DIAGRAMMATIC APPROACH FOR THE TWOFOLD DEGENERATE ANDERSON IMPURITY MODEL

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Abstract

The twofold degenerate Anderson impurity model [1–4] is investigated in normal and superconducting states, and the strong electronic correlations of d-electrons of impurity ion are taken into account by elaborating a suitable diagram technique. We discuss the properties of the Slater–Kanamori model [2–4] of d-impurity electrons. After finding the eigenfunctions and eigenvalues of all 16 local states, we determine the local one-particle propagator. Then we construct the perturbation theory around the atomic limit of the impurity ion and obtain the Dyson type equations between impurity electron propagators and normal and anomalous correlation functions. By summing infinite series of ladder diagrams, the approximation for correlation functions is established. The criterion for appearance of a superconducting state of the model is discussed.

1. Introduction

The theory of strongly correlated electron systems plays a central role in contemporary condensed matter physics. The essence of the problem is the competition between the localization tendency originated by the Coulomb repulsion of *d* electrons and itinerancy tendency arising from the hybridization of electron orbitals.

The orbital degeneracy can be completely eliminated in solid substances, but in many of them, for example, new superconductors based on *Fe* and AnC_{60} materials, orbital degeneracy is not completely eliminated and orbital effects are important.

Many materials with open *d*- or *f*- shells exhibit metal-insulator transitions of Mott–Hubbard type due to strong electron–electron correlations.

Major progress in understanding the physics of the Mott–Hubbard metal–insulator transition has been achieved in the last decade through the development of the dynamical mean-field theory (DMFT) [5]. In the last-mentioned paper, the study of Mott-Hubbard transition is realized within the DMFT at $T = 0$ using Wilson's Numerical Renormalization Group.

The role of the Hund's rule coupling I_H has been investigated in models of magnetic impurities and quantum dots [6]. This has lead to different predictions for the behavior of the Kondo temperature in these systems as a function of I_H. This issue is investigated by applying a combination of numerical renormalization group (NRG) and renormalized perturbation theory (RPT) to some of different models.

In [7, 8] the phase diagram of the Anderson impurity model (AIM) has been studied by employing the Wilson's NRG method. It has been shown that the physical behavior in the vicinity of the nontrivial fixed point of the AIM resembles that of the two-impurity Kondo model. This fixed point is reached in the immediate vicinity of the metal-to-insulator transition upon variation of the Hund parameter.

It is well known that orbital degeneracy plays an essential role in the Mott metal–insulator transition. In the present work, we study the role of Hund rule coupling in the orbital degenerate model using a diagrammatic approach and taking into account the intra-atomic Coulomb interactions of two electrons with opposite spins occupying the same or different orbitals on equal footing with the intra-atomic exchange.

The investigation is based on the diagram theory for strongly correlated electron systems we have earlier developed for the non-degenerated [9–17] and twofold degenerate [18] models.

Our approximation includes only local self-energy terms. It is well known that such approximation is well justified for a large coordination number. The nonlocal [19] terms neglected here correspond to higher order approximation in inverse coordination number.

The paper has the following structure. In Section 1 we describe the twofold degenerate Anderson impurity model. The local properties of the model are considered in Section 2. The perturbation theory around the atomic limit of impurity ion is formulated in Section 3. In this section, we discuss the process of delocalization and renormalization of the dynamical quantities. In Section 4 the simplest irreducible Green's function is calculated. In Section 5 the analysis of the main equations is discussed. In Section 6 the main equations for the superconducting state are formulated and necessary approximations are elaborated. The correlation functions Y, $\overline{Y}$ is determined in both cases when triplet or singlet superconductivity is realized. In Section 7 the conditions that determine the critical temperature are analyzed, and the last Section 8 contains the conclusions.

The Hamiltonian of the two-fold degenerate AIM includes two components: conduction electrons and strongly correlated localized electrons on one side and the term describing their hybridization on the other side [1–4]:

$$H = H^0 + H_{\text{int}}, \tag{1}$$

$$H^0 = H_c^0 + H_d^L, \tag{2}$$

$$H_c^0 = \sum_{\vec{k}l\sigma} \varepsilon_l(\vec{k}) C_{\vec{k}l\sigma}^+ C_{\vec{k}l\sigma}, \tag{3}$$

$$\begin{aligned} H_d^L = {} & \sum_{l,\sigma} \varepsilon^d d_{l\sigma}^+ d_{l\sigma} + U \sum_l n_{l\uparrow} n_{l\downarrow} + U' n_1 n_2 + I_H \sum_{\sigma\sigma'} d_{1\sigma}^+ d_{2\sigma}^+ d_{1\sigma'} d_{2\sigma'} \\ & + I'_H (d_{1\uparrow}^+ d_{1\downarrow}^+ d_{2\downarrow} d_{2\uparrow} + H.C.), \end{aligned} \tag{4}$$

$$H_{int} = \frac{1}{\sqrt{N}} \sum_{\vec{k}l\sigma} (V_{\vec{k}l} d_{l\sigma}^+ C_{\vec{k}l\sigma} + V_{\vec{k}l}^* C_{\vec{k}l\sigma}^+ d_{l\sigma}), \tag{5}$$

where the local Hamiltonian H_d^L is standard in the Slater–Kanamori [2–4] form, $C_{\vec{k}l\sigma}$ is the conduction electron annihilation operator with momentum $\vec{k}$, orbital number l = 1, 2 and spin $\sigma = \pm 1(\uparrow,\downarrow)$, $d_{l\sigma}$ operator for localized d electron. Conduction electron of l–*th* orbital state

hybridizes only with the local electron of the same orbital state, $n_{l\sigma} = d_{l\sigma}^{+} d_{l\sigma}$, $n_l = \sum_{\sigma} n_{l\sigma}$, $V_{\vec{k}l}$ is matrix element of hybridization. U is the Coulomb repulsion between the d-electrons in the same orbital state; U', between electrons in different orbital states. I_H is the Hund's rule coupling constant and pair hopping terms, $\varepsilon_l(\vec{k})$ is the band dispersion and ε^d is the impurity ion energy evaluated from the chemical potential μ. N is the number of lattice sites.

In the following, we assume that the symmetry of the system is such that there exists the relation [20]:

$$U' = U - 2I_H, \; I'_H = I_H. \tag{6}$$

The Coulomb interactions are far too large to be treated as perturbation and they must be included in H^0 - zero order Hamiltonian. The hybridization term (5) is considered as the perturbation of the system. In the following, the main ideas of the perturbation theory elaborated for non-degenerate strongly correlated systems are extended to the case of orbital degeneracy. This generalization has been discussed, e.g., for the twofold degenerate Hubbard model [14]. As is known, the new elements of this perturbation theory of strongly correlated systems are the irreducible correlation functions which contain all charge, spin, and pairing quantum fluctuations.

2. Local properties

In the main approximation of the Anderson model, one has free conduction and strongly interacting localized electrons described by the Hamiltonian H^0. The localized part of the Hamiltonian, H_0^L, can be diagonalized by using Hubbard transfer operators $\chi^{mn}=|m\rangle\langle n|$ where $|m\rangle$ is the eigenvector of operator H_d^L [9].

Because orbital quantum number takes two values l = 1, 2, the total number of local quantum states is 16.

There are the following eigenvectors of operator H_d^L. The first quantum state $|1\rangle$ is the vacuum state $|0\rangle$ with energy E_1=0. There are four one-particle states with spin $S = \frac{1}{2}$ and $S_z = \pm\frac{1}{2}$:

$|2>= d_{1\uparrow}^{+}|0\rangle$, $|3\rangle = d_{2\uparrow}^{+}|0\rangle$, $|4\rangle = d_{1\downarrow}^{+}|0\rangle$ and $|5\rangle = d_{2\downarrow}^{+}|0\rangle$. The energies of all these states are $E_2 = E_3 = E_4 = E_5 = \varepsilon_d$.

Then there are six states with two particles. Three of them are singlet states with spin S=0 and others 3 triplet states with S=1 and $S_z = -1,0,1$,

$$|6\rangle = \frac{1}{\sqrt{2}}\left(d_{1\uparrow}^{+} d_{1\downarrow}^{+} - d_{2\uparrow}^{+} d_{2\downarrow}^{+}\right)|0\rangle, \quad |7\rangle = \frac{1}{\sqrt{2}}\left(d_{1\uparrow}^{+} d_{1\downarrow}^{+} + d_{2\uparrow}^{+} d_{2\downarrow}^{+}\right)|0\rangle, \quad |8\rangle = \frac{1}{\sqrt{2}}\left(d_{1\uparrow}^{+} d_{2\downarrow}^{+} - d_{1\downarrow}^{+} d_{2\uparrow}^{+}\right)|0\rangle,$$

$$|9\rangle = d_{1\uparrow}^{+} d_{2\uparrow}^{+}|0\rangle, \; |10\rangle = \frac{1}{\sqrt{2}}\left(d_{1\uparrow}^{+} d_{2\downarrow}^{+} + d_{1\downarrow}^{+} d_{2\uparrow}^{+}\right)|0\rangle, \; |11\rangle = d_{1\downarrow}^{+} d_{2\downarrow}^{+}|0\rangle.$$

The eigenvalues of these quantum states are

$E_6 = 2\varepsilon_d + U - I'_H$, $E_7 = 2\varepsilon_d + U + I'_H$,

$E_8 = 2\varepsilon_d + U' + I_H$, $E_9 = E_{10} = E_{11} = 2\varepsilon_d + U' - I_H$.

Then there are four states composed from three particles

$|12\rangle = d_{1\uparrow}^+ d_{1\downarrow}^+ d_{2\uparrow}^+ |0\rangle$, $|13\rangle = d_{2\uparrow}^+ d_{2\downarrow}^+ d_{1\uparrow}^+ |0\rangle$,

$|14\rangle = d_{1\uparrow}^+ d_{1\downarrow}^+ d_{2\downarrow}^+ |0\rangle$, $|15\rangle = d_{2\uparrow}^+ d_{2\downarrow}^+ d_{1\downarrow}^+ |0\rangle$

with energy value $E_{12} = E_{13} = E_{14} = E_{15} = 3\varepsilon_d + U + 2U' - I_H$.

The last local state is singlet

$|16\rangle = d_{1\uparrow}^+ d_{1\downarrow}^+ d_{2\uparrow}^+ d_{2\downarrow}^+ |0\rangle$ with energy value $E_{16} = 4\varepsilon_d + 2U + 4U' - 2I_H$.

When equalities (6) take place we obtain more simple forms:

$E_6 = E_8 = 2\varepsilon_d + U - I_H$, $E_7 = 2\varepsilon_d + U + I_H$, $E_9 = 2\varepsilon_d + U - 3I_H$, $E_{12} = 3\varepsilon_d + 3U - 5I_H$, $E_{16} = 4\varepsilon_d + 6U - 10I_H$.

The triplet states $|9\rangle$, $|10\rangle$ and $|11\rangle$ are the lowest in energy.

