

Non-equilibrium transport of two sites anderson impurity model with vertex corrections

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Non-equilibrium Green's Function (NEGF) method at the first principles level has been a powerful tool to examine electron dynamics under external potentials such as electric or magnetic fields¹. However, despite of its success, NEGF based on Density Functional Theory (DFT) is limited by the presence of transition metals or heavy elements because of degenerate strong Coulomb interactions. Here, we introduce a model study of coupled two sites Anderson impurity model including vertex correction (or crossing term) in Non-Crossing Approximation (NCA) impurity solver using auxiliary particle approach². To evaluate the real time green's functions and the steady state observables, we used Keldysh formalism and Landauer-Buttiker formula. We expect that the implementation of the impurity solver with the finite Coulomb interactions U and with the cluster expansion in NEGF-DFT methods can deal with many realistic systems³.

Keywords - Non-equilibrium Green's Function, Non-Crossing Approximation, Keldysh formalism, strong Coulomb interactions

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