Diagrammatic theory for twofold degenerate Anderson impurity model

V. A. Moskalenko\textsuperscript{1,2}, L. A. Dohotaru\textsuperscript{3}, D. F. Digor\textsuperscript{1} and I. D. Cebotari\textsuperscript{1}

December 11, 2013

\textsuperscript{1}Institute of Applied Physics, Moldova Academy of Sciences, Chisinau 2028, Moldova,
\textsuperscript{2}BLTP, Joint Institute for Nuclear Research, 141980 Dubna, Russia,
\textsuperscript{3}Technical University, Chisinau 2004, Moldova

Abstract

The twofold degenerate Anderson impurity model \cite{1-4} is investigated and the strong electronic correlations of d-electrons of impurity ion are taken into account by elaborating suitable diagram technique.

We discuss the properties of the Slater-Kanamori model \cite{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 equation for the renormalized one-particle propagator. Diagrammatic theory has been developed and correlation function determined. Special diagrammatic approximation was discussed and summation of diagram has been considered.

PACS numbers: 71.27.+a, 71.10.Fd

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 as a result of 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\textsubscript{60} materials orbital degeneracy is not completely eliminated and orbital effects are important. For instance, orbital degeneracy plays essential role in the Mott metal-insulator transition. Here the effects of Hund’s rule coupling in our orbitally degenerated model are studied with diagrammatic approach.

We study the influence of the intra-atomic Coulomb interactions of the two electrons with opposite spins situated on the same or different orbitals and intra-atomic exchange is analyzed.

Our investigation is based on the diagram theory elaborated for strongly correlated electron systems as in non-degenerated \cite{5-9,11-14} and as in twofold degenerated ones \cite{10}.

The paper has the following structure. In Sec. 1 we describe the twofold degenerate Anderson impurity model. The local properties of our model are considered in Sec. 2. The perturbation theory around the atomic limit of impurity ion is formulated in Sec. 3. In this section we discuss the process of delocalization and renormalization of the dynamical quantities. In Sec. 4 the simplest irreducible Green’s function is calculated. Sec. 5 is devoted to discussion of the Mott-Hubbard phase transition. Sec. 6 is devoted to the conclusions.
The Anderson Impurity model with twofold orbital degeneracy has the Hamiltonian composed one part of conduction electrons - one part of interacting localized and strongly correlated electrons and of hybridization term between these two parts [1-4]:

\[
\begin{align*}
H &= H^0 + H_{\text{int}}, \\
H^0 &= H^0_c + H^0_d, \\
H^0_c &= \sum_{\vec{k}l\sigma} \epsilon_{l}(\vec{k}) C^+_{\vec{k}l\sigma} C_{\vec{k}l\sigma}, \\
H^0_d &= \sum_{\sigma} \epsilon_{d}(\vec{k}) d^+_{\vec{k}l\sigma} d_{\vec{k}l\sigma} + U \sum_{l} n_{l\uparrow} n_{l\downarrow} + U' n_{1\uparrow} n_{2\downarrow} + I_H \sum_{\sigma} d^+_{1\sigma} a_{2\sigma} d_{1\sigma'} a_{2\sigma'}, \\
H_{\text{int}} &= \frac{1}{\sqrt{N}} \sum_{\vec{k}l\sigma} (V_{\vec{k}l} d^+_{\vec{k}l\sigma} C_{\vec{k}l\sigma} + V_{\vec{k}l}^* C^+_{\vec{k}l\sigma} d_{\vec{k}l\sigma}),
\end{align*}
\]  

(1) (2) (3) (4) (5)

where the local Hamiltonian \(H^0_d\) is standard Slater-Kanamori [2-4] form, \(C_{\vec{k}l\sigma}\) is conduction electron annihilation operator with momentum \(\vec{k}\), orbital number \(l = 1, 2\), and spin \(\sigma = \pm 1(\uparrow, \downarrow)\), \(d_{\vec{k}l\sigma}\) operator for localized \(d\) electron. Conduction electron of \(l - \theta\) 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 Coulomb repulsion between the \(d\)-electrons in the same orbital state and \(U'\) - between electrons in different orbital states. \(I_H\) is coefficient of the Hund’s rule coupling and pair hopping terms, \(\epsilon_{l}(\vec{k})\) is the band dispersion and \(\epsilon^d\) - is impurity ion energy evaluated from the chemical potential \(\mu\). \(N\) is a number of lattice sites.

