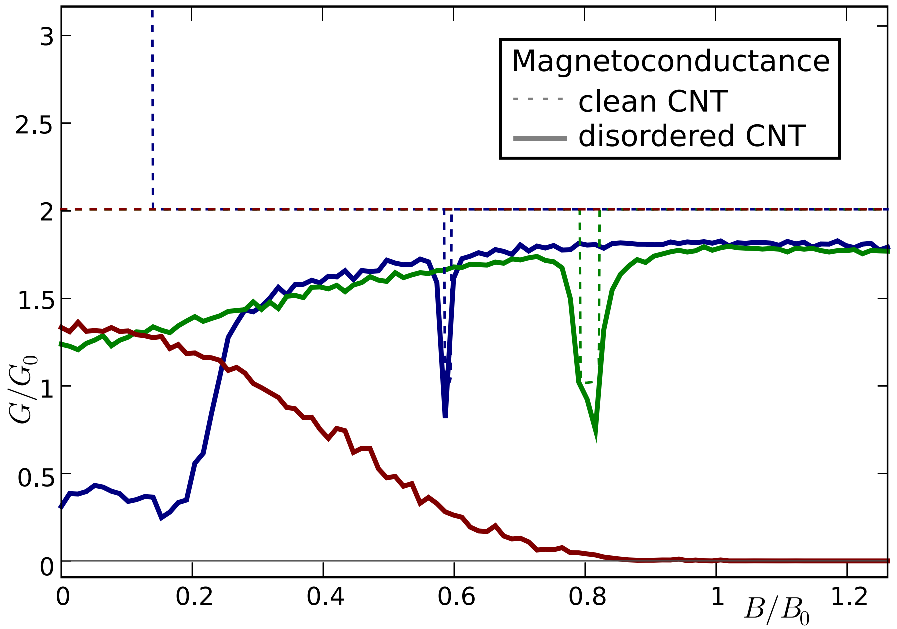




$\longrightarrow$ at $E = 0$: increased scattering due to band quenching

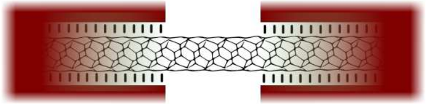
$\Rightarrow$ negative magnetoconductance !!

$\longrightarrow$ increased scattering near bandedges



Characteristic WL-effect:

- $\star$ independent of E
- $\star$ obscured by bandstructure effects



Effects of extended contacts

in cooperation with D. Tománek

Motivation

- contacts in experimental setup:
  CNTs coated by metal over several 100 nm
- Different results about the *effective contact size*
- Palladium gives good contacts, but why?

