KELDYSH DIAGRAM TECHNIQUE FOR STRONGLY CORRELATED SYSTEMS

Leonid DOHOTARU

Technical University of Moldova

***Abstract**: The non - equilibrium 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 for 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.*

***Key words:** Keldysh diagram technique, non-equilibrium state, Green's function, Anderson impurity model.*

We develop a new diagram technique for investigating the non - equilibrium state of strongly correlated electrons systems.

We construct the perturbation theory for Anderson impurity model with the strong electronic correlations of d electrons of the impurity ion taken into account. This theory is based on the Generalized Wick Theorem (GWT) which permits to calculate the thermodynamic averages of the product of contour arranged of electron operators by generalizing the Keldysh diagram technique [1]. The main parameter of theory is considered the Coulomb interaction between impurity electrons and as a perturbation the mixing interaction between impurity and conduction electrons.

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

$$H = H_0 + H_i, H_0 = \sum_{\lambda=L,R}\sum_{\vec{k}\sigma}\varepsilon_{\vec{k}\lambda}C^+_{\vec{k}\lambda\sigma}C_{\vec{k}\lambda\sigma} + \sum_{\sigma}\varepsilon_d n_{d\sigma} + Un_{d\uparrow}n_{d\downarrow}, H_i = \sum_{\lambda=L,R}\sum_{\vec{k}\sigma}(V_{\vec{k}\lambda}d^+_\sigma C_{\vec{k}\lambda\sigma} + V^*_{\vec{k}\lambda}C^+_{\vec{k}\lambda\sigma}d_\sigma),$$

where d_σ and $C_{\vec{k}\lambda\sigma}$ annihilation operators of the dot and leads electrons correspondingly, with spin σ, $\varepsilon_{\vec{k}\lambda}$ is leads electron energy eigenvalues and ε_d is dot's electron on-site energy, U is the Coulomb repulsion,

$$V_{\vec{k}\lambda}$$

is the mixing matrix elements which describe the coupling 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 $b_{\lambda\sigma} = \sum_{\vec{k}} V_{\vec{k}\lambda}C_{\vec{k}\lambda\sigma}$

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 the system is in non-equilibrium state. Therefore we employ the Keldysh formalism [1-2] based on the contour (Fig. 1).

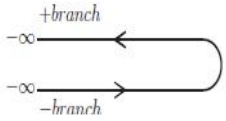

Fig.1. The Keldysh contour of the time evolution.

of the time evolution and the systems of four Green's functions for the both subsystem of localized and free electrons with operator d_σ, d^+_σ and $C_{\vec{k}\sigma}, C^+_{\vec{k}\sigma}$ correspondingly.

We use the time-ordering and anti-time ordering of the Heisenberg operators. For leads conduction electrons we use the localized mode and investigate the influence of the localized electrons of this collective mode $b_{\lambda\sigma} = \sum_{\vec{k}} V_{\vec{k}\lambda}C_{\vec{k}\lambda\sigma}$ on conduction electrons. The system of four Green's function of the lead's electrons has, in the notification of [2], the form

$$g^{--}_{\lambda\lambda'}(t,t') = -i\left\langle Tb_\lambda(t)\,\mathrm{b}^+_{\lambda'}(t')\right\rangle, \mathrm{g}^{-+}_{\lambda\lambda'}(t,t') = i\left\langle \mathrm{b}^+_{\lambda'}(t')b_\lambda(t)\right\rangle,$$
$$g^{+-}_{\lambda\lambda'}(t,t') = -i\left\langle b_\lambda(t)\,\mathrm{b}^+_{\lambda'}(t')\right\rangle, \mathrm{g}^{++}_{\lambda\lambda'}(t,t') = -i\left\langle \tilde{T}b_\lambda(t)\,\mathrm{b}^+_{\lambda'}(t')\right\rangle.$$

Here T and $\tilde{T}$ denote the time and anti-time ordering. The analogous definitions exist for the Green's function of he localized electrons marked in as $G^{--}_{\sigma\sigma'}$ and so on.

