REVISITING CHARGE TRANSPORT AT THE MESOSCOPIC SCALE : *EMERGING QUANTUM PHENOMENA IN THE LIGHT OF ADVANCED COMPUTATIONAL APPROACHES*

Stephan Roche
Commissariat à l'Energie Atomique
MINATEC, CEA-DSM/DRFMC/SPSMS Grenoble
http://www-drfmc.cea.fr/Pisp/22/stephan.roche.html
stephan.roche@cea.fr

In this contribution, we theoretically investigate in-depth the quantum transport properties of two fundamental quasi-1D objects of modern nanoscience and nanotechnologies, namely the carbon nanotubes [1] and the Silicon-based semiconducting nanowires.

In the first part, quantum transport phenomena in chemically doped carbon nanotubes is presented [2], exploring for the first time the transition from weak to strong localization regime at a quantitative level, for a realistic modeling of low dimensional systems. The extraction of transport length scales such as elastic mean free path and localization lengths are efficiently achieved by a computational strategy based on both the Kubo and the Landauer-Buttiker transport formalisms. The fundamental Thouless relationship between both quantities is shown to be well reproduced. Differently, the analysis of surface roughness in semiconducting nanowires evidences the limitations of conventional semi-classical 'effective mass"-based transport approaches [3]. The charge mobility of rough silicon nanowires are quantitatively evaluated, while the limitations of the Thouless relationship are discussed.

The second part of the talk focuses on the effects of electron-(optic) phonon interaction on transport through metallic carbon nanotubes. By using a full quantum description of the joined processes of tunneling and phonon-assisted transport, the interaction between electrons and optical phonons is shown to result in *nonequilibrium energy-gaps* opening at half the phonon energy above (below) the charge neutrality point, owing to phonon emission (absorption) [4].

As a result, an onset of current saturation develops as soon as incoming electrons in the nanotubes gain sufficient kinetic energy to explore the electron-phonon Fock space. This novel inelastic backscattering mechanism yields a novel explanation of the high-bias current saturation, beyond typical semiclassical arguments based on the application of the Fermi golden rule approximation. In the case of semiconducting nanotubes, similar inelastic backscattering phenomena take place, but become strongly diameter-dependent [4].

[1] J.C. Charlier, X. Blase and S. Roche**, Rev. Mod. Phys. 79**, 677 (2007)
[2] R. Avriller, S. Latil, F. Triozon, X. Blase, S. Roche, **Phys. Rev. B 74**, 121406**R** (2006)
Ch. Adessi, S. Roche, X. Blase, **Phys. Rev. B 73**, 125414 (2006).
[3] A. Lherbier, M. Person, F. Triozon, Y.M. Niquet, S. Roche, (submitted)
[4] L. E. F. Foa Torres and S. Roche, **Phys. Rev. Lett. 97**, 076804 (2006)
L. E. F. Foa Torres and S. Roche, **Phys. Rev. B. 75**, 153402 (2007).
S. Roche et al, **J. Phys. Condens. Matter 19**, 183203 (2007).