$\Rightarrow$ **our goal:**

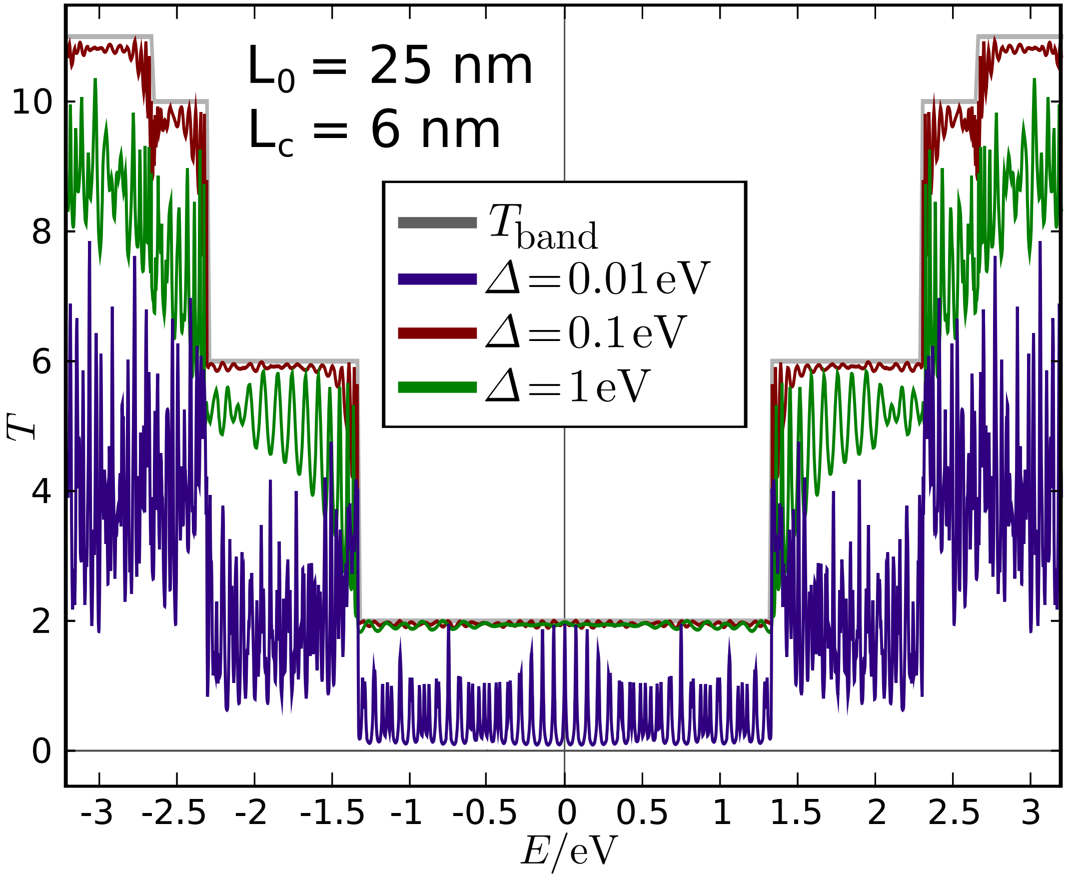
ab initio $\longrightarrow$ TB-parametrization

$\longrightarrow$ large scale transport calculation

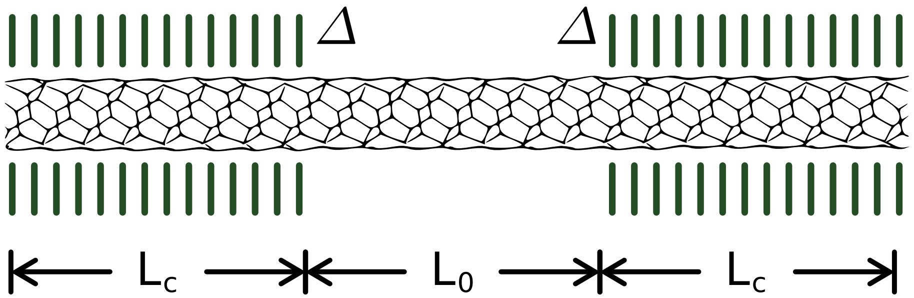
*Javey et al. Nature **424**, 654 (2003)*

Computation method

Raw transmission data $T_\Delta(E)$ and $T_{\rm band}(E)$:



Coating wide-band leads:



$L_0 = 100\mathrm{nm}$ (fixed), $L_c \leqslant 100\mathrm{nm}$ (variable)

Wide-band constant Δ

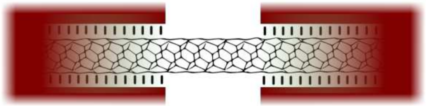
$$\Delta = \left(\gamma_{\substack{\text{carbon}\\\text{metal}}}\right)^2 \times \mathrm{LDOS}_{\text{metal-surface}}$$