In the following we assume that the symmetry of the system is such that exist the relation:

\[
U' = U - 2I_H, \quad I'_H = I_H.
\]  

(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 for degenerated systems. Such generalization has been discussed, for example, in the case of twofold degenerate Hubbard model [10]. 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.

\section{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, \(H^0_d\), can be diagonalized by using Hubbard transfer operators \(\chi^{mn} = |m\rangle\langle n|\) where \(|m\rangle\) is eigenvector of operator \(H^0_d\) [5].

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

There are the following eigenvectors of operator \(H^0_d\). The first quantum state \(|1\rangle\) is the vacuum state \(|0\rangle\) with energy \(E_1 = 0\). There are 4 one particle states with spin \(S = \frac{1}{2}\) and \(S_z = \pm \frac{1}{2}\): \(|2\rangle = d^+_{1\uparrow} |0\rangle, |3\rangle = d^+_{2\uparrow} |0\rangle, |4\rangle = d^+_{1\downarrow} |0\rangle\) and \(|5\rangle = d^+_{2\downarrow} |0\rangle\). The energies of all these states are \(E_2 = E_3 = E_4 = E_5 = \epsilon_d\).
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 $S_z = -1, 0, 1$,

$|6\rangle = \frac{1}{\sqrt{2}} (d^+_{1\uparrow}d^+_{1\downarrow} - d^+_{2\uparrow}d^+_{2\downarrow}) |0\rangle$, $|7\rangle = \frac{1}{\sqrt{2}} (d^+_{1\uparrow}d^+_{1\downarrow} + d^+_{2\uparrow}d^+_{2\downarrow}) |0\rangle$, $|8\rangle = \frac{1}{\sqrt{2}} (d^+_{1\uparrow}d^+_{2\downarrow} - d^+_{1\downarrow}d^+_{2\uparrow}) |0\rangle$, $|9\rangle = d^+_{1\uparrow}d^+_{2\downarrow} |0\rangle$,

$|10\rangle = \frac{1}{\sqrt{2}} (d^+_{1\uparrow}d^+_{2\downarrow} + d^+_{1\downarrow}d^+_{2\uparrow}) |0\rangle$, $|11\rangle = d^+_{1\uparrow}d^+_{2\uparrow} |0\rangle$.

The eigenvalues of these quantum states are

$E_6 = 2\epsilon_d + U - I_H$, $E_7 = 2\epsilon_d + U + I_H$, $E_8 = 2\epsilon_d + U' + I_H$, $E_9 = E_{10} = E_{11} = 2\epsilon_d + U' - I_H$.

Then there are four states composed from three particles

$|12\rangle = d^+_{1\uparrow}d^+_{1\downarrow}d^+_{2\downarrow} |0\rangle$, $|13\rangle = d^+_{1\uparrow}d^+_{2\downarrow}d^+_{2\downarrow} |0\rangle$, $|14\rangle = d^+_{1\uparrow}d^+_{2\uparrow}d^+_{2\downarrow} |0\rangle$, $|15\rangle = d^+_{2\uparrow}d^+_{2\downarrow}d^+_{1\downarrow} |0\rangle$,

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

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 $E_{16} = 4\epsilon_d + 2U + 4U' - 2I_H$.

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

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

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

Quantum states enumerated above permit us to organize Hubbard transfer operators $\chi^{mn}$ and establish the relation with fermion impurity operators $|10\rangle$:

\[
    d^+_{l\sigma} = \chi^{2l-\sigma,1} + \frac{\sigma}{\sqrt{2}} [(-1)^l\chi^{6,2l+\sigma} + \chi^{7,2l+\sigma}] + \frac{1}{\sqrt{2}} [\sigma\chi^{8,5-l+\sigma} + (-1)^{l+1}\chi^{10,5-l+\sigma}]
    + \frac{1}{\sqrt{2}} [-\chi^{12,l-\sigma,8} + \sigma(-1)^{l-1}\chi^{12,l-\sigma,10}] + \frac{1}{\sqrt{2}} [(-1)^l\chi^{15,l-\sigma,6} + \chi^{15,l-\sigma,7}]
    + (-1)^{l+1}\chi^{10,-5-l+\sigma} + (-1)^{l+1}\chi^{12,l+\sigma,10+\sigma} + \sigma\chi^{16,5-l+\sigma}.
\]