Quantum states enumerated above permit us to organize Hubbard transfer operators χ^{mn} and establish the relation with fermions' impurity operators [14]:

$$\begin{aligned} d_{l\sigma}^+ = {} & \chi^{2+l-\sigma,1} + \frac{\sigma}{\sqrt{2}}\left[(-1)^{l+1}\chi^{6,2+l+\sigma} + \chi^{7,2+l+\sigma}\right] + \frac{1}{\sqrt{2}}\left[\sigma\chi^{8,5-l+\sigma} + (-1)^{l+1}\chi^{10,5-l+\sigma}\right] \\ & + \frac{1}{\sqrt{2}}\left[-\chi^{12+l-\sigma,8} + \sigma(-1)^{l+1}\chi^{12+l-\sigma,10}\right] + \frac{1}{\sqrt{2}}\left[(-1)^{l}\chi^{15-l-\sigma,6} + \chi^{15-l-\sigma,7}\right] \\ & + (-1)^{l+1}\chi^{10-\sigma,5-l-\sigma} + (-1)^{l+1}\sigma\chi^{12+l+\sigma,10+\sigma} + \sigma\chi^{16,15-l+\sigma}. \end{aligned} \tag{7}$$

Equation (7) allows calculating all the local dynamical quantities. For example, quantum electron number has the form:

$$\begin{aligned} n_{l\sigma} = {} & \chi^{2+l-\sigma,2+l-\sigma} + \frac{1}{2}\left[\chi^{6,6} + (-1)^{l+1}\chi^{6,7} + (-1)^{l+1}\chi^{7,6} + \chi^{7,7}\right] \\ & + \frac{1}{2}\left[\chi^{8,8} + \sigma(-1)^{l+1}\chi^{8,10} + \sigma(-1)^{l+1}\chi^{10,8} + \chi^{10,10}\right] + \chi^{10-\sigma,10-\sigma} \\ & + \chi^{12+l-\sigma,12+l-\sigma} + \chi^{12+l+\sigma,12+l+\sigma} + \chi^{15-l-\sigma,15-l-\sigma} + \chi^{16,16} \end{aligned} \tag{8}$$

and

$$n_{l\uparrow} - n_{l\downarrow} = \chi^{1+l,1+l} - \chi^{3+l,3+l} + (-1)^{l+1}\left[\chi^{8,10} + \chi^{10,8}\right] + \chi^{9,9} - \chi^{11,11} + \chi^{14-l,14-l} - \chi^{16-l,16-l}. \tag{9}$$

For τ dependent quantity $A(\tau) = e^{\tau H_0} A e^{-\tau H_0}$, we have the equation

$$\begin{aligned} n_{l\uparrow}(\tau) - n_{l\downarrow}(\tau) = {} & \chi^{1+l,1+l} - \chi^{3+l,3+l} + (-1)^{l+1}\left[\chi^{8,10}e^{\tau(E_8-E_{10})} + \chi^{10,8}e^{\tau(E_{10}-E_8)}\right] \\ & + \chi^{9,9} - \chi^{11,11} + \chi^{14-l,14-l} - \chi^{16-l,16-l}. \end{aligned} \tag{10}$$

The correlation between quantities with different orbital numbers is determined by the equation (l = 1, 2):

$$\begin{aligned} (n_{l\uparrow}(\tau) - n_{l\downarrow}(\tau))(n_{l'\uparrow}(0) - n_{l'\downarrow}(0)) = {} & \delta_{ll'}\left[\chi^{1+l,1+l} + \chi^{3+l,3+l} + \chi^{14-l,14-l} + \chi^{16-l,16-l}\right] \\ & + (-1)^{l+l'}\left[\chi^{8,8}e^{\tau(E_8-E_{10})} + \chi^{10,10}e^{\tau(E_{10}-E_8)}\right] + \chi^{9,9} + \chi^{11,11}, \end{aligned} \tag{11}$$

$$\sum_{ll'}(n_{l\uparrow}(\tau)-n_{l\downarrow}(\tau))(n_{l'\uparrow}(0)-n_{l'\downarrow}(0))=\frac{4}{Z_0}\left(e^{-\beta E_2}+e^{-\beta E_{12}}+2e^{-\beta E_9}\right) \tag{12}$$

In special case $l=1,\ l'=2$, we have

$$(n_{1\uparrow}(\tau)-n_{1\downarrow}(\tau))(n_{2\uparrow}(0)-n_{2\downarrow}(0))=-\left[\chi^{8,8}e^{\tau(E_8-E_{10})}+\chi^{10,10}e^{\tau(E_{10}-E_8)}\right]+\chi^{9,9}+\chi^{11,11}, \tag{13}$$

which is the *d* electron susceptibility [2–4].

We now define the Matsubara one-particle Green's function of localized *d*-electrons:

$$\mathcal{G}^0(l\sigma\tau,l'\sigma'\tau')=\mathcal{G}^0_{l\sigma,l'\sigma'}(\tau-\tau')=-\left\langle Td_{l\sigma}(\tau)\bar{d}_{l'\sigma'}(\tau')\right\rangle_0, \tag{14}$$

where

$$\bar{d}_{l\sigma}(\tau)=e^{\tau H_0}d^+_{l\sigma}e^{-\tau H_0},\ d_{l\sigma}(\tau)=e^{\tau H_0}d_{l\sigma}e^{-\tau H_0}\ .$$

The Fourier components of this Green's function are

$$\mathcal{G}_0(\tau)=\frac{1}{\beta}\sum_{\omega_n}e^{-i\omega_n\tau}\mathcal{G}_0(i\omega_n). \tag{15}$$

Using (8) and the properties of Hubbard operators we obtain the equation for local function:

$$\begin{aligned}\mathcal{G}^{(0)}_{l\sigma l'\sigma'}(i\omega_n)=\frac{\delta_{ll'}\delta_{\sigma\sigma'}}{Z_0}\Bigg\{&\frac{e^{-\beta E_1}+e^{-\beta E_2}}{i\omega_n+E_1-E_2}+\frac{e^{-\beta E_2}+e^{-\beta E_6}}{i\omega_n+E_2-E_6}\\&+\frac{1}{2}\frac{e^{-\beta E_2}+e^{-\beta E_7}}{i\omega_n+E_2-E_7}+\frac{3}{2}\frac{e^{-\beta E_2}+e^{-\beta E_9}}{i\omega_n+E_2-E_9}+\frac{e^{-\beta E_6}+e^{-\beta E_{12}}}{i\omega_n+E_6-E_{12}}\\&+\frac{1}{2}\frac{e^{-\beta E_7}+e^{-\beta E_{12}}}{i\omega_n+E_7-E_{12}}+\frac{3}{2}\frac{e^{-\beta E_9}+e^{-\beta E_{12}}}{i\omega_n+E_9-E_{12}}+\frac{e^{-\beta E_{12}}+e^{-\beta E_{16}}}{i\omega_n+E_{12}-E_{16}}\Bigg\},\end{aligned} \tag{16}$$

where Z_0 is partition function in atomic limit

$$Z_0=e^{-\beta E_1}+4e^{-\beta E_2}+2e^{-\beta E_6}+e^{-\beta E_7}+3e^{-\beta E_9}+4e^{-\beta E_{12}}+e^{-\beta E_{16}}. \tag{17}$$

The spectral function of impurity *d*-electron in local approximation is as follows:

$$A^{(0)}(E)=-2\,\mathrm{Im}\,\mathcal{G}^0(E+i\delta) \tag{18}$$

where $\mathcal{G}^0(E+i\delta)$ with δ=+0 is the analytical continuation of the Matsubara to retarded Green's function.

Using (14) we obtain

$$A^{(0)}(E)=\frac{2\pi}{Z_0}\Big\{(e^{-\beta E_1}+e^{-\beta E_2})\delta(E+E_1-E_2)+(e^{-\beta E_2}+e^{-\beta E_6})\delta(E+E_2-E_6)$$
$$+\frac{1}{2}(e^{-\beta E_2}+e^{-\beta E_7})\delta(E+E_2-E_7)+\frac{3}{2}(e^{-\beta E_2}+e^{-\beta E_9})\delta(E+E_2-E_9)$$
$$+(e^{-\beta E_6}+e^{-\beta E_{12}})\delta(E+E_6-E_{12})+\frac{1}{2}(e^{-\beta E_7}+e^{-\beta E_{12}})\delta(E+E_7-E_{12}) \quad (19)$$
$$+\frac{3}{2}(e^{-\beta E_9}+e^{-\beta E_{12}})\delta(E+E_9-E_{12})+(e^{-\beta E_{12}}+e^{-\beta E_{16}})\delta(E+E_{12}-E_{16}),$$

with property

$$\int_{-\infty}^{\infty}A^{(0)}(E)dE=2\pi. \quad (20)$$

3. Delocalization processes

We use the perturbation theory elaborated previously for strongly correlated electron systems both of non degenerate [9–13, 15–18] and of degenerate forms [14]. We study the process of renormalization of Green's function resulting from intra- and inter-orbital flips of tunneling electrons.

The full Matsubara Green's function in the interaction representation for conduction and impurity electrons are

$$G(\vec{k}l\sigma\tau\,|\,\vec{k}'l'\sigma'\tau')=-\left\langle TC_{\vec{k}l\sigma}(\tau)\bar{C}_{\vec{k}'l'\sigma'}(\tau')U(\beta)\right\rangle_0^c,$$
$$\mathcal{G}(l\sigma\tau\,|\,l'\sigma'\tau')=-\left\langle Td_{l\sigma}(\tau)\bar{d}_{l'\sigma'}(\tau')U(\beta)\right\rangle_0^c. \quad (21)$$

The anomalous functions are defined as

$$F(\vec{k}l\sigma\tau\,|\,\vec{k}'l'\sigma'\tau')=-\left\langle TC_{\vec{k}l\sigma}(\tau)C_{\vec{k}'l'\sigma'}(\tau')U(\beta)\right\rangle_0^c$$
$$\bar{F}(\vec{k}l\sigma\tau\,|\,\vec{k}'l'\sigma'\tau')=-\left\langle T\bar{C}_{\vec{k}l\sigma}(\tau)\bar{C}_{\vec{k}'l'\sigma'}(\tau')U(\beta)\right\rangle_0^c$$
$$f(l\sigma\tau\,|\,l'\sigma'\tau')=-\left\langle Td_{l\sigma}(\tau)d_{l'\sigma'}(\tau')U(\beta)\right\rangle_0^c \quad (22)$$
$$\bar{f}(l\sigma\tau\,|\,l'\sigma'\tau')=-\left\langle T\bar{d}_{l\sigma}(\tau)\bar{d}_{l'\sigma'}(\tau')U(\beta)\right\rangle_0^c.$$

Here τ and τ' stand for imaginary time with $0\le\tau\le\beta$, β is the inverse temperature, T is the chronological ordering operator.

The evolution operator is

$$U(\beta)=T\exp(-\int_0^{\beta}H_{\rm int}(\tau)d\tau). \quad (23)$$

The statistical averaging is carried out in (21) and (22) with respect to the zero-order density matrix of the conduction and impurity electrons. Index c means connected diagrams.

In the zero order approximation we have

$$H_0^L=\sum_{n=1}^{16}E_n\chi^{nn},\quad \sum_{n=1}^{16}\chi^{nn}=1,$$

$$G^{(0)}_{l\sigma l'\sigma'}(\vec{k}\vec{k}' \mid \tau-\tau') = \delta_{\vec{k}\vec{k}'}\delta_{ll'}\delta_{\sigma\sigma'}G^{(0)}_{l\sigma}(\vec{k} \mid \tau-\tau'),, \tag{24}$$

$$G^{(0)}_{l\sigma}(\vec{k} \mid i\omega_n) = \frac{1}{i\omega_n - \varepsilon(\vec{k})},\ \omega_n = \frac{(2n+1)\pi}{\beta},$$

and $\mathcal{G}^{(0)}(i\omega_n)$ is determined by equation (16).

Hybridization between the conduction and *d* impurity electrons results in renormalization of their propagators. Because the number of conduction electrons *N* is much larger than the single impurity state, the effect of the latter on the conduction band scales as $\frac{1}{N}$.

The renormalized conduction electron propagator is

$$\begin{aligned} G_{l\sigma l'\sigma'}(\vec{k}\vec{k}' \mid i\omega_n) &= \delta_{\vec{k}\vec{k}'}\delta_{ll'}\delta_{\sigma\sigma'}G^{(0)}_{l\sigma}(\vec{k} \mid i\omega_n) \\ &+ \frac{V^*_{\vec{k}l}V_{\vec{k}'l'}}{N}G^{(0)}_{l\sigma}(\vec{k} \mid i\omega_n)\mathcal{g}_{l\sigma l'\sigma'}(i\omega_n)G^{(0)}_{l'\sigma'}(\vec{k}' \mid i\omega_n), \end{aligned} \tag{25}$$

where $\mathcal{g}_{l\sigma l'\sigma'}(i\omega_n)$ is the full impurity electron propagator.

A similar equation holds for the anomalous function of conduction electrons in superconducting state:

$$F_{l\sigma l'\sigma'}(\vec{k},-\vec{k}' \mid i\omega_n) = \frac{V^*_{\vec{k}l}V_{\vec{k}'l'}}{N}G^{(0)}_{l\sigma}(\vec{k} \mid i\omega_n)\, f_{l\sigma l'\sigma'}(i\omega_n)G^{(0)}_{l'\sigma'}(-\vec{k}' \mid -i\omega_n).$$

The equations for the full functions $\mathcal{g}$ and *f* of impurity electrons have the diagrammatical form shown in Fig.1.

