TT8.1

Spin transport in disordered single wall carbon nanotubes

Nitesh Ranjan, Norbert Nemec and Gianaurelio Cuniberti

Molecular Computing Group, Institute for Theoretical Physics, Universtity of Regensburg, D-93047 Regensburg, Germany

Abstract

The effect of disorder on spin transport through single wall carbon nanotubes (SWCNT) is investigated.
Model disorder in SWCNTs is is expected to capture the presence of fabrication related inpurities, vibrations [1] and even the effects of intershell interaction in incommensurate multi wall carbon nanotubes (MWCNT) [2]
With this motivation, we study spin transport in ferromagnetically contacted disordered single wall carbon nanotubes in the coherent regime up to experimentally relevant tube lengths of several 100 nm.

Modelling a two-probe setup

Conductance in the linear regime at zero temperature (Landauer formula):

$$G = \frac{2e^2}{h} T(E_F) \qquad (1)$$

The transmission coefficient $T(E)$ can be obtained from the Fisher-Lee relation [3]:

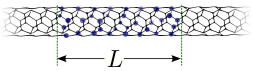
$$T(E) = tr\left\{\Gamma_L G_c^a \Gamma_R G_c^r\right\} \qquad (2)$$

$\Gamma_{L/R} = i(\Sigma_{L/R} - \Sigma_{L/R}^\dagger)$
$\Sigma_{L/R}$: self energy coming from the left (right) lead
$G_c^{r/a}$ projection of Green function onto the conductor.

For the leads efficient algorithms exist [4].
To calculate the Green function of the conductor, we developed a highly efficient decimation algorithm that allows us to handle CNT of several hundred nanometers in length ($\sim$ 20,000 atoms).

Anderson disordered CNTs

Anderson disorder is a good model of various kinds of physical disorder (defects, adsorbants, thermal vibrations [1], etc.). For our calculations, disorder is introduced only in the conductor:



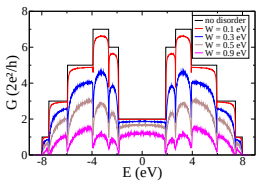
Hamiltonian in π-orbital tight-binding approximation:

$$H = \sum_i \epsilon_i c_i^\dagger c_i + \sum_{\langle i,j \rangle} t_{ij} c_j^\dagger c_i \qquad (3)$$

$t_{ij} = -2.66$ eV: hopping parameter between neighboring atoms
Disorder: random onsite potential ϵ_i:

$$\epsilon_i = \epsilon_0 + \delta\epsilon_i \qquad (4)$$

$\delta\epsilon_i$: chosen randomly from the interval $[-W/2, W/2]$ (uncorrelated)
$\epsilon_0 = eV_g$ constant energy offset (here: $V_g = 0$)
Conductance for various strengths of disorder W:



(4,4)-CNT, $L \approx 100$nm

Similar results have been obtained before by Anantram and Govindan [5]

Spin Transport

Julliere's model [6] gives a *Stoner shift* ΔE of the band-structure for the different spin-channels, depending on the magnetization of the leads.
Two configurations of magnetization:

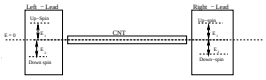
parallel (p) or *anti-parallel* (ap)

In each case two transport channels:

spin-up ($\uparrow$) and *spin-down* ($\downarrow$)

Measured conductance:

$$G^{\text{total}} = G^\uparrow + G^\downarrow \qquad (5)$$



Parallel magnetization:

$$\Delta E_{\text{L}}^\uparrow = \Delta E_{\text{R}}^\uparrow = +|\Delta E| \Rightarrow G_{\text{p}}^\uparrow = G^{++}$$
$$\Delta E_{\text{L}}^\downarrow = \Delta E_{\text{R}}^\downarrow = -|\Delta E| \Rightarrow G_{\text{p}}^\downarrow = G^{--}$$

$$G^{\text{p}} = G_{\text{p}}^\uparrow + G_{\text{p}}^\downarrow = G^{++} + G^{--}$$

Anti-parallel magnetization:

$$\Delta E_{\text{L}}^\uparrow = +|\Delta E|\,; \Delta E_{\text{R}}^\uparrow = -|\Delta E| \Rightarrow G_{\text{ap}}^\uparrow = G^{+-}$$
$$\Delta E_{\text{L}}^\downarrow = -|\Delta E|\,; \Delta E_{\text{R}}^\downarrow = +|\Delta E| \Rightarrow G_{\text{ap}}^\downarrow = G^{-+}$$