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

\[
    n_{l\sigma} = \chi^{2l-\sigma,2l+\sigma} + \frac{1}{\sqrt{2}} [\chi^{6,6} + (-1)^l\chi^{6,7} + (-1)^{l+1}\chi^{7,6} + X^{7,7}]
    + \frac{1}{2} [\chi^{8,8} + \sigma(-1)^{l+1}\chi^{8,10} + \sigma(-1)^{l+1}\chi^{10,8} + \chi^{10,10}]
    + \chi^{10,-5-\sigma,10-\sigma} + \chi^{12,l+\sigma,12,l-\sigma} + \chi^{12,l+\sigma,12,l+\sigma}
    + \chi^{15,l-\sigma,15,l-\sigma} + \chi^{16,16},
\]

and

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

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

\[
    n_{l\uparrow}(\tau) - n_{l\downarrow}(\tau) = \chi^{1+l,1+l} - \chi^{3+l,3+l} + (-1)^{l+1}[\chi^{8,10} e^{\tau(E_6 - E_{10})}
    + \chi^{10,8} e^{\tau(E_{10} - E_8)}] + \chi^{9,9} - \chi^{11,11} + \chi^{14-l,14-l} - \chi^{16-l,16-l}.
\]

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

\[
    (n_{l\uparrow}(\tau) - n_{l\downarrow}(\tau))(n_{l'\uparrow}(0) - n_{l'\downarrow}(0)) = \delta_{ll'} [\chi^{1+l,1+l} + \chi^{3+l,3+l} + \chi^{14-l,14-l} + \chi^{16-l,16-l}]
    + (-1)^{l+l'} [\chi^{8,8} e^{\tau(E_6 - E_{10})} + \chi^{10,10} e^{\tau(E_{10} - E_8)}] + \chi^{9,9} + \chi^{11,11},
\]
\[
\sum_{ll'} (n_{l\uparrow}(\tau) - n_{l\downarrow}(\tau))(n_{l'\uparrow}(0) - n_{l'\downarrow}(0)) = \frac{4}{Z_0} (e^{-\beta E_2} + e^{-\beta E_1} + 2e^{-\beta E_0}). \tag{12}
\]

In special case \(l = 1, l' = 2\) we have:
\[
(n_{1\uparrow}(\tau) - n_{1\downarrow}(\tau))(n_{2\uparrow}(0) - n_{2\downarrow}(0)) = -[\chi_{8,8}e^{\tau(E_8-E_{10})} + \chi_{10,10}e^{\tau(E_{10}-E_8)}] + \chi_{9,9} + \chi_{11,11}, \tag{13}
\]
which is the \(d\) electron susceptibility [2-4].

We now define the Matsubara one-particle Green’s function of localized \(d\)-electrons:
\[
g^{0}(l\sigma, l'\sigma'; \tau - \tau') = g^{0}_{l\sigma,l'\sigma'}(\tau - \tau') = -\langle T d_{l\sigma}(\tau) d_{l'\sigma'}(\tau') \rangle_0, \tag{14}
\]
where \(d_{l\sigma}(\tau) = e^{\tau H_0} d_{l\sigma} e^{-\tau H_0}, \; \tilde{d}_{l\sigma}(\tau) = e^{\tau H_0} d_{l\sigma} e^{-\tau H_0}.\)

The Fourier components of this Green’s function are:
\[
g^{(0)}(\tau) = \frac{1}{\beta} \sum_{\omega_n} e^{-i\omega_n \tau} g^{(0)}(i\omega_n). \tag{15}
\]

Using (8) and the properties of Hubbard operators we obtain the equation for local function:
\[
g^{(0)}_{l\sigma,l'\sigma'}(i\omega_n) = \frac{\delta_{ll'}\delta_{\sigma\sigma'}}{Z_0} \left\{ \frac{e^{-\beta E_1} + e^{-\beta E_2}}{i\omega_n + E_1 - E_2} + \frac{e^{-\beta E_2} + e^{-\beta E_6}}{i\omega_n + E_2 - E_6} + \frac{e^{-\beta E_7} + e^{-\beta E_0}}{i\omega_n + E_7 - E_0} \right\}, \tag{16}
\]
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 equal to
\[
A^{(0)}(E) = -2Img^{0}(E + i\delta), \tag{18}
\]
where \(g^{0}(E + i\delta)\) with \(\delta = +0\) is analytical continuation of the Matsubara to retarded Green’s function.