The structure representative of the diagrams in Fig. 1 is given by the following equation

$$\begin{aligned} \sum_{\vec{k}_1}\sum_{\vec{k}_2}\frac{V_{\vec{k}_1 l_1}V^*_{\vec{k}_2 l_2}}{N}G^0_{l_1\sigma_1 l_2\sigma_2}(\vec{k}_1\vec{k}_2 \mid i\omega_n) &= \frac{1}{N}\sum_{\vec{k}_1}\left|V_{\vec{k}_1 l_1}\right|^2 G^{(0)}_{l_1\sigma_1}(\vec{k}_1 \mid i\omega_n)\delta_{l_1 l_2}\delta_{\sigma_1\sigma_2} \\ &= \delta_{l_1 l_2}\delta_{\sigma_1\sigma_2}\mathcal{G}^{(0)}_{l_1\sigma_1}(i\omega_n), \end{aligned} \tag{26}$$

where

$$\mathcal{G}^{(0)}_{l\sigma}(i\omega_n) = \frac{1}{N}\sum_{\vec{k}}\left|V_{\vec{k}l}\right|^2 G^{(0)}_{l\sigma}(\vec{k} \mid i\omega_n) = \frac{1}{N}\sum_{\vec{k}}\frac{|V_{\vec{k}l}|^2}{i\omega_n - \varepsilon(\vec{k})}. \tag{27}$$

The renormalization quantity is

$$\mathcal{G}_{l\sigma l'\sigma'}(i\omega_n) = \frac{1}{N}\sum_{\vec{k}\vec{k}'}V_{\vec{k}l}V^*_{\vec{k}'l'}G_{l\sigma l'\sigma'}(\vec{k}\vec{k}' \mid i\omega_n). \tag{28}$$

In Fig. 1, the double dashed lines with arrows depict renormalized $\mathcal{g}$ and *f* propagators of localized electrons and solid thin lines represent $\mathcal{G}^0$ function of conduction electrons. The function V_1 means $V_{\vec{k}_1 l_1}$ and summation by repeated indices is assumed.

Λ and $\overline{Y}$ are correlation functions. They contain a sum of strongly connected irreducible diagrams. The simplest examples of these diagrams are shown in Fig. 2.

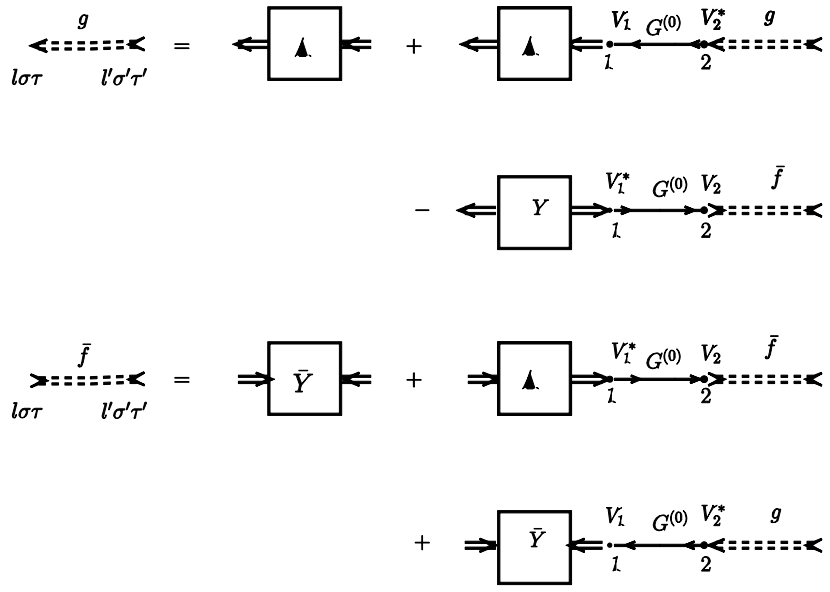

Fig. 1. Dyson type equation for Green's function of impurity electrons. Λ, *Y*, $\bar{Y}$ are correlation functions.

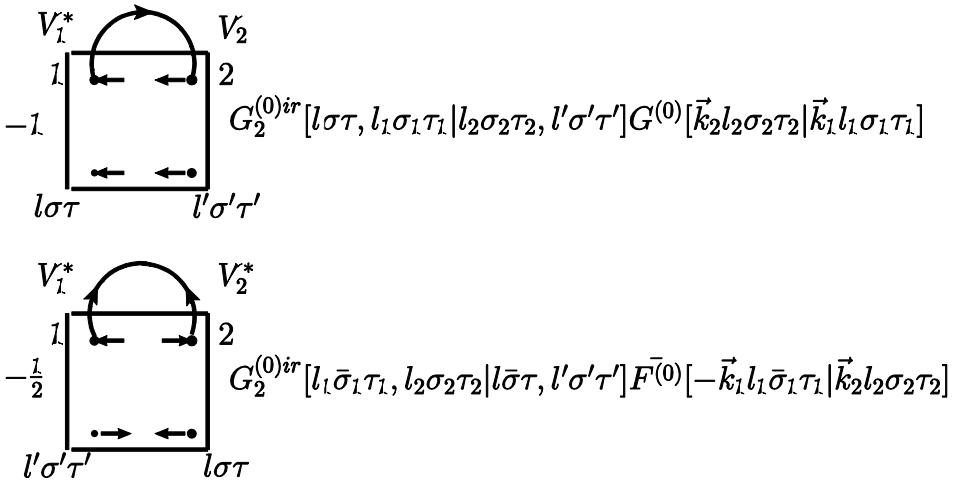

Fig. 2. Simplest examples of correlation functions Λ and $\bar{Y}$.

The analytical form of equations in Fig.1 is the following:

$$\begin{aligned} \mathcal{G}_{l\sigma l'\sigma'}(i\omega_n) &= \Lambda_{l\sigma l'\sigma'}(i\omega_n) + \Lambda_{l\sigma l_1\sigma_1}(i\omega_n)\mathcal{G}^{(0)}_{l_1\sigma_1}(i\omega_n)\mathcal{G}_{l_1\sigma_1 l'\sigma'}(i\omega_n) \\ &\quad -Y_{l\sigma l_1\sigma_1}(i\omega_n)\mathcal{G}^{(0)}_{l_1\sigma_1}(-i\omega_n)\,\bar{f}_{l_1\sigma_1 l'\sigma'}(i\omega_n), \\ \bar{f}_{l\sigma l'\sigma'}(i\omega_n) &= \bar{Y}_{l\sigma l'\sigma'}(i\omega_n) + \Lambda_{l_1\sigma_1 l\sigma}(-i\omega_n)\mathcal{G}^{(0)}_{l_1\sigma_1}(-i\omega_n)\,\bar{f}_{l_1\sigma_1 l'\sigma'}(i\omega_n) \\ &\quad +\bar{Y}_{l\sigma l_1\sigma_1}(i\omega_n)\mathcal{G}^{(0)}_{l_1\sigma_1}(i\omega_n)\mathcal{G}_{l_1\sigma_1 l'\sigma'}(i\omega_n). \end{aligned} \tag{29}$$

This system of equations is rather general and admits different phases. We shall discuss one of the most simple forms with singlet superconductivity on the paramagnetic background.

For this special case, we use the new notations ($\bar{\sigma} = -\sigma$):

$$\begin{gathered} g_{l\sigma l'\sigma'}(i\omega_n) = \delta_{\sigma\sigma'} g_\sigma^{ll'}(i\omega_n), \quad \bar{f}_{l\sigma l'\sigma'}(i\omega_n) = \delta_{\sigma\bar{\sigma}'} \bar{f}_{\bar{\sigma}\sigma}^{ll'}(i\omega_n), \\ \Lambda_{l\sigma l'\sigma'}(i\omega_n) = \delta_{\sigma\sigma'} \Lambda_\sigma^{ll'}(i\omega_n), \quad \bar{Y}_{l\sigma l'\sigma'}(i\omega_n) = \delta_{\sigma\bar{\sigma}'} \bar{Y}_{\bar{\sigma}\sigma}^{ll'}(i\omega_n), \\ g_{l\sigma}^{(0)}(i\omega_n) = g_\sigma^{(0)l}(i\omega_n). \end{gathered} \tag{30}$$

With these definitions, we obtain:

$$\begin{gathered} g_\sigma^{ll'}(i\omega_n) = \Lambda_\sigma^{ll'}(i\omega_n) + \Lambda_\sigma^{ll'}(i\omega_n) G_\sigma^{l_1(0)}(i\omega_n) g_\sigma^{l_1 l'}(i\omega_n) - Y_{\sigma\bar{\sigma}}^{ll_1}(i\omega_n) G_{\bar{\sigma}}^{l_1(0)}(-i\omega_n) \bar{f}_{\bar{\sigma}\sigma}^{l_1 l'}(i\omega_n), \\ \bar{f}_{\bar{\sigma}\sigma}^{ll'}(i\omega_n) = \bar{Y}_{\bar{\sigma}\sigma}^{ll'}(i\omega_n) + \Lambda_{\bar{\sigma}}^{l_1 l}(-i\omega_n) G_{\bar{\sigma}}^{l_1(0)}(-i\omega_n) \bar{f}_{\bar{\sigma}\sigma}^{l_1 l'}(i\omega_n) + \bar{Y}_{\bar{\sigma}\sigma}^{ll_1}(i\omega_n) G_\sigma^{l_1(0)}(i\omega_n) g_\sigma^{l_1 l'}(i\omega_n). \end{gathered} \tag{31}$$

In the absence of orbital degeneracy, this system of equation has the known solution [18]:

$$\begin{gathered} g_\sigma(i\omega_n) = \frac{\Lambda_\sigma(i\omega_n) + G_\sigma^{(0)}(-i\omega_n)\left[\Lambda_\sigma(i\omega_n)\Lambda_{\bar{\sigma}}(-i\omega_n) + Y_{\sigma\bar{\sigma}}(i\omega_n)\bar{Y}_{\bar{\sigma}\sigma}(i\omega_n)\right]}{d_\sigma(i\omega_n)}, \\ \bar{f}_{\bar{\sigma}\sigma}(i\omega_n) = \frac{\bar{Y}_{\bar{\sigma}\sigma}(i\omega_n)}{d_\sigma(i\omega_n)}, , \quad f_{\sigma\bar{\sigma}}(i\omega_n) = \frac{Y_{\sigma\bar{\sigma}}(i\omega_n)}{d_\sigma(i\omega_n)}, \\ d_\sigma(i\omega_n) = \left(1 - \Lambda_\sigma(i\omega_n) G_\sigma^{(0)}(i\omega_n)\right)\left(1 - \Lambda_{\bar{\sigma}}(-i\omega_n) G_{\bar{\sigma}}^{(0)}(-i\omega_n)\right) \\ + G_\sigma^{(0)}(i\omega_n) G_{\bar{\sigma}}^{(0)}(-i\omega_n) Y_{\sigma\bar{\sigma}}(i\omega_n) \bar{Y}_{\bar{\sigma}\sigma}(i\omega_n). \end{gathered} \tag{32}$$

Solutions of equation (31) for the normal state of the degenerate system have the form:

$$\begin{gathered} g_\sigma^{11}(i\omega_n) = \frac{\Lambda_\sigma^{11}(i\omega_n) + G_\sigma^{2(0)}(-i\omega_n)\left[\Lambda_\sigma^{11}(i\omega_n)\Lambda_\sigma^{22}(i\omega_n) + \Lambda_\sigma^{12}(i\omega_n)\Lambda_\sigma^{21}(i\omega_n)\right]}{d_\sigma(i\omega_n)}, , \\ g_\sigma^{21}(i\omega_n) = \frac{\Lambda_\sigma^{21}(i\omega_n)}{d_\sigma(i\omega_n)}, , \quad \begin{gathered} d_\sigma(i\omega_n) = \left(1 - G_\sigma^{1(0)}(i\omega_n)\Lambda_\sigma^{11}(i\omega_n)\right)\left(1 - G_\sigma^{2(0)}(i\omega_n)\Lambda_\sigma^{22}(i\omega_n)\right) \\ - G_\sigma^{1(0)}(i\omega_n) G_\sigma^{2(0)}(i\omega_n) \Lambda_\sigma^{12}(i\omega_n)\Lambda_\sigma^{21}(i\omega_n). \end{gathered} \end{gathered} \tag{33}$$

The other two functions are obtained by changing the indexes $1 \leftrightarrow 2$. These equations are of Dyson type. They determine Green's functions through correlation functions $\Lambda = g^{(0)} + Z$, Y and $\bar{Y}$ ones. The last three can only be given in a form of infinite diagram series, since an exact solution does not exist.

An example of efficient summation of diagram and determination of the correlation functions *Z*, *Y* and $\bar{Y}$ is presented in Fig. 3.

