Report on a Short Collaborative Visit of S. Kurth (San Sebastian) to G. Stefanucci (Rome) October 20-27, 2012

In recent work (Phys.Rev. Lett. **107**, 216401 (2012)), Dr. Stefanucci and myself showed that, at zero temperature, the Kondo plateau in the conductance of the Anderson impurity model can be obtained correctly within density functional theory (DFT) combined with Landauer theory if an exchange-correlation (xc) potential with a rapid (almost discontinuous) density dependence is used. We also showed that at finite temperature, the DFT+Landauer approach is not sufficient in order to obtain the correct suppression of the Kondo plateau and the appearance of Coulomb blockade peaks. If the problem is formulated in the framework of time-dependent DFT (TDDFT), the Landauer formula has to be modified due to the presence of dynamical xc effects and the correction can be expressed in terms of the xc kernel of TDDFT.

During this visit we were investigating how to correctly describe these dynamical xc corrections by studying simple model systems. One focus of discussion was on the nonlocality of both the xc potential and the xc kernel. In particular, we are interested in the case when a non-interacting and an interacting subsystem are brought into contact. Here the non-locality manifests itself as a non-vanishing xc potential in the non-interacting subsystem. At the same time, the discontinuous behavior of the xc potential of the interacting subsystem is smoothened due to the presence of the contact. Numerical calculations indicate that there is a connection between the xc kernel in the non-interacting region and the change of the xc potential in the interacting region. However, this observation still has to be confirmed by more detailed investigations.

While at present our studies are concerned with model systems, we expect our findings to be relevant also for a more realistic description of transport through nanoscale systems. We also feel that the discussions we had during this visit were extermely useful. They gave a fresh boost to our collaboration which we certainly will continue in the future.