Scientific Report "Short Visit Grant"

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Purpose of the visit: Prof. Stefan Kurth and myself recently published a paper [Phys. Rev. Lett. **107**, 216401 (2011)] on the possibility of describing the conductance of the Anderson model in the Kondo regime using Time-Dependent (TD) Density Functional Theory (DFT). We showed that static DFT combined with the Landauer formula exactly reproduces the Kondo plateau at zero temperature provided that the exchange-correlation (xc) potential exhibits a derivative discontinuity. We further showed that at temperatures above the Kondo temperature the very same approach fails dramatically and we traced back the problem to the absence of dynamical xc corrections. The purpose of the visit was to understand how to estimate these corrections so as to suppress the Kondo peak without suppressing the Coulomb blockade side peaks. Even though the research is, at present, limited to rather simple model systems we believe that the qualitative features of the TDDFT xc potential are present also in more realistic situations and can help to shed some light on the current discrepancies between theory and experiments.

Description of the work carried out during the visit: In order to estimate the dynamical xc corrections we modeled the leads as finite size clusters and calculated the TDDFT and the exact density response function by exact diagonalization. These response functions are indeed the basic quantities according to the results derived in Phys. Rev. Lett. **107**, 216401 (2011). We wrote a code to solve finite size Anderson models. We then inserted the xc correction into the exact TDDFT formula and study the dependence on temperature, coupling to the leads, Coulomb repulsion U and on site energy at the impurity. The results revealed a strong connection between the TDDFT kernel with space arguments on the leads and the TDDFT kernel with arguments on the impurity. We spend the rest of the time in trying to justify this finding and got some preliminary results. The basic ideas developed during the visit need, however, to be further studied and checked.

Description of main results obtained: The main remarkable result is that the dynamical xc corrections calculated as described above do indeed suppress the Kondo peak. At present this is only a numerical evidence but we have elaborated preliminary explanations on how to justify this result in general. The interesting thing of our results is that they can be cast into a formula that seems to be independent of the underlying physical system, and hence is universal. More work is needed to check the correctness of this universality.

Future collaboration with the host institution: We believe that the progress we made during this week holds promise for an 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: Before the end of the visit we made a list of things to do. This list involves both theoretical and numerical analysis. We are confident that after the analysis we will have enough publishable material to submit at least one paper in an international peer reviewed journal.