The diagrams of Fig. 3 differ from the ones of Fig. 2 by the presence of the full conduction electron Green's function instead of the bare one of Fig. 2. This difference is the result of ladder summation of main diagrams.

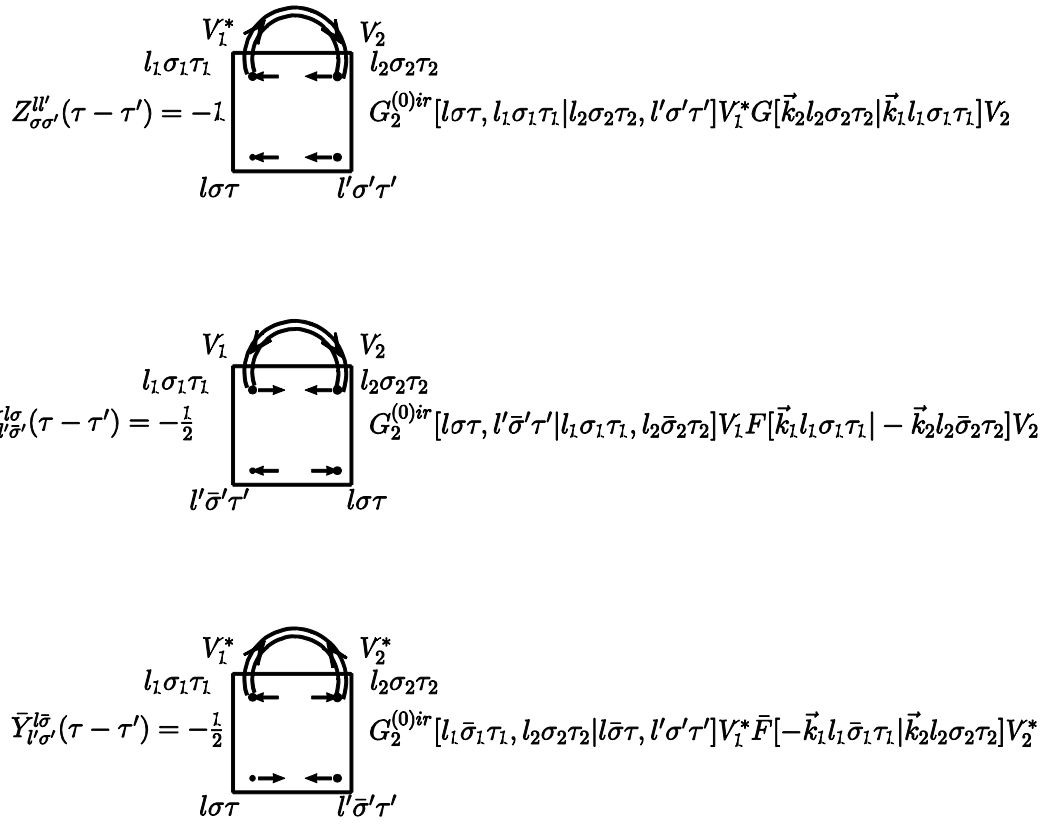

Fig. 3. The main approximation for the correlation functions. The solid double lines with arrows depict the full Green's functions of conduction electrons. The rectangles depict the irreducible Green's functions of the impurity electrons.

4. Correlation functions

The main approximation is based on calculation of simplest normal and anomalous correlation functions in order to establish its dependence on spin and orbital quantum numbers.

The simplest correlation function is determined as

$$G_2^{irr}[1,2\,|\,\overline{3},\overline{4}] = g_2^{(0)}(1,2\,|\,\overline{3},\overline{4}) - g_1^{(0)}(1\,|\,\overline{4})g_1^{(0)}(2\,|\,\overline{3}) + g_1^{(0)}(1\,|\,\overline{3})g_1^{(0)}(2\,|\,\overline{4}),,$$

$$g_2^{(0)}(1,2\,|\,\overline{3},\overline{4}) = \left\langle Td_1d_2\overline{d}_3\overline{d}_4\right\rangle_0,\quad g_1^{(0)}(1\,|\,\overline{4}) = -\left\langle Td_1\overline{d}_4\right\rangle_0,\ 1=(l_1,\sigma_1,\tau_1), \tag{34}$$

with two- and one-particle bare Green's functions of localized electrons.

Owing to the presence of Coulomb interaction terms in zero order Hamiltonian, the r.h.s. of equation (34) does not vanish and contains charge, spin, and pairing fluctuations.

The two-particle Green's function $g_2^{(0)}$ is the sum of 4! terms of different time ordered electron operators products. The statistical averages of these quantities are calculated by using Hubbard transfer operator's representation.

We need the Fourier representation of these functions

$$G_2^{irr}[l_1\sigma_1\tau_1;l_2\sigma_2\tau_2\,|\,l_3\sigma_3\tau_3;l_4\sigma_4\tau_4]=$$

$$=\frac{1}{\beta^4}\sum_{\omega_1\omega_2\omega_3\omega_4}G_2^{irr}[l_1\sigma_1 i\omega_1;l_2\sigma_2 i\omega_2\,|\,l_3\sigma_3 i\omega_3;l_4\sigma_4 i\omega_4]e^{-i\omega_1\tau_1-i\omega_2\tau_2+i\omega_3\tau_3+i\omega_4\tau_4},$$

$$g_1^{(0)}(l_1\sigma_1\tau_1\,|\,l_2\sigma_2\tau_2)=\frac{1}{\beta}\sum_{\omega_1}g_1^{(0)}(l_1\sigma_1;l_2\sigma_2\,|\,i\omega_1)e^{-i\omega_1(\tau_1-\tau_2)},, \tag{35}$$

$$g_1^{(0)}(l_1\sigma_1;l_2\sigma_2\,|\,i\omega_1)\approx\delta_{l_1l_2}\delta_{\sigma_1\sigma_2}m(i\omega_1)=\frac{\delta_{l_1l_2}\delta_{\sigma_1\sigma_2}}{2}\left(\frac{1}{i\omega_1+E_2-E_9}+\frac{1}{i\omega_1+E_9-E_{12}}\right).$$

$$\begin{aligned}&G_2^{irr}[l_1\sigma_1 i\omega_1;l_2\sigma_2 i\omega_2\,|\,l_3\sigma_3 i\omega_3;l_4\sigma_4 i\omega_4]=\\&=g_2^{(0)}[l_1\sigma_1 i\omega_1;l_2\sigma_2 i\omega_2\,|\,l_3\sigma_3 i\omega_3;l_4\sigma_4 i\omega_4]-\beta\delta(\omega_1+\omega_2-\omega_3-\omega_4)\\&\left[\beta\delta(\omega_1-\omega_4)\,g_1^{(0)}(l_1\sigma_1;l_4\sigma_4\,|\,i\omega_1)g_1^{(0)}(l_2\sigma_2;l_3\sigma_3\,|\,i\omega_2)\right.\\&\left.-\beta\delta(\omega_1-\omega_3)g_1^{(0)}(l_1\sigma_1;l_3\sigma_3\,|\,i\omega_1)\,g_1^{(0)}(l_2\sigma_2;l_4\sigma_4\,|\,i\omega_2)\right].\end{aligned} \tag{36}$$

There exists the law of frequency conservation

$$\begin{aligned}&G_2^{irr}[l_1\sigma_1 i\omega_1;l_2\sigma_2 i\omega_2\,|\,l_3\sigma_3 i\omega_3;l_4\sigma_4 i\omega_4]=\\&=\beta\delta(\omega_1+\omega_2-\omega_3-\omega_4)\tilde{G}_2^{irr}[l_1\sigma_1 i\omega_1;l_2\sigma_2 i\omega_2\,|\,l_3\sigma_3 i\omega_3;l_4\sigma_4 i\omega_4].\end{aligned} \tag{37}$$

The statistical averages of chronologically ordered products of the electron operators of the function $g_2^{(0)}$ have different weights of the form $\frac{e^{-\beta E_n}}{Z_0}$, where E_n are the energies determined in the previous section. Because E_9 is the lowest in energy, its weight $e^{-\beta E_n}$ is dominant over the others and therefore only these terms are taken into account.

Motivated by these arguments, we use the approximate value (35) instead of initial exact equation (16) for zero order Green's function $g_{l\sigma l'\sigma'}^{(0)}$. Zero order partition function Z_0 (17) is approximated as $3e^{-\beta E_9}$.

For example, the contribution to function $g_2^{(0)}[l_1\sigma_1 i\omega_1;l_2\sigma_2 i\omega_2\,|\,l_3\sigma_3 i\omega_3;l_4\sigma_4 i\omega_4]$ with time order $\beta>\tau_1>\tau_3>\tau_2>\tau_4>0$ and with weight $e^{-\beta E_9}$ is

$$\begin{aligned}&-\delta_{l_1l_3}\delta_{l_2l_4}(\frac{1}{4}\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}+\delta_{\sigma_1,-\sigma_3}\delta_{\sigma_2,-\sigma_4}\delta_{\sigma_2\sigma_3}+\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}\delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3})I_{1\bar{3}2\bar{4}}^{(1)}\\&-(\delta_{3-l_1-l_3,0}\delta_{3-l_2-l_4,0}+(-1)^{l_1+l_4}\delta_{l_1l_3}\delta_{l_2l_4})(\frac{1}{4}\sigma_1\sigma_4\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}+\frac{1}{2}\delta_{\sigma_1,-\sigma_3}\delta_{\sigma_2,-\sigma_4}\delta_{\sigma_1\sigma_4})I_{1\bar{3}2\bar{4}}^{(2)}\\&-(-1)^{l_1+l_4}\delta_{3-l_1-l_3,0}\delta_{3-l_2-l_4,0})(\frac{1}{4}\sigma_1\sigma_4\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}+\frac{1}{2}\delta_{\sigma_1,-\sigma_3}\delta_{\sigma_2,-\sigma_4}\delta_{\sigma_1\sigma_4})I_{1\bar{3}2\bar{4}}^{(3)},\end{aligned} \tag{38}$$

where

$$I_{1\bar{3}2\bar{4}}^{(1)}=\frac{e^{-\beta E_9}}{Z_0}\int_0^\beta d\tau_1\int_0^{\tau_1}d\tau_3\int_0^{\tau_3}d\tau_2\int_0^{\tau_2}d\tau_4 e^{(E_9-E_{12})(\tau_1+\tau_2-\tau_3-\tau_4)}e^{i\omega_1\tau_1+i\omega_2\tau_2-i\omega_3\tau_3-i\omega_4\tau_4},$$

$$I^{(2)}_{1\bar{3}2\bar{4}}=\frac{e^{-\beta E_9}}{Z_0}\int_0^\beta d\tau_1\int_0^{\tau_1}d\tau_3\int_0^{\tau_3}d\tau_2\int_0^{\tau_2}d\tau_4 e^{(E_9-E_{12})(\tau_1-\tau_4)+(E_6-E_{12})(\tau_2-\tau_3)}e^{i\omega_1\tau_1+i\omega_2\tau_2-i\omega_3\tau_3-i\omega_4\tau_4}, \tag{39}$$

$$I^{(3)}_{1\bar{3}2\bar{4}}=\frac{e^{-\beta E_9}}{Z_0}\int_0^\beta d\tau_1\int_0^{\tau_1}d\tau_3\int_0^{\tau_3}d\tau_2\int_0^{\tau_2}d\tau_4 e^{(E_9-E_{12})(\tau_1-\tau_4)+(E_7-E_{12})(\tau_2-\tau_3)}e^{i\omega_1\tau_1+i\omega_2\tau_2-i\omega_3\tau_3-i\omega_4\tau_4}.$$

These fourfold multiple integrals by time variable τ can be transformed in contour integral by using the method of Claude Bloch [21]. With this purpose, it is necessary to introduce the exponential form

$$e^{(\beta-\tau_1)\bar{E}_0+(\tau_1-\tau_3)\bar{E}_1+(\tau_3-\tau_2)\bar{E}_2+(\tau_2-\tau_4)\bar{E}_3+(\tau_3-0)\bar{E}_4},, \tag{40}$$

which must be compared with the exponential form of our integrals $I^{(n)}_{1\bar{3}2\bar{4}}$. Comparison with $I^{(1)}_{1\bar{3}2\bar{4}}$ give us the result

$$\bar{E}_0=-E_9,\ \bar{E}_2=-E_9+i\omega_1-i\omega_3,\ \bar{E}_4=-E_9+i\Omega,\ \bar{E}_1=-E_{12}+i\omega_1,$$
$$\bar{E}_3=-E_{12}+i\omega_1+i\omega_2-i\omega_3,\quad \Omega=\omega_1+\omega_2-\omega_3-\omega_4 \tag{41}$$

Our integral $I^{(1)}_{1\bar{3}2\bar{4}}$ is transformed in the contour integral

$$I^{(1)}=\frac{1}{2\pi i}\frac{1}{Z_0}\oint_{C^+}\frac{dze^{-\beta z}}{(z+\bar{E}_0)(z+\bar{E}_1)(z+\bar{E}_2)(z+\bar{E}_3)(z+\bar{E}_4)}, \tag{42}$$

where contour C^+ surrounds the real axis in the positive direction. The integrals $I^{(2)}$ and $I^{(3)}$ have the same form (42) but differ in the definition of energy $\bar{E}_2$. For $I^{(2)}$ the energy $\bar{E}_2=-\mathrm{E}_6+i\omega_1-i\omega_3$ and for $I^{(3)}$, $\bar{E}_2=-\mathrm{E}_7+i\omega_1-i\omega_3$. Other parameters coincide.