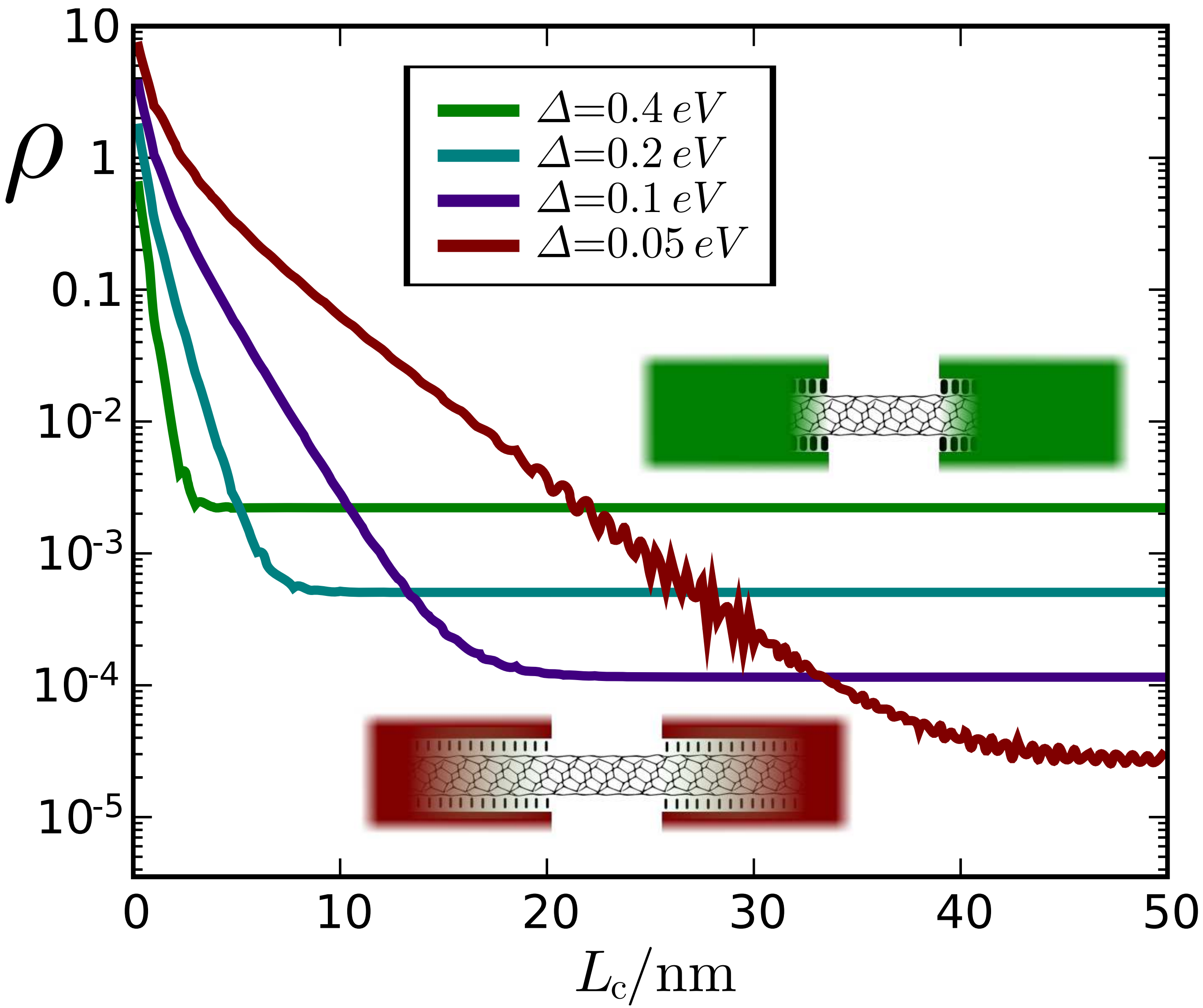
From ab initio calculation:

$\Delta_{\rm Pd} \approx 0.02\,\mathrm{eV}$, $\Delta_{\rm Ti} \approx 0.1\,\mathrm{eV}$