Using (14) we obtain
\[
A^{(0)}(E) = \frac{2\pi}{Z_0} \left\{ \frac{(e^{-\beta E_1} + e^{-\beta E_2})\delta(E + E_1 - E_2)}{2} + \frac{(e^{-\beta E_2} + e^{-\beta E_6})\delta(E + E_2 - E_6)}{2} + \frac{(e^{-\beta E_6} + e^{-\beta E_7})\delta(E + E_6 - E_7)}{2} + \frac{(e^{-\beta E_7} + e^{-\beta E_0})\delta(E + E_7 - E_0)}{2} + \frac{(e^{-\beta E_0} + e^{-\beta E_12})\delta(E + E_0 - E_12)}{2} + \frac{(e^{-\beta E_12} + e^{-\beta E_{16}})\delta(E + E_{12} - E_{16})}{2} \right\} \tag{19}
\]
with property
\[
\int_{-\infty}^{\infty} A^{(0)}(E) dE = 2\pi. \tag{20}
\]
3 Delocalization processes

We use the perturbation theory elaborated previously for strongly correlated electron systems both of non degenerate [5-9,11-14] and of degenerate forms [10]. 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:

\[ \tilde{G}(\tilde{k}\sigma|\tilde{k}'\sigma') = -\langle TC_{\tilde{k}\sigma}(\tau)\tilde{C}_{\tilde{k}'\sigma'}(\tau')U(\beta)\rangle_0, \]
\[ g(l\sigma|l'\sigma') = -\langle Td_{l\sigma}(\tau)d_{l'\sigma'}(\tau')U(\beta)\rangle_0. \]  
(21)

The anomalous functions are defined as

\[ F(\tilde{k}\sigma|\tilde{k}'\sigma') = -\langle TC_{\tilde{k}\sigma}(\tau)C_{\tilde{k}'\sigma'}(\tau')U(\beta)\rangle_0, \]
\[ \tilde{F}(\tilde{k}\sigma|\tilde{k}'\sigma') = -\langle TC_{\tilde{k}\sigma}(\tau)\tilde{C}_{\tilde{k}'\sigma'}(\tau')U(\beta)\rangle_0, \]
\[ f(l\sigma|l'\sigma') = -\langle Td_{l\sigma}(\tau)d_{l'\sigma'}(\tau')U(\beta)\rangle_0, \]
\[ \tilde{f}(l\sigma|l'\sigma') = -\langle T\tilde{d}_{l\sigma}(\tau)\tilde{d}_{l'\sigma'}(\tau')U(\beta)\rangle_0. \]  
(22)

Here \( \tau \) and \( \tau' \) stand for imaginary time with \( 0 \leq \tau \leq \beta \), \( \beta \) is inverse temperature, \( T \) is chronological ordering operator.

The evolution operator is

\[ U(\beta) = T \exp(-\int_0^\beta H_{\text{int}}(\tau)d\tau). \]  
(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

\[ H_0^L = \sum_{n=1}^{16} E_n \chi_{nn}, \quad \sum_{n=1}^{16} \chi_{nn} = 1, \]  
(24)

\[ G_{l\sigma\sigma'}^{(0)}(\tilde{k}\tilde{k}'|\tau - \tau') = \delta_{\tilde{k}\tilde{k}'}, \delta_{\sigma\sigma'}G_{l\sigma}^{(0)}(\tilde{k}|\tau - \tau'), \]
\[ G_{l\sigma}^{(0)}(\tilde{k}|i\omega_n) = \frac{1}{i\omega_n - \epsilon(\tilde{k})}, \omega_n = \frac{(2n + 1)\pi}{\beta}. \]

and \( g^{(0)}(i\omega_n) \) is determined by the 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

\[ G_{l\sigma\sigma'}(\tilde{k}\tilde{k}'|i\omega_n) = \delta_{\tilde{k}\tilde{k}'}, \delta_{\sigma\sigma'}G_{l\sigma}^{(0)}(\tilde{k}|i\omega_n) + \frac{V_{kl}^*V_{k'l'}}{N}G_{l\sigma}^{(0)}(\tilde{k}|i\omega_n)g_{l\sigma\sigma'}(i\omega_n)G_{l'\sigma'}^{(0)}(\tilde{k}'|i\omega_n), \]  
(25)

where \( g_{l\sigma\sigma'}(i\omega_n) \) is the full impurity electron propagator.