The contour integral (42) is evaluated by the method of residues. The simple results are obtained when the parameters $\bar{E}_n$ are different. The existence of multiple poles is possible for the special values of frequencies ω_n.

For example, in the case where $\omega_1-\omega_3=0$ and Ω=0, we have $\bar{E}_0=\bar{E}_2=\bar{E}_4$ and the pole $z=-\bar{E}_0$ is threefold multiple with the residue

$$\frac{1}{2}\left(\frac{e^{-\beta z}}{(z+\bar{E}_1)(z+\bar{E}_3)}\right)''_{z=-\bar{E}_0} \tag{43}$$

To find all possible multiple poles, we consider different values of frequencies using the identity 1=δ(ω)+ψ(ω), where ψ(ω)=1−δ(ω). For example, we consider the possibility when Ω can be equal to zero and $\omega_1=\omega_3$. We have the identity

$$\begin{aligned}1&=(\delta(\Omega)+\psi(\Omega))(\delta(\omega_1-\omega_3)+\psi(\omega_1-\omega_3))\\&=\delta(\Omega)\delta(\omega_1-\omega_3)+\delta(\Omega)\psi(\omega_1-\omega_3)+\psi(\Omega)\delta(\omega_1-\omega_3)+\psi(\Omega)\psi(\omega_1-\omega_3)\end{aligned} \tag{44}$$

The first term in the right-hand part of this equation admits the existence of a triple pole; the next two terms admit double poles, and last term admits double and single poles.

We shall take into account these residues, statistical weights of which is $\frac{e^{-\beta Z_0}}{Z_0}$, and shall omit the other ones. In this approximation, we have

$$
\begin{aligned}
Z_0 I^{(1)}_{1\bar{3}2\bar{4}} &= \frac{1}{2}\delta(\Omega)\delta(\omega_1-\omega_3)\left(\frac{e^{-\beta Z}}{(z+\bar{E}_1)(z+\bar{E}_3)}\right)''_{z=-\bar{E}_0} \\
&+\delta(\Omega)\psi(\omega_1-\omega_3)\left[\left(\frac{e^{-\beta Z}}{(z+\bar{E}_1)(z+\bar{E}_2)(z+\bar{E}_3)}\right)'_{z=-\bar{E}_0}+\left(\frac{e^{-\beta Z}}{(z+\bar{E}_0)^2(z+\bar{E}_1)(z+\bar{E}_3)}\right)'_{z=-\bar{E}_2}\right] \\
&+\delta(\omega_1-\omega_3)\psi(\Omega)\left[\left(\frac{e^{-\beta Z}}{(z+\bar{E}_1)(z+\bar{E}_3)(z+\bar{E}_4)}\right)'_{z=-\bar{E}_0}+\left(\frac{e^{-\beta Z}}{(z+\bar{E}_0)^2(z+\bar{E}_1)(z+\bar{E}_3)}\right)'_{z=-\bar{E}_4}\right] \\
&+\psi(\omega_1-\omega_3)\psi(\Omega)\delta(\omega_2-\omega_4)\left[\left(\frac{e^{-\beta Z}}{(z+\bar{E}_0)(z+\bar{E}_1)(z+\bar{E}_3)}\right)'_{z=-\bar{E}_2}\right. \\
&\left.+\left(\frac{e^{-\beta Z}}{(z+\bar{E}_2)^2(z+\bar{E}_1)(z+\bar{E}_3)}\right)'_{z=-\bar{E}_0}\right]+\psi(\Omega)\psi(\omega_1-\omega_3)\psi(\omega_2-\omega_4)\times \\
&\times\left[\left(\frac{e^{-\beta Z}}{(z+\bar{E}_1)(z+\bar{E}_2)(z+\bar{E}_3)(z+\bar{E}_4)}\right)'_{z=-\bar{E}_0}+\left(\frac{e^{-\beta Z}}{(z+\bar{E}_0)(z+\bar{E}_1)(z+\bar{E}_3)(z+\bar{E}_4)}\right)'_{z=-\bar{E}_2}\right. \\
&\left.+\left(\frac{e^{-\beta Z}}{(z+\bar{E}_0)(z+\bar{E}_1)(z+\bar{E}_2)(z+\bar{E}_3)}\right)'_{z=-\bar{E}_4}\right].
\end{aligned}
\tag{45}
$$

The contribution of other poles is negligible. Our next approximation consists in preserving, in the case of a low temperature, of the main part of the second derivative (43) just of the form

$$
\Delta I = \frac{\beta^2 e^{-\beta E_9}}{2Z_0(\bar{E}_1-\bar{E}_0)(\bar{E}_3-\bar{E}_0)} \tag{46}
$$

This contribution, together with contribution (36) of the product of one-particle Green's functions, determines the main part of the correlation function. This part is designed as $G_2^{(0)irr}$.

After some transformation and summation of different contributions, we obtain the main approximation for the correlation function:

$$G_2^{(0)irr}[l_1\sigma_1 i\omega_1; l_2\sigma_2 i\omega_2 \mid l_3\sigma_3 i\omega_3; l_4\sigma_4 i\omega_4] = \frac{\beta}{6}\delta(\omega_1+\omega_2-\omega_3-\omega_4)\,p(i\omega_1)\,p(i\omega_2)\times$$
$$\times(\beta\delta(\omega_1-\omega_4)\delta_{l_1l_4}\delta_{l_2l_3}[2\delta_{\sigma_1,-\sigma_4}\delta_{\sigma_2,-\sigma_3}\delta_{\sigma_2\sigma_4}+\delta_{\sigma_1\sigma_3}\delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3}-\delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3}\delta_{\sigma_3,-\sigma_1}] \qquad (47)$$
$$-\beta\delta(\omega_1-\omega_3)\delta_{l_1l_3}\delta_{l_2l_4}[2\delta_{\sigma_1,-\sigma_3}\delta_{\sigma_2,-\sigma_4}\delta_{\sigma_2\sigma_3}+\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}\delta_{\sigma_1\sigma_4}-\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}\delta_{\sigma_4,-\sigma_1}]),$$

with

$$p(i\omega)=\left(\frac{1}{i\omega+E_2-E_9}-\frac{1}{i\omega+E_9-E_{12}}\right) \qquad (48)$$

5. Analysis of the main equations

As noted above, one example of efficient summation of diagrams which determine correlation function Z and Λ is presented in Fig. 4. It has the form

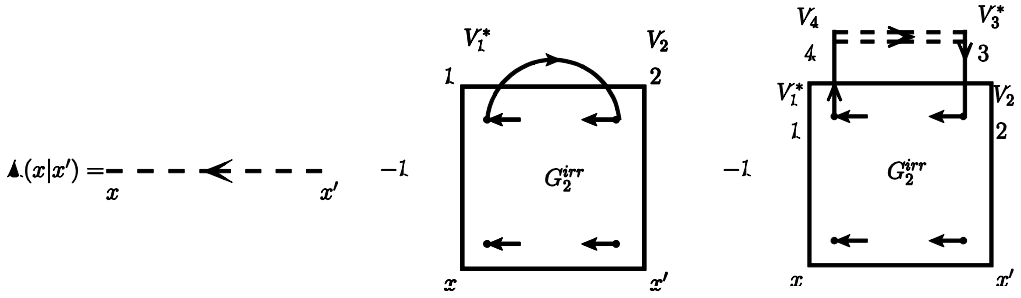

Fig. 4. The main equation for the function $\Lambda(x|x')$. Here x is $(l,\sigma,i\omega)$. The thin dashed line represents the bare local one-particle Green's function and the double dashed the renormalized one. The thin solid line represents the conduction propagator.

First of all, we shall discuss the approximation with zero order correlation function $G_2^{(0)irr}$ Using the result (47), we obtain

$$\frac{1}{\beta}\sum_{\omega_1}\sum_{l_1\sigma_1}\tilde{G}_2^{(0)irr}[l\sigma i\omega; l_1\sigma_1 i\omega_1 \mid l_1\sigma_1 i\omega_1; l'\sigma' i\omega]\mathcal{G}^{(0)}_{l_1\sigma_1}(i\omega_1)=-\frac{1}{2}\delta_{\sigma\sigma'}\delta_{ll'}[p(i\omega)]^2\mathcal{G}^{(0)}_{l\sigma}(i\omega), \qquad (49)$$

$$\sum_{l_1\sigma_1 l_2\sigma_2}\tilde{G}_2^{(0)irr}[l\sigma i\omega; l_1\sigma_1 i\omega_1 \mid l_2\sigma_2 i\omega_1; l'\sigma' i\omega]\mathcal{G}^{(0)}_{l_2\sigma_2}(i\omega_1)\mathcal{g}_{l_2\sigma_2 l_1\sigma_1}(i\omega_1)\mathcal{G}^{(0)}_{l_1\sigma_1}(i\omega_1)$$
$$=\frac{1}{6}p(i\omega)\,p(i\omega_1)\{\beta\delta(\omega-\omega)\,\delta_{ll'}\sum_{l_1}(2\delta_{\sigma',-\sigma}\mathcal{g}^{(0)}_{l_1\sigma}(i\omega_1)$$
$$\times\mathcal{g}_{l_1\sigma l_1,-\sigma}(i\omega_1)\mathcal{G}^{(0)}_{l_1,-\sigma}(i\omega_1)+\delta_{\sigma\sigma'}\mathcal{G}^{(0)}_{l_1\sigma}(i\omega_1)\mathcal{g}_{l_1\sigma l_1\sigma}(i\omega_1)\mathcal{G}^{(0)}_{l_1\sigma}(i\omega_1) \qquad (50)$$
$$-\delta_{\sigma\sigma'}\mathcal{G}^{(0)}_{l_1,-\sigma}(i\omega_1)\mathcal{g}_{l_1,-\sigma l_1,-\sigma}(i\omega_1)\mathcal{G}^{(0)}_{l,-\sigma}(i\omega_1))$$
$$-\beta\delta(\omega-\omega_1)[2\delta_{\sigma\sigma'}\mathcal{G}^{(0)}_{l_1,-\sigma}(i\omega_1)\mathcal{g}_{l,-\sigma l',-\sigma}(i\omega_1)\mathcal{G}^{(0)}_{l',-\sigma}(i\omega_1)$$
$$+\delta_{\sigma\sigma'}\mathcal{G}^{(0)}_{l\sigma}(i\omega_1)\mathcal{g}_{l\sigma l'\sigma}(i\omega_1)\mathcal{G}^{(0)}_{l'\sigma}(i\omega_1)-\delta_{\sigma,-\sigma'}\mathcal{G}^{(0)}_{l\sigma}(i\omega_1)\mathcal{g}_{l\sigma l'\sigma'}(i\omega_1)\mathcal{G}^{(0)}_{l'\sigma'}(i\omega_1)]\}.$$

We keep the terms that preserve the spin and have the form $\delta_{\sigma\sigma'}$ and omit the terms with spin-flip

of the form $\delta_{\sigma',-\sigma}$ and also omit the terms that are reciprocally subtracted and differ only by the sign of spin. We take into account that the function $\mathcal{G}_l^{(0)}(i\omega)$ does not depend on spin index and

$$\sum_{\sigma_1}\sigma_1\sigma\mathcal{G}_{l\sigma_1}^{(0)}(i\omega)=0. \tag{51}$$