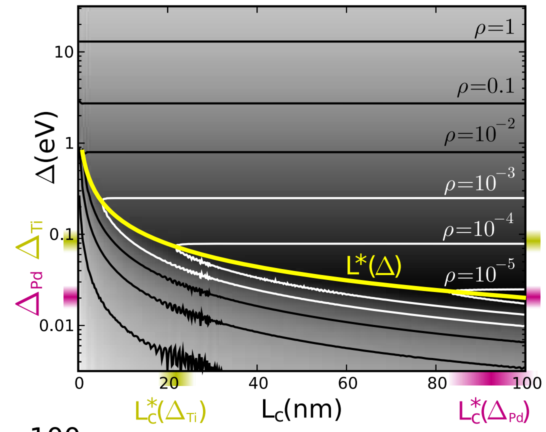
Contact reflection defined as: $\rho = \left\langle \frac{T_{\rm band} - T_\Delta}{T_{\rm band} T_\Delta} \right\rangle_E$ (Avg. for massless bands only)

Results

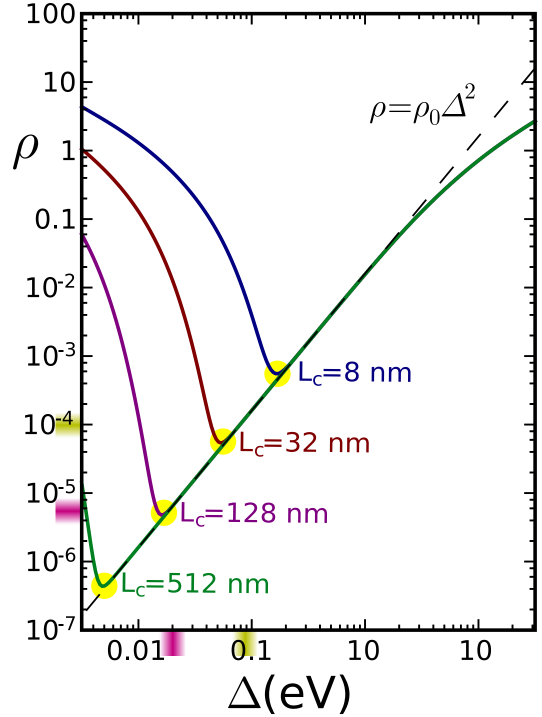




10
1
0.1
10^{-2}
10^{-3}
10^{-4}
10^{-5}
ρ
Δ=0.4 eV
Δ=0.2 eV
Δ=0.1 eV
Δ=0.05 eV
0
10
20
30
40
50
L_c/nm



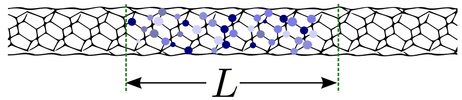
ρ=1
ρ=0.1
$\rho=10^{-2}$
$\rho=10^{-3}$
$\rho=10^{-4}$
$\rho=10^{-5}$
L*(Δ)
Δ(eV)
Δ_{Ti}
Δ_{Pd}
L_c(nm)
$L_c^*(\Delta_{Ti})$
$L_c^*(\Delta_{Pd})$



$\rho=\rho_0\Delta^2$
ρ
L_c=8 nm
L_c=32 nm
L_c=128 nm
L_c=512 nm
Δ(eV)

Summary

Length dependence in disordered CNTs



- increased $\ell_{\mathrm{loc}}/\ell_{\mathrm{el}}$-ratio at band-edges

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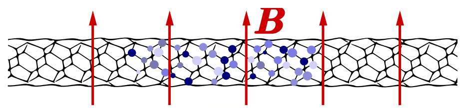
Magnetoresistance in CNTs



- weak localization effect visible, obscured by bandstructure
- *positive magnetoresistance* caused by *band-quenching* at $E = 0$

