

Scientific Report “Short Visit Grant”

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Purpose of the visit: In a recent paper [Phys. Rev. Lett. **111**, 030601 (2013)] Prof. Stefan Kurth and myself showed that the exact conductance of molecular junctions in the Coulomb blockade regime is orders of magnitude smaller than the corresponding Kohn-Sham conductance of Density Functional Theory (DFT), and proposed a simple and implementable formula to correct the latter. During the visit we extended this work to molecular junctions with degenerate orbital states. In particular we investigated a paradigmatic situation where some of the degenerate orbitals are only weakly coupled to the leads. In this case anomalies in the conductance are expected due to a multi-orbital Kondo effect.

Description of the work carried out during the visit: In the first part of the visit we generalize the previously published formula of the conductance to molecular junctions with degenerate orbital states. Then we focussed on the simplest non-trivial case (degeneracy two) and calculated the spectral function by modelling the leads as finite size clusters and performing exact-diagonalization calculations. The spectral function was used to extract the exact conductance (used for benchmarks) and an accurate exchange-correlation potential for DFT calculations.

Description of main results obtained: The main result is that degenerate orbitals with different coupling to the leads are shifted by the Kohn-Sham potential in a substantially different way when the gate voltage is varied. Nevertheless for the calculation of the conductance only the variation of the local exchange-correlation potential with respect to the total number of electrons is needed. Thus our formula seems to be general and applicable to more complicated molecular junctions like those with orbital degeneracy.

Future collaboration with the host institution: We believe that the progress we made during this week holds promise for another important result in the TDDFT approach to quantum transport. It is therefore our intention to continue the collaboration possibly with other short visits.

Projected publications: As a result of the visit a clear scenario for the drawing up of a paper emerged. We still need to complete the numerical analysis of the outcomes but the main obstacles (generalization of the conductance formula and derivation of an accurate exchange-correlation potential) have been overtaken. After this analysis we will submit at least one paper in an international peer reviewed journal.