Abstract submitted to the
RESEARCH WORKSHOP ON SPIN, CHARGE, AND ENERGY CURRENTS IN NOVEL MATERIALS
October 1 - 7, 2017 Hvar, Croatia

Non-equilibrium inhomogeneous DMFT for correlated heterostuctures

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Submitted : August 4, 2017

Keywords : strong correlations, DMFT, non-equilibrium steady state, Hetterostucture

Here we present our results for the system consisting of correlated monoatomic layers, sandwiched between two metallic leads. In addition to the local Hubbard interaction we also take into account long-range Coulomb interaction, which causes electronic charge reconstruction not only in the correlated layers, but also in the leads. We investigate the steady-state behavior of the system, which is driven by applying a bias-voltage to the leads.

In particular we present results for the steady-state current, spectral functions, and electronic charge reconstruction. We investigate them for different set of parameters (bias voltage, interaction strength, hybridization between leads and correlated heterostructure). Depending on the parameter set we obtain the Coulomb blockade.

In order to investigate steady-state properties we use Non-equilibrium inhomogeneous (real-space) dynamical mean-field theory (R-DMFT) [1, 2] combined with the Poisson equation. Using Poisson equation we determine onsite energies, while R-DMFT is used to find many body solution. Problem has to be solved self-consistently. To take into account charge reconstruction in the leads we take some lead layers explicitly in addition to the correlated layers. Number of the leads layers has to be chosen such that electron number density, far from the correlated region has to converge to the bulk filling of the leads. As an impurity solver for R-DMFT we use recently developed auxiliary master equation approach, 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, 4, 5, 6].

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