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

\[ F_{l\sigma\sigma'}(\tilde{k}, -\tilde{k}'|i\omega_n) = \frac{V_{kl}^*V_{k'l'}}{N}G_{l\sigma}^{(0)}(\tilde{k}|i\omega_n)f_{l\sigma\sigma'}(i\omega_n)G_{l'\sigma'}^{(0)}(-\tilde{k}' - i\omega_n). \]
The equations for the full functions $g$ 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

$$
\sum \sum \frac{V_{k_1i_1}V_{k_2i_2}^*}{N} G^{(0)}_{l_1\sigma_1l_2\sigma_2}(\vec{k}_1\vec{k}_2)|i\omega_n) =
\frac{1}{N} \sum_{k_1} |V_{k_1i_1}|^2 G^{(0)}_{l_1\sigma_1}(\vec{k}_1|i\omega_n) \delta_{l_1l_2} \delta_{\sigma_1\sigma_2} = \delta_{l_1l_2} \delta_{\sigma_1\sigma_2} G^{(0)}_{l_1\sigma_1}(i\omega_n),
$$

where

$$
G^{(0)}_{l\sigma}(i\omega_n) = \frac{1}{N} \sum_k |V_{kli}|^2 G^{(0)}_{l\sigma}(\vec{k}|i\omega_n) = \frac{1}{N} \sum_k \frac{|V_{kli}|^2}{i\omega_n - \epsilon(\vec{k})}.
$$

The renormalization quantity is

$$
G_{l\sigma l'\sigma'}(i\omega_n) = \frac{1}{N} \sum_{k_1k_2} V_{k_1l_1}^* V_{k_2l_2} G_{l\sigma l'\sigma'}(\vec{k_1} \vec{k_2}|i\omega_n).
$$

In the Fig. 1 the double dashed lines with arrows depict renormalized $g$ and $f$ propagators of localized electrons and solid thin lines represent $G^0$ function of conduction electrons. The function $V_1$ means $V_{k_1l_1}$ and summation by repeated indices is assumed.

$\Lambda$ and $\bar{Y}$ are correlation functions. They contain a sum of strongly connected irreducible diagrams. The simplest examples of such diagrams are shown on Fig. 2.

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

$$
g_{l\sigma l'\sigma'}(i\omega_n) = \Lambda_{l\sigma l'\sigma'}(i\omega_n) + \Lambda_{l_1 \sigma_1 l_2 \sigma_2} G^{(0)}_{l_1 \sigma_1}(i\omega_n) g_{l_1 \sigma_1 l' \sigma'}(i\omega_n) -
$$
Solutions of the equation (31) for the normal state of the degenerate system has the form:

\[ \sigma \]

For this special case we use the new notations (\( \bar{\sigma} \) the most simple form with singlet superconductivity on the paramagnetic background.

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

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

\[
\begin{align*}
g_{\bar{\sigma}l\bar{\sigma}}(i\omega_n) &= g_{\bar{\sigma}l\bar{\sigma}}^+(i\omega_n) + \Lambda_{\bar{\sigma}l\bar{\sigma}l\bar{\sigma}}(i\omega_n)g_{\bar{\sigma}l\bar{\sigma}}^+(i\omega_n) - Y_{\bar{\sigma}l\bar{\sigma}l\bar{\sigma}}(i\omega_n)g_{\bar{\sigma}l\bar{\sigma}}^+(i\omega_n), \\
\bar{f}_{\bar{\sigma}l\bar{\sigma}}(i\omega_n) &= \bar{f}_{\bar{\sigma}l\bar{\sigma}}(i\omega_n) + \Lambda_{\bar{\sigma}l\bar{\sigma}l\bar{\sigma}}(i\omega_n)\bar{f}_{\bar{\sigma}l\bar{\sigma}}(i\omega_n) - Y_{\bar{\sigma}l\bar{\sigma}l\bar{\sigma}}(i\omega_n)\bar{f}_{\bar{\sigma}l\bar{\sigma}}(i\omega_n).
\end{align*}
\]

