**Research Networking Programmes**

## Short Visit Grant ☒ or Exchange Visit Grant ☐

*(please tick the relevant box)*

## Scientific Report

**The scientific report (WORD or PDF file – maximum of eight A4 pages) should be submitted online within one month of the event. It will be published on the ESF website.**

***Proposal Title***: Dynamical exchange-correlation corrections to Kohn-Sham conductances

***Application Reference N°:*** 6950

### 1) Purpose of the visit

The purpose of my visit to Dr. Stefanucci was to continue our long-standing collaboration and investigate dynamical exchange-correlation (xc) effects in the description of electron transport within the frame-work of density functional theory (DFT). We feel that we made important progress in the description of these corrections in the *finite-bias* regime.

### 2) Description of the work carried out during the visit

On the formal level, we were able to set up a DFT framwork for steady-state transport at finite bias. In a Kohn-Sham description this gives rise to two xc potentials, the xc gate potential and the xc bias. These quantities are needed to recover the total number of electrons in the central region in the steady state as well as the steady state current of an interacting system in terms of an auxiliary non-interacting system. Formally they are also closely related to the corresponding xc potentials of time-dependent DFT. However, since in the present setup we are only interested in *steady-state* quantities, it is easier to find good approximations for these xc potentials.

**3) Description of the main results obtained**

Based on numerical studies of the single-impurity Anderson model we were able to construct accurate approximations for the xc gate and xc bias and we are now able to correctly reproduce both total density and total current of this model for any external gate and bias potential within our DFT framework (naturally including the Coulomb blockade diamonds in the differential conductance). We are now generalizing these xc potentials to systems with more than one level in the spirit of a similar, recently suggested, extension (Phys.Rev. Lett. **111**, 030601 (2013)) for the *zero-bias* conductance. Independently of the outcome of this multi-level extension, we feel that already now we have enough material to be presented in a nice publication which we just started to write.

**4) Future collaboration with host institution (if applicable)**

We certainly will continue our longstanding fruitful collaboration.

**5) Projected publications / articles resulting or to result from the grant *(ESF must be acknowledged in publications resulting from the grantee's work in relation with the grant)***

We already started writing one publication directly resulting from this visit. Further publications are possible since there are many possible ideas to explore which make use of the new results.

**6) Other comments (if any)**

We feel that compared with previous collaborative visits between the two of us, the present one was particularly successful and productive. Apart from the results we already have, we have been discussing many ideas and possible applications of our findings to time-dependent DFT in general, even in situations which have nothing to do with transport.Therefore we hope that the present visit in the future will lead to even more results than the ones we will present in the paper described above.