Effects of extended contact

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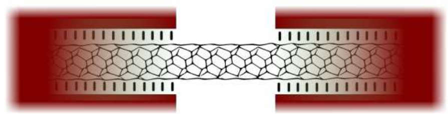
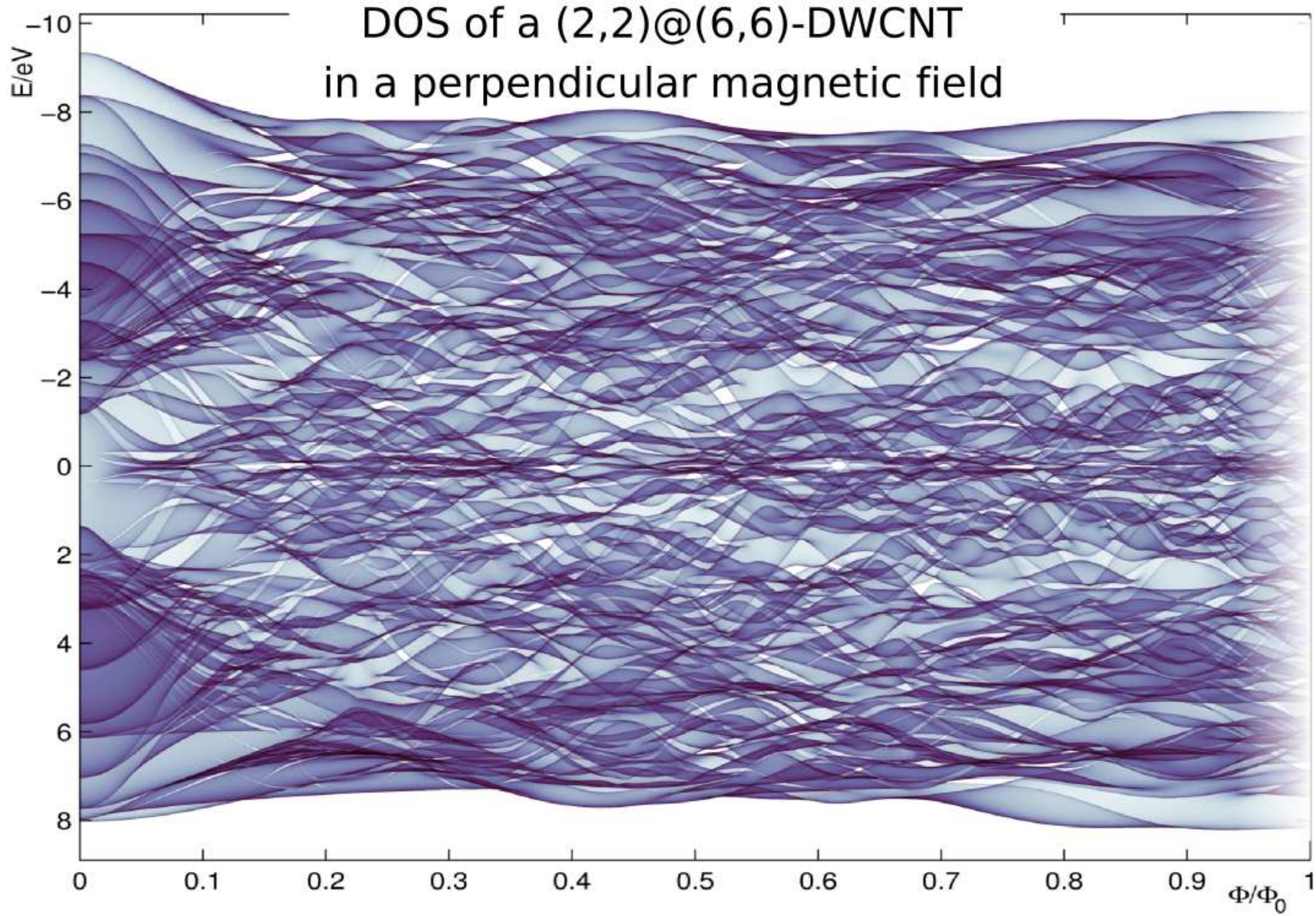


- Pd-CNT coupling weaker then Ti-CNT
- weak metal-CNT coupling leads to high contact transparency

$\longrightarrow$ disorder in contact region?	$\longrightarrow$ MWCNTs?


DOS of a (2,2)@(6,6)-DWCNT
in a perpendicular magnetic field
E/eV
−10
−8
−6
−4
−2
0
2
4
6
8
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Φ/Φ0