In the absence of orbital degeneracy this system of equation has the known solution [14]

\[
\begin{align*}
g_{\sigma}(i\omega_n) &= \frac{\Lambda_{\sigma}(i\omega_n) - G_{\sigma}^0(0)(i\omega_n)[\Lambda_{\sigma}(i\omega_n)\Lambda_{\sigma}(i\omega_n) - Y_{\sigma\sigma}(i\omega_n)\bar{Y}_{\sigma\sigma}(i\omega_n)]}{d_{\sigma}(i\omega_n)}, \\
\bar{f}_{\bar{\sigma}}(i\omega_n) &= \frac{Y_{\bar{\sigma}\bar{\sigma}}(i\omega_n)}{d_{\bar{\sigma}}(i\omega_n)}, \\
d_{\sigma}(i\omega_n) &= \frac{(1 - \Lambda_{\sigma}(i\omega_n)G_{\sigma}^0(i\omega_n))(1 - \Lambda_{\bar{\sigma}}(i\omega_n)G_{\bar{\sigma}}^0(i\omega_n)) + G_{\sigma}^0(i\omega_n)G_{\bar{\sigma}}^0(i\omega_n)}{d_{\sigma}(i\omega_n)}.
\end{align*}
\]

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

\[
\begin{align*}
g_{\sigma}^{11}(i\omega_n) &= \frac{\Lambda_{\sigma}^{11}(i\omega_n) - G_{\sigma}^{20}(0)(i\omega_n)[\Lambda_{\sigma}^{11}(i\omega_n)\Lambda_{\sigma}^{22}(i\omega_n) - \Lambda_{\sigma}^{12}(i\omega_n)\Lambda_{\sigma}^{21}(i\omega_n)]}{d_{\sigma}(i\omega_n)}, \\
g_{\sigma}^{21}(i\omega_n) &= \frac{\Lambda_{\sigma}^{21}(i\omega_n)}{d_{\sigma}(i\omega_n)}, \\
d_{\sigma}(i\omega_n) &= (1 - G_{\sigma}^{10}(0)(i\omega_n) \times \Lambda_{\sigma}^{11}(i\omega_n))(1 - G_{\sigma}^{20}(0)(i\omega_n)\Lambda_{\sigma}^{22}(i\omega_n)) - G_{\sigma}^{10}(0)(i\omega_n)G_{\sigma}^{20}(0)(i\omega_n)\Lambda_{\sigma}^{12}(i\omega_n)\Lambda_{\sigma}^{21}(i\omega_n).
\end{align*}
\]
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 the exact solution does not exist.

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

$$Z^{(0)}_{\sigma\tau}(\tau - \tau') = \langle l_1 \sigma_1 \tau_1 l_2 \sigma_2 \tau_2 | \sigma \tau, l_1 \sigma_1 \tau_1 l_2 \sigma_2 \tau_2, l' \sigma' \tau' | V_1^* G_{l_1 \sigma_1 \tau_1 l_2 \sigma_2 \tau_2, l' \sigma', \tau'} G_{l_2 l_2 \sigma_2 \tau_2 | l_1 \sigma_1 \tau_1, v} V_2 \rangle$$

$$Y^{(0)}_{\sigma\tau}(\tau - \tau') = \langle l_1 \sigma_1 \tau_1 l_2 \sigma_2 \tau_2 | \sigma \tau, l_1 \sigma_1 \tau_1 l_2 \sigma_2 \tau_2, l' \sigma' \tau' | V_1^* F_{l_1 \sigma_1 \tau_1 l_2 \sigma_2 \tau_2, l' \sigma', \tau'} G_{l_2 l_2 \sigma_2 \tau_2 | l_1 \sigma_1 \tau_1, v} V_2 \rangle$$

$$\bar{Y}^{(0)}_{\sigma\tau}(\tau - \tau') = \langle l_1 \sigma_1 \tau_1 l_2 \sigma_2 \tau_2 | \sigma \tau, l_1 \sigma_1 \tau_1 l_2 \sigma_2 \tau_2, l' \sigma' \tau' | V_1^* \bar{F}_{l_1 \sigma_1 \tau_1 l_2 \sigma_2 \tau_2, l' \sigma', \tau'} G_{l_2 l_2 \sigma_2 \tau_2 | l_1 \sigma_1 \tau_1, v} V_2 \rangle$$

Figure 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.

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.

