Report on a Short Collaborative Visit of S. Kurth (San Sebastian) to G. Stefanucci (Rome) October 12-19, 2013

During this visit, Dr. Stefanucci and myself continued our long-standing collaboration on the description of electron transport using time-dependent density functional theory. Our focus is on the dynamical exchange-correlation corrections to the conductance obtained with the Landauer formalism. In recent work (Phys.Rev. Lett. **111**, 030601 (2013)) we have demonstrated the importance of these corrections to correctly describe the Coulomb blockade peaks in the zero-bias conductance of weakly coupled molecules/quantum dots at temperatures above the Kondo temperature.

During the visit we were aiming to construct improved approximations to the exchange-correlation potential for multi-level systems weakly coupled to leads. We describe these multi-level systems in the constant-interaction model. For the isolated multi-level system at finite temperature we were able to recast the equations in a form such that the exact Green function (and thus the level occupations) can be obtained by solving a linear system. One technical problem we encountered with this approach is that at low temperatures this linear system becomes numerically ill-conditioned. On the other hand, the solution is trivial at zero temperature. Since our approach yields the Green function (or, alternatively, the spectral function), one can model in a straightforward manner the broadening of the spectral peaks when coupling the system to leads. This coupling alleviates the problem of the ill-conditioned linear system. Unfortunately, however, it can for certain parameter ranges lead to total occupations on the multi-level dot which are not monotonously dependent on an external gate potential. We have traced this clearly unphysical behaviour to the incorrect asymptotic form of certain integrals originating from our simple way to model the level broadening. In an improved model of this broadening the correct asymptotics needs to be incorporated.

During this visit we have encountered some unexpected, mostly technical/numerical problems which still need to be fully resolved. However, we also have made significant progress in understanding the exact solution of our multi-level model which will lead to better approximations to the exchange-correlation potential needed to calculate the dynamical corrections to transport. Like on previous occasions, this visit also strengthened our collaboration which will be maintained in the future.