(symmetric system $\Rightarrow G^{+-} = G^{-+}$)

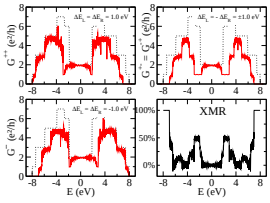
$$G^{\text{ap}} = G_{\text{ap}}^\uparrow + G_{\text{ap}}^\downarrow = G^{+-} + G^{-+}$$

XMR: coherent magnetoresistance
normalized ratio between the two values, measuring the signal strength:

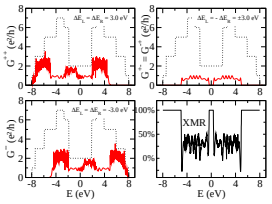
$$\text{XMR} = \frac{G^{\text{p}} - G^{\text{ap}}}{G^{\text{p}} + G^{\text{ap}}}$$

Spin transport in embedded leads

Two semi-infinite, magnetically inert CNTs embedded into ferromagnetic material like cobalt.
We only consider what effect the ferromagnetic nature of the contacting material has on the tube itself.
Assumption: Stoner shift is carried over the the embedded CNT.
Weak coupling between metal and carbon $\Rightarrow$ CNT itself can be considered as lead.
Results for different values of ΔE:



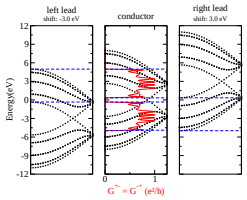
(4,4)-CNT, $L \approx 100$ nm, $W = 0$ eV, $\Delta E = \pm 1.0$ eV



(4,4)-CNT, $L \approx 100$ nm, $W = 0$ eV, $\Delta E = \pm 3.0$ eV

Band Analysis

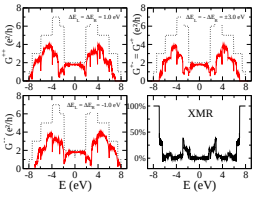
Band structure shifted differently (by the same amount) in various tube sections:



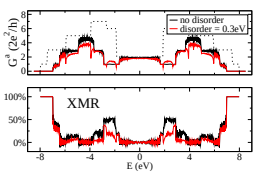
The band mismatch between the regions causes blocking of transport. (No transport between bands of different angular momentum.)

Disorder assisted transport

Anderson disorder reduces symmetry $\Rightarrow$ Scattering between states of different angular momentum becomes possible.

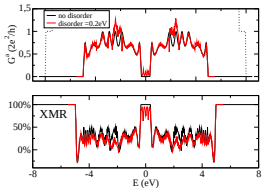


(4,4)-CNT, $L \approx 100$ nm, $W = 0.3$ eV, $\Delta E = \pm 1.0$ eV



(4,4)-CNT, $L \approx 100$ nm, $\Delta E = \pm 3.0$ eV

For stronger energy splits, the gap of the clean system is bridged. (XMR-value is reduced)

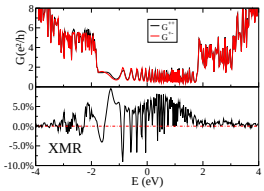


(4,4)-CNT, $L \approx 100$ nm, $\Delta E = \pm 3.0$ eV

Spin transport in fcc-surface leads

Alternative approach for leads, fcc surfaces contacting a CNT on both ends (surfaces not shown figure).

Different hopping parameters in the electrodes (metal-metal) and in the contact (metal-carbon)



(6,6)-CNT, $L \approx 200$ nm, $W = 0$ eV, $\Delta E = \pm 1.0$ eV

$\Rightarrow$ contacts do matter! Further investigation needed.

Conclusions

- Disorder decreases the transmission with more pronounced effects at the van Hove singularities.
- Disorder can enhance transmission and even bridge band-gaps.
- For fcc leads the Julliere's model may gives highly fluctuating XMR. The effect of disorder can be evaluated.

References

[1] M. Gheorghe *et al.*, `cond-mat/0411192`, Poster `TT8.2`.

[2] R. Egger and A. O. Gogolin, Phys. Rev. Lett. **87**, (2001).

[3] D. S. Fisher and P. A. Lee, Phys Rev. B **23**, 6851 (1981).

[4] M. P. L. Sancho, J. M. L. Sancho, and J. Rubio, J. Phys. F: Metal Physics **14**, 1205 (1984).

[5] M. P. Anantram and T. R. Govindan, Phys. Rev. B **58**, 4882 (1998).

[6] M. Julliere, Phys. Lett. A **54**, 225 (1975).