GOETHE UNIVERSITÄT FRANKFURT AM MAIN

Fachbereich Physik
Institut für Theoretische Physik

CONDENSED MATTER THEORY SEMINAR

Subject: **Non-equilibrium real-space DMFT for correlated heterostructures with long-range Coulomb interaction**

Speaker: **Dr. Irakli Titvinidze (Universität Graz)**

Date & time: **Thursday, May 3rd, 2018 at 2 p.m.**

Venue: **Seminar room 1.101**

We consider a system consisting of several correlated monoatomic layers sandwiched between two metallic leads. In addition to the local Hubbard interaction we also take the long-range Coulomb interaction into account, which causes electronic charge reconstruction in the correlated layers, as well as in the leads. The non-equilibrium situation is driven by applying a bias-voltage to the leads. We investigate the steady-state behavior of the system for different parameters (bias voltage, interaction strength, hybridization strength between leads and the correlated heterostructure).

In particular, we present results for the steady-state current, spectral functions, and electronic charge reconstruction. Depending on the particular parameters we either observe a capacitor-like behavior or one dominated by charge transport. Furthermore, the Hubbard interaction has significant effect on the charge reconstruction.
In order to investigate steady-state properties we use real-space Dynamical mean-field theory (R-DMFT)[1, 2, 3, 4] combined with the Poisson equation, both solved in a self-consistent fashion. To account for the charge reconstruction in the leads we include some lead layers explicitly in R-DMFT in addition to the correlated layers. As impurity solver for R-DMFT we use the recently developed auxiliary master equation approach (AMEA), which addresses the DMFT impurity problem within an auxiliary system consisting of a correlated impurity, a small number of uncorrelated bath sites and two Markovian environments described by a generalized Master equation.[3, 5, 6, 7]

References

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[4] M. Snoek, I. Titvinidze, C. Toke, K. Byczuk, W. Hofstetter, New J. Phys. 10, 093008 (2008).
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