## 4 Correlation functions

The simplest correlation function is determined as

$$G^{(0)}_{l_1 l_2 l_3 l_4} = g_{l_1 l_2 l_3 l_4}^{(0)} = g_{l_1 l_2 l_3 l_4}^{(0)} + g_{l_1 l_2 l_3 l_4}^{(0)}$$

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

Because the presence of the Coulomb interactions in zero order Hamiltonian, equation (34) is different of zero and contains charge, spin and pairing fluctuations.

The two-particle Green’s function $g_{l_1 l_2 l_3 l_4}^{(0)}$ 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 operators representation.
We need the Fourier representation of these functions

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

\[
g_1^{(0)}(l_1 \sigma_1 \tau_1 | l_2 \sigma_2 \tau_2) = \frac{1}{\beta} \sum_{\omega} g_1^{(0)}(l_1 \sigma_1; l_2 \sigma_2 | \omega_1) e^{-i \omega_1 (\tau_1 - \tau_2)}
\]

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

\[
G_2^{irr}[l_1 \sigma_1 \omega_1; l_2 \sigma_2 \omega_2 | l_3 \sigma_3 \omega_3; l_4 \sigma_4 \omega_4] = g_2^{(0)}[l_1 \sigma_1 \omega_1; l_2 \sigma_2 \omega_2 | l_3 \sigma_3 \omega_3; l_4 \sigma_4 \omega_4] - \beta \delta(\omega_1 + \omega_2 - \omega_3 - \omega_4) [\delta(\omega_1 - \omega_4) g_1^{(0)}(l_1 \sigma_1; l_4 \sigma_4 | \omega_1) g_1^{(0)}(l_2 \sigma_2; l_3 \sigma_3 | \omega_2) - \delta(\omega_1 - \omega_3) g_1^{(0)}(l_1 \sigma_1; l_3 \sigma_3 | \omega_1) g_1^{(0)}(l_2 \sigma_2; l_4 \sigma_4 | \omega_2)].
\]

There exists the law of frequency conservation

\[
G_2^{irr}[l_1 \sigma_1 \omega_1; l_2 \sigma_2 \omega_2 | l_3 \sigma_3 \omega_3; l_4 \sigma_4 \omega_4] = \beta \delta(\omega_1 + \omega_2 - \omega_3 - \omega_4) G_2^{irr}[l_1 \sigma_1 \omega_1; l_2 \sigma_2 \omega_2 | l_3 \sigma_3 \omega_3; l_4 \sigma_4 \omega_4].
\]

The statistical averages of chronologically ordered products of the electron operators of the function \( g_2^{(0)} \) have different weights of the form \( e^{-\beta E_n} / Z_0 \), where \( E_n \) are the energies determined in previous sections. Because \( E_9 \) is the lowest energy the weight \( e^{-\beta E_9} \) is the main of them and only such terms are taken into account.

Just such considerations determined us to use instead initial exact equation (16) for zero order Green’s function \( g_{\sigma \sigma'}^{(0)} \) the approximate value (35). Zero order partition function \( Z_0 \) (17) concomitant is approximated as \( 3 e^{-\beta E_9} \).

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

\[
- \delta_{l_1 l_3} \delta_{l_2 l_4} \left( \frac{1}{4} \delta_{\sigma_1 \sigma_3} \delta_{\sigma_2 \sigma_4} + \delta_{\sigma_1, -\sigma_3} \delta_{\sigma_2, -\sigma_4} \delta_{\sigma_3, \sigma_4} + \delta_{\sigma_1, \sigma_3} \delta_{\sigma_2, \sigma_4} \delta_{\sigma_3, \sigma_4} + \delta_{\sigma_1, \sigma_3} \delta_{\sigma_2, \sigma_4} \delta_{\sigma_3, \sigma_4} \right) I_{1324}^{(1)} -
\]

\[
(\delta_3 - l_1 - l_3, 0) \delta_3 - l_2 - l_4, 0 + (1) l_1 l_4 \delta_{l_1 l_4} \left( \frac{1}{4} \epsilon_{\sigma_1 \sigma_4} \delta_{\sigma_1 \sigma_3} \delta_{\sigma_4 \sigma_2} + \frac{1}{2} \delta_{\sigma_1, -\sigma_3} \delta_{\sigma_2, -\sigma_4} \delta_{\sigma_1, \sigma_4} \right) I_{1324}^{(2)} -
\]