As a result of these simplifications, we obtain

$$\begin{aligned}&\sum_{l_1\sigma_1 l_2\sigma_2}\tilde{G}_2^{(0)irr}[l\sigma i\omega;l_1\sigma_1 i\omega_1\,|\,l_2\sigma_2 i\omega_2;l'\sigma' i\omega]\mathcal{G}_{l_2\sigma_2}^{(0)}(i\omega_1)\mathcal{g}_{l_2\sigma_2 l_1\sigma_1}(i\omega_1)\mathcal{G}_{l_1\sigma_1}^{(0)}(i\omega_1)\\&=-\frac{1}{2}\beta\delta(\omega-\omega_1)p(i\omega)p(i\omega_1)\delta_{\sigma\sigma'}\mathcal{G}_{l\sigma}^{(0)}(i\omega_1)\mathcal{g}_{l\sigma l'\sigma}(i\omega_1)\mathcal{G}_{l'\sigma}^{(0)}(i\omega_1),\end{aligned} \tag{52}$$

$$\Lambda_{l\sigma l'\sigma'}(i\omega)=\delta_{ll'}\delta_{\sigma\sigma'}[m_l(i\omega)+\frac{p^2(i\omega)}{2}\mathcal{G}_l^{(0)}(i\omega)]+\frac{p^2(i\omega)}{2}\mathcal{G}_l^{(0)}(i\omega)\mathcal{G}_{l'}^{(0)}(i\omega)\mathcal{g}_{l\sigma l'\sigma'}(i\omega), \tag{53}$$

with the following realizations

$$\begin{aligned}\Lambda_{11}(i\omega)&=m_1(i\omega)+\frac{p^2(i\omega)}{2}\mathcal{G}_1^{(0)}(i\omega)+\frac{p^2(i\omega)}{2}[\mathcal{G}_1^{(0)}(i\omega)]^2\mathcal{g}_{11}(i\omega),\\\Lambda_{22}(i\omega)&=m_2(i\omega)+\frac{p^2(i\omega)}{2}\mathcal{G}_2^{(0)}(i\omega)+\frac{p^2(i\omega)}{2}[\mathcal{G}_2^{(0)}(i\omega)]^2\mathcal{g}_{22}(i\omega),\\\Lambda_{12}(i\omega)&=\frac{p^2(i\omega)}{2}\mathcal{G}_1^{(0)}(i\omega)\mathcal{G}_2^{(0)}(i\omega)\mathcal{g}_{12}(i\omega),\end{aligned} \tag{54}$$

We take into account the Dyson type equation

$$\mathcal{g}_{11}(i\omega)=\frac{\Lambda_{11}(i\omega)-\mathcal{G}_2^{(0)}(i\omega)(\Lambda_{11}(i\omega)\Lambda_{22}(i\omega)-\Lambda_{12}(i\omega)\Lambda_{21}(i\omega))}{d(i\omega)},\quad \mathcal{g}_{12}(i\omega)=\frac{\Lambda_{12}(i\omega)}{d(i\omega)},$$

$$d(i\omega)=(1-\Lambda_{11}(i\omega)\mathcal{G}_1^{(0)}(i\omega))(1-\Lambda_{22}(i\omega)\mathcal{G}_2^{(0)}(i\omega))-\mathcal{G}_1^{(0)}(i\omega)\mathcal{G}_2^{(0)}(i\omega)\Lambda_{12}(i\omega)\Lambda_{21}(i\omega)).. \tag{55}$$

We make some generalization by considering function $m(i\omega)$ dependent on orbital quantum number l even if it is really not. The function $\mathcal{g}_{22}$ is obtained from equation (55) by changing indices 1 and 2.

We have found two solutions of equations (54) and (55).

The first of them is

$$\Lambda_{11}(i\omega)=m_1(i\omega),\quad \mathcal{g}_{11}(i\omega)=-\frac{1}{\mathcal{G}_1^{(0)}(i\omega)},$$

$$\Lambda_{22}(i\omega)=\frac{1}{\mathcal{G}_2^{(0)}(i\omega)},\quad \mathcal{g}_{22}(i\omega)=-\frac{1}{\mathcal{G}_2^{(0)}(i\omega)}\left(1+\frac{m_2(i\omega)\mathcal{G}_2^{(0)}(i\omega)-1}{\frac{p^2(i\omega)}{2}(\mathcal{G}_2^{(0)}(i\omega))^2}\right), \tag{56}$$

$$\Lambda_{12}(i\omega)=\Lambda_{21}(i\omega)=\pm\frac{ip(i\omega)}{\sqrt{2}},\ \mathcal{g}_{12}(i\omega)=\pm\frac{i\sqrt{2}}{p(i\omega)\mathcal{G}_1^{(0)}(i\omega)\mathcal{G}_2^{(0)}(i\omega)},$$

with the condition that

$$\frac{1}{\mathcal{G}_1^{(0)}(i\omega)} - m_1(\omega) = \frac{1}{\mathcal{G}_2^{(0)}(i\omega)} - m_2(\omega)\,. \tag{57}$$

The second solution is obtained from (56) by changing indices 1 and 2.

The analytical continuation of obtained solutions in upper half-plane gives us the possibility to determine spectral function of localized electrons:

$$\rho_{ll'}(E) = -2\,\mathrm{Im}\,\mathcal{g}_{ll'}(E + i\delta) \tag{58}$$

For example, the intra-orbital contribution has the form

$$\rho_{11}(E) = -\frac{2\,\mathrm{Im}\,\mathcal{G}_1^{(0)}(E + i\delta)}{\mathrm{Re}(\mathcal{G}_1^{(0)})^2 + \mathrm{Im}(\mathcal{G}_1^{(0)})^2}\,, \tag{59}$$

where

$$\mathrm{Im}\,\mathcal{G}_1^{(0)}(E + i\delta) = -\pi\rho_0(E)\,|V_1|^2 \tag{60}$$

The quantity $\rho_{11}(E)$ differs from zero owing to the existence of the matrix element of hybridization and of the zero order density of states $\rho_0(E)$. This intra-orbital contribution to the impurity states transferred to the Fermi level due to hybridization with band electrons is a direct extension of the result known for the single orbital model.

However, there exists an additional contribution to this transfer caused by inter-orbital correlation effect, which follows from our solution:

$$\rho_{12}(E) = -\,\mathrm{Im}\,\mathcal{g}_{12}(E + i\delta) = \frac{2(E + \Delta E_1)(\Delta E_2 - E)}{\mathrm{Im}\,\mathcal{G}_1^{(0)}(0)\,\mathrm{Im}\,\mathcal{G}_2^{(0)}(0)(\Delta E_1 + \Delta E_2)}, \tag{61}$$

where

$\Delta E_1 = E_2 - E_9 > 0$, $\Delta E_2 = E_{12} - E_9 > 0$.

This quantity is positive for $-\Delta E_1 < E < \Delta E_2$.

Thus, for these energy values, the inter-orbital excitations give a positive contribution to the metallic state.

6. Superconducting state

We shall discuss now the generalization of our previous theory for the case of superconductivity.

Because the orbital quantum number *l* takes, in our model, two values *l* = 1, 2, we can rewrite equation (31) in the form

$$
\begin{aligned}
g_\sigma^{11}(i\omega_n) &= \Lambda_\sigma^{11}(i\omega_n) + \Lambda_\sigma^{11}(i\omega_n)\mathcal{G}_1^{(0)}(i\omega_n)g_\sigma^{11}(i\omega_n) + \Lambda_\sigma^{12}(i\omega)\mathcal{G}_2^{(0)}(i\omega_n)g_\sigma^{21}(i\omega_n) - \\
&\quad Y_{\sigma\bar\sigma}^{11}(i\omega_n)\mathcal{G}_1^{(0)}(-i\omega_n)\,\bar f_{\bar\sigma\sigma}^{11}(i\omega_n) - Y_{\sigma\bar\sigma}^{12}(i\omega_n)\mathcal{G}_2^{(0)}(-i\omega_n)\,\bar f_{\bar\sigma\sigma}^{21}(i\omega_n), \\
g_\sigma^{21}(i\omega_n) &= \Lambda_\sigma^{21}(i\omega_n) + \Lambda_\sigma^{21}(i\omega_n)\mathcal{G}_1^{(0)}(i\omega_n)g_\sigma^{11}(i\omega_n) + \\
&\quad \Lambda_\sigma^{22}(i\omega)\mathcal{G}_2^{(0)}(i\omega_n)g_\sigma^{21}(i\omega_n) - Y_{\sigma\bar\sigma}^{21}(i\omega_n)\mathcal{G}_1^{(0)}(-i\omega_n)\,\bar f_{\bar\sigma\sigma}^{11}(i\omega_n) - \\
&\quad Y_{\sigma\bar\sigma}^{22}(i\omega_n)\mathcal{G}_2^{(0)}(-i\omega_n)\,\bar f_{\bar\sigma\sigma}^{21}(i\omega_n), \\
\bar f_{\bar\sigma\sigma}^{11}(i\omega_n) &= \bar Y_{\bar\sigma\sigma}^{11}(i\omega_n) + \bar Y_{\bar\sigma\sigma}^{11}\mathcal{G}_1^{(0)}(i\omega_n)g_\sigma^{11}(i\omega_n) + \Lambda_{\bar\sigma}^{11}(-i\omega_n)\mathcal{G}_1^{(0)}(-i\omega_n)\,\bar f_{\bar\sigma\sigma}^{11}(i\omega_n) + \\
&\quad \bar Y_{\bar\sigma\sigma}^{12}(i\omega_n)\mathcal{G}_2^{(0)}(i\omega_n)g_\sigma^{21}(i\omega_n) + \Lambda_{\bar\sigma}^{21}(-i\omega_n)\mathcal{G}_2^{(0)}(-i\omega_n)\,\bar f_{\bar\sigma\sigma}^{21}(i\omega_n), \\
\bar f_{\bar\sigma\sigma}^{21}(i\omega_n) &= \bar Y_{\bar\sigma\sigma}^{21}(i\omega_n) + \bar Y_{\bar\sigma\sigma}^{21}(i\omega_n)\mathcal{G}_1^{(0)}(i\omega_n)g_\sigma^{11}(i\omega_n) + \Lambda_{\bar\sigma}^{12}(-i\omega_n)\mathcal{G}_1^{(0)}(-i\omega_n)\,\bar f_{\bar\sigma\sigma}^{11}(i\omega_n) + \\
&\quad \bar Y_{\bar\sigma\sigma}^{22}(i\omega_n)\mathcal{G}_2^{(0)}(i\omega_n)g_\sigma^{21}(i\omega_n) + \Lambda_{\bar\sigma}^{22}(-i\omega_n)\mathcal{G}_2^{(0)}(-i\omega_n)\,\bar f_{\bar\sigma\sigma}^{21}(i\omega_n).
\end{aligned}
\tag{62}
$$

Here $\Lambda_\sigma^{ll'}(i\omega_n)$, $Y_{\sigma\bar\sigma}^{ll'}(i\omega_n)$ and $\bar Y_{\bar\sigma\sigma}^{ll'}(i\omega_n)$ are the correlation functions of superconducting state and $g_\sigma^{ll'}(i\omega_n)$ and $\bar f_{\bar\sigma\sigma}^{ll'}(i\omega_n)$ are the full normal and anomalous one-particle Green's functions.

The other system of four equations for quantities g_σ^{12}, g_σ^{22}, $\bar f_{\bar\sigma\sigma}^{12}$, and $\bar f_{\bar\sigma\sigma}^{22}$ can be formulated. We introduce the definition

$$
Q_\sigma^l(i\omega_n) = 1 - \Lambda_\sigma^{ll}(i\omega_n)\mathcal{G}_\sigma^{l(0)}(i\omega_n) \tag{63}
$$

and find the determinant of fourth order $D_4(i\omega_n)$:

$$
D_4(i\omega_n) = \begin{vmatrix}
Q_\sigma^1(i\omega_n), & -\Lambda_\sigma^{12}(i\omega_n)\mathcal{G}_2^{(0)}(i\omega_n) & Y_{\sigma\bar\sigma}^{11}(i\omega_n)\mathcal{G}_1^{(0)}(-i\omega_n) & Y_{\sigma\bar\sigma}^{12}(i\omega_n)\mathcal{G}_2^{(0)}(-i\omega_n) \\
-\Lambda_\sigma^{21}(i\omega_n)\mathcal{G}_1^{(0)}(i\omega_n) & Q_\sigma^2(i\omega_n) & Y_{\sigma\bar\sigma}^{21}(i\omega_n)\mathcal{G}_1^{(0)}(-i\omega_n) & Y_{\sigma\bar\sigma}^{22}(i\omega_n)\mathcal{G}_2^{(0)}(-i\omega_n) \\
-\bar Y_{\bar\sigma\sigma}^{11}(i\omega_n)\mathcal{G}_1^{(0)}(i\omega_n) & -\bar Y_{\bar\sigma\sigma}^{12}(i\omega_n)\mathcal{G}_2^{(0)}(i\omega_n) & Q_{\bar\sigma}^1(-i\omega_n) & -\Lambda_{\bar\sigma}^{21}(-i\omega_n)\mathcal{G}_2^{(0)}(-i\omega_n) \\
-\bar Y_{\bar\sigma\sigma}^{21}(i\omega_n)\mathcal{G}_1^{(0)}(i\omega_n) & -\bar Y_{\bar\sigma\sigma}^{22}(i\omega_n)\mathcal{G}_2^{(0)}(i\omega_n) & -\Lambda_{\bar\sigma}^{12}(-i\omega_n)\mathcal{G}_1^{(0)}(-i\omega_n) & Q_{\bar\sigma}^2(-i\omega_n)
\end{vmatrix}
\tag{64}
$$

These equations are the Dyson-type equations and they establish the relations between propagators g, f and $\bar f$ and correlation functions Λ, Y and $\bar Y$. Anomalous correlation functions have the properties of the order parameters Y and $\bar Y$ of the superconducting state.

