Electron transport in large systems including fluctuating environment and many body effects

Stefano Sanvito

School of Physics and CRANN, Trinity College, Dublin 2, Ireland

The non-equilibrium Green's function (NEGF) method combined with density functional theory (DFT) is at present the workhorse algorithm for investigating electron transport in complex systems. In general the realism of these calculations depend heavily on our ability to deal with three fundamental issues: 1) the systems to investigate are typically large (in excess of 10,000 atoms); 2) the electrostatic potential may be determined by a dynamical environment (for instance a solvent); 3) many body effects may dominate the electrical response.

In this contribution I will present the development of a large scale electronic transport code based on NEGF+DFT and its application to systems containing a large number of atoms and possibly including inelastic effects of various origin. The code builds on SMEAGOL [1] and consists of three main elements: i) a parallel and threaded library to calculate the Green's function of the system based on the recursive Green's function method combined with an efficient and accurate calculation of the electrodes' self-energies [2], ii) an adaptive mesh algorithm to integrate the non-equilibrium Green's function to give the charge density, and iii) a many body expansion for incorporating non-elastic effects.

Then I will present three rather different examples of how the method works. First I will consider electron transport in nanostructures constructed on the Si (100) surface and show that our scheme is ideal to explain non-local STM experiments. Then I will briefly discuss how electron transport in large bio-molecules such as DNA [3] can be tackled and finally I will consider the competition between spin-flip inelastic electron tunneling spectroscopy and the Kondo effect in single magnetic atoms on insulating surfaces [4].

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[3] C. D. Pemmaraju, I. Rungger, X. Chen, A. R. Rocha and S. Sanvito, Phys. Rev. B 82, 125426 (2010)

[4] A. Hurley, N. Baadji and S. Sanvito, arXiv:1103.2652 (2011)