The theory of nonequilibrium Anderson impurity model for strongly correlated electron systems

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The nonequilibrium theory of strongly correlated systems is proposed theory which is grounded on the generalized Wick theorem. This theorem is employed for calculation of the thermal averages of the contour arranged products of electron operators by generalizing Keldysh formalism. Perturbation expansion is realized for Anderson impurity model in which we consider the Coulomb interaction of the impurity electrons as a main parameter of the model and the mixing interaction between impurity and conduction electrons as a perturbation. The first two approximations are used and is obtained the value of the current between one of the leads and central region of interacting electrons. The contribution of the strong correlations and of irreducible diagrams is analyzed.

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1. Introduction

We start with single Anderson impurity model connected to two leads named left (L) and right (R) with Hamiltonian

$$H = H^0 + H_i, \tag{1}$$

$$H^{0} = \sum_{\lambda = L,R} \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}\lambda} C^{+}_{\mathbf{k}\lambda\sigma} C_{\mathbf{k}\lambda\sigma} + \sum_{\sigma} \epsilon_{d} n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow}, \quad (2)$$

$$H_{i} = \sum_{\lambda = L, R} \sum_{\mathbf{k}\sigma} (V_{\mathbf{k}\lambda} d_{\sigma}^{+} C_{\mathbf{k}\lambda\sigma} + V_{\mathbf{k}\lambda}^{*} C_{\mathbf{k}\lambda\sigma}^{+} d_{\sigma}), \qquad (3)$$

where d_{σ} and $C_{\mathbf{k}\lambda\sigma}$ are the annihilation operators of the dot and leads electrons, correspondingly, with spin σ , $\epsilon_{\mathbf{k}\lambda}$ is the leads electron energy eigenvalues, ϵ_d is the dot's electron on site energy, U is the Coulomb repulsion, $V_{\mathbf{k}\lambda}$ is the mixing matrix elements which describe the couplings between dot and leads, $n_{\sigma} = d_{\sigma}^+ d_{\sigma}$.

We shall use the operators $b_{\lambda\sigma}$ of the localized mode of leads conduction electrons

$$b_{\lambda\sigma} = \sum_{\mathbf{k}} V_{\mathbf{k}\lambda} C_{\mathbf{k}\lambda\sigma} \tag{4}$$

and investigate the influence of the localized electrons of impurity on this collective mode of conduction electrons.

The chemical potentials of both leads are supposed to be different and system is in nonequilibrium state. Therefore we employ the Keldysh [1–3] formalism based on the contour of the time evolution of the Fig. 1 and four local Green's functions for every of both subsystems of electrons:

$$G_{\sigma\sigma'}^{--}(t,t') = -i \left\langle Td_{\sigma}(t)d_{\sigma'}^{+}(t') \right\rangle,$$

$$G_{\sigma\sigma'}^{-+}(t,t') = i \left\langle d_{\sigma'}^{+}(t')d_{\sigma}(t) \right\rangle,$$

$$G_{\sigma\sigma'}^{+-}(t,t') = -i \left\langle d_{\sigma}(t)d_{\sigma'}^{+}(t') \right\rangle,$$

$$G_{\sigma\sigma'}^{++}(t,t') = -i \left\langle \tilde{T}d_{\sigma}(t)d_{\sigma'}^{+}(t') \right\rangle,$$
(5)

and



Fig. 1. The Keldysh contour of the time evolution.