The system of equation (62) permits us to obtain for $T = T_c$ such linear dependences:

$$
\begin{aligned}
\Delta_4(i\omega_n)\,\bar f_{\bar\sigma\sigma}^{11}(i\omega_n) &= \bar Y_{\bar\sigma\sigma}^{11}Q_\sigma^2(i\omega_n)Q_{\bar\sigma}^2(-i\omega_n) + \bar Y_{\bar\sigma\sigma}^{12}(i\omega_n)Q_{\bar\sigma}^2(-i\omega_n)\Lambda_\sigma^{21}(i\omega_n)\mathcal{G}_2^{(0)}(i\omega_n) + \\
&\quad \bar Y_{\bar\sigma\sigma}^{21}(i\omega_n)\Lambda_{\bar\sigma}^{21}(-i\omega_n)\mathcal{G}_2^{(0)}(-i\omega_n)Q_\sigma^2(i\omega_n) + \\
&\quad \bar Y_{\bar\sigma\sigma}^{22}(i\omega_n)\Lambda_{\bar\sigma}^{21}(-i\omega_n)\Lambda_\sigma^{21}(i\omega_n)\mathcal{G}_2^{(0)}(i\omega_n)\mathcal{G}_2^{(0)}(-i\omega_n), \\
\Delta_4(i\omega_n)\,\bar f_{\bar\sigma\sigma}^{21}(i\omega_n) &= Q_\sigma^2(i\omega_n)\bar Y_{\bar\sigma\sigma}^{11}(i\omega_n)\Lambda_{\bar\sigma}^{12}(-i\omega_n)\mathcal{G}_1^{(0)}(-i\omega_n) + Q_\sigma^2(i\omega_n)\bar Y_{\bar\sigma\sigma}^{21}(i\omega_n)Q_{\bar\sigma}^1(-i\omega_n) + \\
&\quad \bar Y_{\bar\sigma\sigma}^{12}(i\omega_n)\Lambda_{\bar\sigma}^{12}(-i\omega_n)\Lambda_\sigma^{21}(i\omega_n)\mathcal{G}_2^{(0)}(i\omega_n)\mathcal{G}_1^{(0)}(-i\omega_n) + \\
&\quad \bar Y_{\bar\sigma\sigma}^{22}(i\omega_n)Q_{\bar\sigma}^1(-i\omega_n)\Lambda_\sigma^{21}(i\omega_n)\mathcal{G}_2^{(0)}(i\omega_n), \\
\Delta_4(i\omega_n)\,\bar f_{\bar\sigma\sigma}^{22}(i\omega_n) &= \bar Y_{\bar\sigma\sigma}^{22}Q_\sigma^1(i\omega_n)Q_{\bar\sigma}^1(-i\omega_n) + \bar Y_{\bar\sigma\sigma}^{21}(i\omega_n)Q_{\bar\sigma}^1(-i\omega_n)\Lambda_\sigma^{12}(i\omega_n)\mathcal{G}_1^{(0)}(i\omega_n) + \\
&\quad \bar Y_{\bar\sigma\sigma}^{12}(i\omega_n)\Lambda_{\bar\sigma}^{12}(-i\omega_n)\mathcal{G}_1^{(0)}(-i\omega_n)Q_\sigma^1(i\omega_n) + \\
&\quad \bar Y_{\bar\sigma\sigma}^{22}(i\omega_n)\Lambda_{\bar\sigma}^{12}(-i\omega_n)\Lambda_\sigma^{12}(i\omega_n)\mathcal{G}_1^{(0)}(i\omega_n)\mathcal{G}_1^{(0)}(-i\omega_n), \\
\Delta_4(i\omega_n)\,\bar f_{\bar\sigma\sigma}^{12}(i\omega_n) &= Q_\sigma^1(i\omega_n)\bar Y_{\bar\sigma\sigma}^{22}(i\omega_n)\Lambda_{\bar\sigma}^{21}(-i\omega_n)\mathcal{G}_2^{(0)}(-i\omega_n) + Q_\sigma^1(i\omega_n)\bar Y_{\bar\sigma\sigma}^{12}(i\omega_n)Q_{\bar\sigma}^2(-i\omega_n) + \\
&\quad \bar Y_{\bar\sigma\sigma}^{21}(i\omega_n)\Lambda_{\bar\sigma}^{21}(-i\omega_n)\Lambda_\sigma^{12}(i\omega_n)\mathcal{G}_1^{(0)}(i\omega_n)\mathcal{G}_2^{(0)}(-i\omega_n) + \\
&\quad \bar Y_{\bar\sigma\sigma}^{11}(i\omega_n)Q_{\bar\sigma}^2(-i\omega_n)\Lambda_\sigma^{12}(i\omega_n)\mathcal{G}_1^{(0)}(i\omega_n),
\end{aligned}
\tag{65}
$$

where $\Delta_4(i\omega_n)$ is equal to $D_4(i\omega_n)$ with equated to zero the order parameters Y and $\bar{Y}$:

$$\Delta_4(i\omega_n) = (Q^1_\sigma(i\omega_n)Q^2_\sigma(i\omega_n) - \Lambda^{12}_\sigma(i\omega_n)\Lambda^{21}_\sigma(i\omega_n)\mathcal{G}^{(0)}_1(i\omega_n)\mathcal{G}^{(0)}_2(i\omega_n))\times$$
$$(Q^1_{\bar\sigma}(-i\omega_n)Q^2_{\bar\sigma}(-i\omega_n) - \Lambda^{12}_{\bar\sigma}(-i\omega_n)\Lambda^{21}_{\bar\sigma}(-i\omega_n)\mathcal{G}^{(0)}_1(-i\omega_n)\mathcal{G}^{(0)}_2(-i\omega_n)). \tag{66}$$

The system of equations (65) is not closed because up till now we have not the dependence of the correlation functions Λ, Y and $\bar{Y}$ on the electron propagators.

This dependence can be the result of infinite summation of the diagrams and certainly is a consequence of some approximations. Our main approximations are depicted in Fig. 3.

We shall now make our approximation (see Fig. 5), which determines the correlation function $\bar{Y}$ as a result of summing a class of ladder diagrams, more precise.

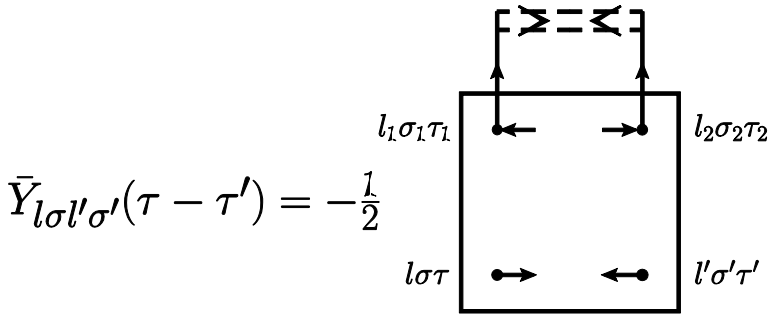

Fig. 5. The ladder approximation for $\bar{Y}$ correlation function. The double dashed line is the full anomalous Green's function of impurity electrons. The solid thin lines are conduction electron Green's functions. The rectangle depicts the simplest irreducible Green's function.

The approximation leads to the following analytical result

$$\bar{Y}^{ll'}_{\sigma\sigma'}(i\omega) \approx -\frac{1}{2\beta}\sum_{\omega_1}\sum_{l_1\sigma_1 l_2\sigma_2}\tilde{G}^{(0)irr}_2[l_1\sigma_1, -i\omega_1; l_2\sigma_2 i\omega_1 \,|\, l\sigma, -i\omega; l'\sigma' i\omega]\times$$
$$\mathcal{G}^{(0)}_{l_1\sigma_1}(-i\omega_1)\,\bar{f}^{l_1 l_2}_{\sigma_1\sigma_2}(i\omega_1)\mathcal{G}^{(0)}_{l_2\sigma_2}(i\omega_1), \tag{67}$$

where

$$G^{irr}_2[l_1\sigma_1 i\omega_1; l_2\sigma_2 i\omega_2 \,|\, l_3\sigma_3 i\omega_3; l_4\sigma_4 i\omega_4] = \beta\delta(\omega_1+\omega_2-\omega_3-\omega_4)\times$$
$$\tilde{G}^{(0)irr}_2[l_1\sigma_1 i\omega_1; l_2\sigma_2 i\omega_2 \,|\, l_3\sigma_3 i\omega_3; l_4\sigma_4 i\omega_4], \tag{68}$$

$$\tilde{G}^{(0)irr}_2[l_1\sigma_1 i\omega_1; l_2\sigma_2 i\omega_2 \,|\, l_3\sigma_3 i\omega_3; l_4\sigma_4 i\omega_4] = \frac{1}{6}p(i\omega_1)p(i\omega_2)\times$$
$$(\beta\delta(\omega_1-\omega_4)\delta_{l_1l_4}\delta_{l_2l_3}[2\delta_{\sigma_1,-\sigma_4}\delta_{\sigma_2,-\sigma_3}\delta_{\sigma_2\sigma_4} + \delta_{\sigma_1\sigma_3}\delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3} - \delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3}\delta_{\sigma_3,-\sigma_1}] -$$
$$\beta\delta(\omega_1-\omega_3)\delta_{l_1l_3}\delta_{l_2l_4}[2\delta_{\sigma_1,-\sigma_3}\delta_{\sigma_2,-\sigma_4}\delta_{\sigma_2\sigma_3} + \delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}\delta_{\sigma_1\sigma_4} - \delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}\delta_{\sigma_4,-\sigma_1}]). \tag{69}$$

By using the anti-symmetry property which is the consequence of the Pauli principle

$$\bar{f}^{ll'}_{\sigma\sigma'}(i\omega_n) = -\bar{f}^{l'l}_{\sigma'\sigma}(-i\omega_n), \tag{70}$$

we can transform the above equation and obtain a more simple one:

$$\bar{Y}^{ll'}_{\sigma\sigma'}(i\omega_n) = \frac{1}{6}[\delta_{\sigma\sigma'} q_{l'\sigma}(i\omega_n) q_{l\sigma}(-i\omega_n)\, \bar{f}^{ll'}_{\sigma\sigma}(i\omega_n) - \\ -\delta_{\sigma'\bar{\sigma}} q_{l\sigma}(-i\omega_n) q_{l'\bar{\sigma}}(i\omega_n)\, \bar{f}^{ll'}_{\sigma\bar{\sigma}}(i\omega_n) + 2\delta_{\sigma'\bar{\sigma}} q_{l'\sigma}(i\omega_n) q_{l\bar{\sigma}}(-i\omega_n)\, \bar{f}^{ll'}_{\bar{\sigma}\sigma}(i\omega_n)], \tag{71}$$

where

$$q_{l\sigma} = p(i\omega_n) G^{(0)}_{l\sigma}(i\omega_n). \tag{72}$$

As can be seen there are two different possibilities for correlation function $\bar{Y}$:
one diagonal by spin indices

$$\bar{Y}^{ll'}_{\sigma\sigma}(i\omega_n) = \frac{1}{6} q_{l\sigma}(-i\omega_n) q_{l'\sigma}(i\omega_n)\, \bar{f}^{ll'}_{\sigma\sigma}(i\omega_n), \tag{73}$$

and second non diagonal by spin indices

$$\bar{Y}^{ll'}_{\sigma\bar{\sigma}}(i\omega_n) = \frac{1}{6} q_{l\sigma}(-i\omega_n) q_{l'\bar{\sigma}}(i\omega_n)(2\,\bar{f}^{ll'}_{\bar{\sigma}\sigma}(i\omega_n) - \bar{f}^{ll'}_{\sigma\bar{\sigma}}(i\omega_n)). \tag{74}$$

The diagonal solution belongs to the triplet superconductivity; the non diagonal, to the singlet case.