In Keldysh formalism we use the matrix Green's functions composed from different elements of the evolution in contour space. We have the matrices

$$\hat{g}_0 = \begin{pmatrix} g_0^{--} & g_0^{-+} \\ g_0^{+-} & g_0^{++} \end{pmatrix}, \hat{\Lambda} = \begin{pmatrix} \Lambda^{--} & \Lambda^{-+} \\ \Lambda^{+-} & \Lambda^{++} \end{pmatrix},$$

and also such one for the full propagator G. Here Λ is correlation function and g_0 is bare propagator of free itinerant electrons.

Dyson-type equation for non-equilibrium strong correlated electron systems has the form

$\hat{G} = \hat{\Lambda} + \hat{\Lambda}\hat{g}_0\hat{G}.$

We formulated the non-equilibrium perturbation theory supposing that the time evolution is realized along the real-time contour, which starts and ends at $t = -\infty$.

The thermal average at $t = 0$ can be obtained in the form

$$\left\langle A(t,t')\right\rangle = \left\langle \hat{S}^{-1}T\tilde{A}(t,t')\hat{S}\right\rangle, \hat{S} = S(-\infty,\infty) = T\exp(-i\int_{-\infty}^{\infty}\tilde{H}_i(t)dt), \hat{S}^{-1} = \hat{S}^+ = \tilde{T}\exp(i\int_{-\infty}^{\infty}\tilde{H}_i(t)dt), (1)$$

where operators with tilde $\tilde{H}_i$ are in interaction representation.

In the next we shall use two forms of operator A

$$A_1(t,t') = ib^+_{\lambda\sigma}(t'^+)d_\sigma(t^-), A_2(t,t') = id^+_\sigma(t'^+)\,\mathrm{b}_{\lambda\sigma}(t^-)$$

and determine the Green's functions

$$\mathrm{G}^{-+}_{\sigma\lambda\sigma'}(t,t') = i\left\langle b^+_{\lambda\sigma'}(t'^+)d_\sigma(t^-)\right\rangle, \mathrm{G}^{-+}_{\lambda\sigma\sigma'}(t,t') = i\left\langle d^+_{\sigma'}(t'^+)\,\mathrm{b}_{\lambda\sigma}(t^-)\right\rangle.$$

The expansion of the exponents in the Eq.(1) is the realization of the perturbation theory.

In the Fig.2 is presented the two contributions of the values $A_1^{(1)}$ and $A_2^{(1)}$ in the first order of perturbation theory

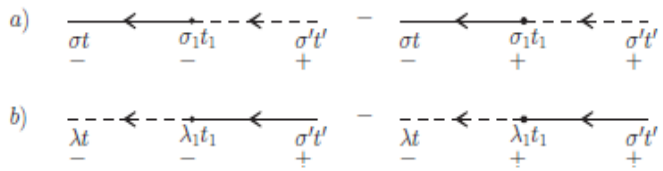

Fig. 2. Diagrams of the first order of perturbation theory. a) for $A_1^{(1)}$ and b) for $A_2^{(1)}$.

Thin solid line is G propagator and dashed line is g propagator.

The analytical expressions for these quantities is the following

$$A_1^{(1)}(t,t') = \int_{-\infty}^{\infty} dt_1 \sum_{\lambda_1\sigma_1}[\mathrm{G}^{--}_{\sigma\sigma_1}(t,t_1)\,\mathrm{g}^{-+}_{\lambda_1\sigma_1\lambda\sigma}(t_1,t') - \mathrm{G}^{-+}_{\sigma\sigma_1}(t,t_1)\,\mathrm{g}^{++}_{\lambda_1\sigma_1\lambda\sigma}(t_1,t')],$$

$$A_2^{(1)}(t,t') = \int_{-\infty}^{\infty} dt_1 \sum_{\lambda_1\sigma_1}[\mathrm{g}^{--}_{\lambda\sigma\lambda_1\sigma_1}(t,t_1)\,\mathrm{G}^{-+}_{\sigma_1\sigma}(t_1,t') - \mathrm{g}^{-+}_{\lambda\sigma\lambda_1\sigma_1}(t,t_1)\,\mathrm{G}^{++}_{\sigma_1\sigma}(t,t')].$$

New elements of diagrammatic theory of our strongly correlated systems are the irreducible Green's functions or Kubo cumulants, which appear in the high order of perturbation theory.

References

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