We suppose that, in the last case, the change in the order of the spin indices is accompanied by a change in the sign of the function.

In this way, we obtain

$$\bar{Y}^{ll'}_{\bar{\sigma}\sigma}(i\omega_n) = \frac{1}{2} q_l(-i\omega_n) q_{l'}(i\omega_n)\, \bar{f}^{ll'}_{\bar{\sigma}\sigma}(i\omega_n). \tag{75}$$

Both possibilities can be joined in the form

$$\bar{Y}^{ll'}(i\omega_n) = \lambda q_l(-i\omega_n) q_{l'}(i\omega_n)\, \bar{f}^{ll'}(i\omega_n), \tag{76}$$

where $\lambda = -\frac{1}{2}$ for singlet and $\lambda = \frac{1}{6}$ for triplet superconductivity.

7. Critical temperature

Now we come back to the system of linearized equations (65) and substitute the propagators $\bar{f}^{ll'}_{\bar{\sigma}\sigma}$ by their values obtained from equation (76). The result of this substitution is the following system of linear equations for the components of order parameter $\bar{Y}^{ll'}_{\bar{\sigma}\sigma}$

$$\left[Q_\sigma^2(i\omega_n)Q_{\bar\sigma}^2(-i\omega_n)-\frac{\Delta_4}{\lambda q_1(-i\omega_n)q_1(i\omega_n)}\right]\bar Y_{\bar\sigma\sigma}^{11}(i\omega_n)+\mathcal{G}_2^{(0)}(i\omega_n)(Q_\sigma^2(-i\omega_n)\Lambda_\sigma^{21}(i\omega_n)\bar Y_{\bar\sigma\sigma}^{12}(i\omega_n)+$$
$$\mathcal{G}_2^{(0)}(-i\omega_n)Q_\sigma^2(i\omega_n)\Lambda_{\bar\sigma}^{21}(-i\omega_n)\bar Y_{\bar\sigma\sigma}^{21}(i\omega_n)+$$
$$\mathcal{G}_2^{(0)}(-i\omega_n)\mathcal{G}_2^{(0)}(i\omega_n)\Lambda_\sigma^{21}(i\omega_n)\Lambda_{\bar\sigma}^{21}(-i\omega_n)\bar Y_{\bar\sigma\sigma}^{22}(i\omega_n)=0,$$
$$\mathcal{G}_1^{(0)}(i\omega_n)(Q_{\bar\sigma}^2(-i\omega_n)\Lambda_\sigma^{12}(i\omega_n)\bar Y_{\bar\sigma\sigma}^{11}(i\omega_n)+\left[Q_\sigma^1(i\omega_n)Q_{\bar\sigma}^2(-i\omega_n)-\frac{\Delta_4}{\lambda q_1(-i\omega_n)q_2(i\omega_n)}\right]\bar Y_{\bar\sigma\sigma}^{12}(i\omega_n))+$$
$$\mathcal{G}_2^{(0)}(-i\omega_n)\mathcal{G}_1^{(0)}(i\omega_n)\Lambda_\sigma^{12}(i\omega_n)\bar Y_{\bar\sigma\sigma}^{21}(i\omega_n)+$$
$$\mathcal{G}_2^{(0)}(-i\omega_n)Q_\sigma^1(i\omega_n)\Lambda_{\bar\sigma}^{21}(-i\omega_n)\bar Y_{\bar\sigma\sigma}^{22}(i\omega_n)=0,$$
$$\mathcal{G}_1^{(0)}(-i\omega_n)Q_\sigma^2(i\omega_n)\Lambda_{\bar\sigma}^{21}(-i\omega_n)\bar Y_{\bar\sigma\sigma}^{11}(i\omega_n)+\mathcal{G}_1^{(0)}(-i\omega_n)\mathcal{G}_2^{(0)}(i\omega_n)\Lambda_\sigma^{21}(i\omega_n)\Lambda_{\bar\sigma}^{12}(-i\omega_n)\bar Y_{\bar\sigma\sigma}^{12}(i\omega_n)+$$
$$\left[Q_\sigma^2(i\omega_n)Q_{\bar\sigma}^1(-i\omega_n)-\frac{\Delta_4}{\lambda q_2(-i\omega_n)q_1(i\omega_n)}\right]\bar Y_{\bar\sigma\sigma}^{21}(i\omega_n)+$$
$$\mathcal{G}_2^{(0)}(i\omega_n)Q_{\bar\sigma}^1(-i\omega_n)\Lambda_\sigma^{21}(i\omega_n)\bar Y_{\bar\sigma\sigma}^{22}(i\omega_n)=0,$$
$$\mathcal{G}_1^{(0)}(-i\omega_n)\mathcal{G}_1^{(0)}(i\omega_n)\Lambda_\sigma^{12}(i\omega_n)\Lambda_{\bar\sigma}^{12}(-i\omega_n)\bar Y_{\bar\sigma\sigma}^{11}(i\omega_n)+\mathcal{G}_1^{(0)}(-i\omega_n)Q_\sigma^1(i\omega_n)\Lambda_{\bar\sigma}^{12}(-i\omega_n)\bar Y_{\bar\sigma\sigma}^{12}(i\omega_n)+$$
$$\mathcal{G}_1^{(0)}(i\omega_n)Q_{\bar\sigma}^1(-i\omega_n)\Lambda_\sigma^{12}(i\omega_n)\bar Y_{\bar\sigma\sigma}^{21}(i\omega_n)+$$
$$\left[Q_\sigma^1(i\omega_n)Q_{\bar\sigma}^1(-i\omega_n)-\frac{\Delta_4}{\lambda q_2(-i\omega_n)q_2(i\omega_n)}\right]\bar Y_{\bar\sigma\sigma}^{22}(i\omega_n)=0, \tag{77}$$

where Δ_4 is equal to (66).

Determinant D_s of this linear system of equations must be zero:

$$\begin{vmatrix} Q_\sigma^2(k)Q_{\bar\sigma}^2(-k)-\frac{\Delta_4}{\lambda q_1(-k)q_1(k)} & \mathcal{G}_2^{(0)}(k)Q_{\bar\sigma}^2(-k)\Lambda_\sigma^{21}(k) & \mathcal{G}_2^{(0)}(-k)Q_\sigma^2(k)\Lambda_{\bar\sigma}^{21}(-k) & \mathcal{G}_2^{(0)}(-k)\mathcal{G}_2^{(0)}(k)\Lambda_\sigma^{21}(k)\Lambda_{\bar\sigma}^{21}(-k) \\ \mathcal{G}_1^{(0)}(k)Q_{\bar\sigma}^2(-k)\Lambda_\sigma^{12}(k) & Q_\sigma^1(k)Q_{\bar\sigma}^2(-k)-\frac{\Delta_4}{\lambda q_1(-k)q_2(k)} & \mathcal{G}_2^{(0)}(-k)\mathcal{G}_1^{(0)}(k)\Lambda_\sigma^{12}(k)\Lambda_{\bar\sigma}^{21}(-k) & \mathcal{G}_2^{(0)}(-k)Q_\sigma^1(k)\Lambda_{\bar\sigma}^{21}(-k) \\ \mathcal{G}_1^{(0)}(-k)Q_\sigma^2(k)\Lambda_{\bar\sigma}^{21}(-k) & \mathcal{G}_1^{(0)}(-k)\mathcal{G}_2^{(0)}(k)\Lambda_\sigma^{21}(k)\Lambda_{\bar\sigma}^{12}(-k) & Q_\sigma^2(k)Q_{\bar\sigma}^1(-k)-\frac{\Delta_4}{\lambda q_2(-k)q_1(k)} & \mathcal{G}_2^{(0)}(k)Q_{\bar\sigma}^1(-k)\Lambda_\sigma^{21}(k) \\ \mathcal{G}_1^{(0)}(-k)\mathcal{G}_1^{(0)}(k)\Lambda_\sigma^{12}(k)\Lambda_{\bar\sigma}^{12}(-k) & \mathcal{G}_1^{(0)}(-k)Q_\sigma^1(k)\Lambda_{\bar\sigma}^{12}(-k) & \mathcal{G}_1^{(0)}(k)Q_{\bar\sigma}^1(-k)\Lambda_\sigma^{12}(k) & Q_\sigma^1(k)Q_{\bar\sigma}^1(-k)-\frac{\Delta_4}{\lambda q_2(-k)q_2(k)} \end{vmatrix}=0, \tag{78}$$

where $k=i\omega_n$.

This condition determines the free parameter of the theory and, as usual, defines the critical temperature T_c. In our case, the critical temperature is present in the dependence of the Matsubara frequencies on T_c: $\omega_n=(2n+1)\pi k_B T_c$.

To determine the value of T_c, we put λ equal to value $-\frac{1}{2}$ which corresponds to the singlet state and preserve equation (78).

The other argument that supports the choice of $\lambda=-\frac{1}{2}$ is the approximation based on the equality to zero of the functions $Q_\sigma^l(i\omega_n)=0$. In this special case, equation (78) is reduced to the simple form

$$D_s=(\Delta_4^{(0)})^2\left[\frac{\Delta_4^{(0)}}{\lambda^2 q_1(-i\omega_n)q_1(i\omega_n)q_2(-i\omega_n)q_2(i\omega_n)}-1\right]^2 \tag{79}$$

where $\Delta_4^{(0)}$ is Δ_4 with the condition $Q_\sigma^l(i\omega_n)=0$:

$$\Delta_4^{(0)}=\mathcal{G}_1^{(0)}(i\omega_n)\mathcal{G}_1^{(0)}(-i\omega_n)\mathcal{G}_2^{(0)}(i\omega_n)\mathcal{G}_2^{(0)}(-i\omega_n)\Lambda_\sigma^{12}(i\omega_n)\Lambda_{\bar\sigma}^{12}(-i\omega_n)\Lambda_\sigma^{21}(i\omega_n)\Lambda_{\bar\sigma}^{21}(-i\omega_n).$$

By taking into account the solutions (56)

$$\Lambda_\sigma^{12}(i\omega_n)\Lambda_\sigma^{21}(i\omega_n)=-\frac{p^2(i\omega_n)}{2}$$

and the definition of q_σ^l, we obtain

$$D_s=(\Delta_4^{(0)})^2\left(\frac{1}{(2\lambda)^2}-1\right)^2=0, \tag{80}$$

that is, the condition $\lambda=-\frac{1}{2}$.

8. Conclusions

We have constructed the strong-coupling diagram perturbation theory approach for the investigation of the twofold degenerate Anderson impurity model.

First of all, the eigenfunctions and eigenvalues of energy of the localized *d*-electron part of the Hamiltonian have been determined. Their dependence of intra- and inter-orbital Coulomb interactions and of Hund rule coupling constant was established.

The perturbation theory around the atomic limit has been developed, and Matsubara Green's functions in the normal and superconducting states have been defined.

Dyson-type equations for these functions have been obtained for both states, and their analytic solutions have been discussed in detail.

Since the main elements of our diagram technique are the irreducible Green's functions, we have carried out the calculation of simplest two-particle irreducible Green's function and determined its dependence on the spin and orbital quantum numbers. This quantity, which has been found only in the low temperature limit, is approximated by taking into account the contributions of statistical weight $e^{-\beta E_9}$, by assuming that the ground state of our system is dominated by the two-particle triplet state E_9.

Having this quantity and summing some class of diagrams, we have obtained the $\Lambda_{l\sigma l'\sigma'}$ correlation function.

We found two solutions for the renormalized Green's functions of the *d*-electrons and determined the spectral weight.

We have proved that orbital degeneracy gives an additional contribution to "metallization" of the impurity states, i.e., to an enhanced transfer of spectral weight to the Fermi level.

We have obtained an approximate expression for anomalous correlation functions and, in particular, for superconducting order parameters.

We have investigated the linearized equations for order parameters and formulated the condition for the realization of singlet superconductivity and determination of the critical temperature.

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