\[
(1) l_1 l_4 \delta_{l_1 l_4} \left( \frac{1}{4} \epsilon_{\sigma_1 \sigma_4} \delta_{\sigma_1 \sigma_3} \delta_{\sigma_4 \sigma_2} + \frac{1}{2} \delta_{\sigma_1, -\sigma_3} \delta_{\sigma_2, -\sigma_4} \delta_{\sigma_1, \sigma_4} \right) I_{1324}^{(3)}
\]

where

\[
I_{1324}^{(1)} = \frac{e^{-\beta E_9}}{Z_0} \int_{0}^{\beta} d\tau_1 \int_{0}^{\tau_1} d\tau_3 \int_{0}^{\tau_3} d\tau_2 \int_{0}^{\tau_2} d\tau_4 e^{(E_9 - E_{12})(\tau_1 + \tau_2 - \tau_3 - \tau_4)} e^{i \omega_1 \tau_1 + i \omega_2 \tau_2 - i \omega_3 \tau_3 - i \omega_4 \tau_4},
\]

\[
I_{1324}^{(2)} = \frac{e^{-\beta E_9}}{Z_0} \int_{0}^{\beta} d\tau_1 \int_{0}^{\tau_1} d\tau_3 \int_{0}^{\tau_3} d\tau_2 \int_{0}^{\tau_2} d\tau_4 e^{(E_9 - E_{12})(\tau_1 - \tau_3) + (E_6 - E_{12})(\tau_2 - \tau_3)} e^{i \omega_1 \tau_1 + i \omega_2 \tau_2 - i \omega_3 \tau_3 - i \omega_4 \tau_4},
\]

\[
I_{1324}^{(3)} = \frac{e^{-\beta E_9}}{Z_0} \int_{0}^{\beta} d\tau_1 \int_{0}^{\tau_1} d\tau_3 \int_{0}^{\tau_3} d\tau_2 \int_{0}^{\tau_2} d\tau_4 e^{(E_9 - E_{12})(\tau_1 - \tau_2) + (E_7 - E_{12})(\tau_2 - \tau_3)} e^{i \omega_1 \tau_1 + i \omega_2 \tau_2 - i \omega_3 \tau_3 - i \omega_4 \tau_4}.
\]

These 4-fold multiple integrals by time variable \( \tau \) can be transformed in contour integral by using the method of Claude Bloch [15]. With this purpose it is necessary to introduce the exponential form

\[
e^{(\beta - \tau_1) E_9 + (\tau_1 - \tau_3) E_1 + (\tau_3 - \tau_2) E_2 + (\tau_2 - \tau_4) E_3 + (\tau_4 - 0) E_4},
\]

(40)
which must be compared with exponential form of our integrals \( I^{(n)}_{1324} \). Comparison with \( I^{(1)}_{1324} \) give us the result

\[
\begin{align*}
\bar{\delta}_0 &= -E_9, \quad \bar{\delta}_2 = -E_9 + i\omega_1 - i\omega_3, \quad \bar{\delta}_4 = -E_9 + i\Omega, \quad \bar{\delta}_1 = -E_{12} + i\omega_1, \\
\bar{\delta}_3 &= -E_{12} + i\omega_1 + i\omega_2 - i\omega_3, \quad \Omega = \omega_1 + \omega_2 - \omega_3 - \omega_4.
\end{align*}
\]

(41)

Our integral \( I^{(1)}_{1324} \) is transformed in the contour integral

\[
I^{(1)} = \frac{1}{2\pi i} \frac{1}{Z_0} \oint_C dz e^{-\beta z} \left( \frac{e^{-\beta Z}}{(z + \bar{\delta}_0)(z + \bar{\delta}_1)(z + \bar{\delta}_3)(z + \bar{\delta}_4)} \right),
\]

(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 \( \bar{\delta}_2 \). For \( I^{(2)} \) the energy \( \bar{\delta}_2 = -E_6 + i\omega_1 - i\omega_3 \) and for \( I^{(3)} \) \( \bar{\delta}_2 = -E_7 + i\omega_1 - i\omega_3 \). Other parameters coincide.

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

For example in the case when \( \omega_1 - \omega_3 = 0 \) and \( \Omega = 0 \) we have \( \bar{\delta}_0 = \bar{\delta}_2 = \bar{\delta}_4 \) and the pole \( z = -\bar{\delta}_0 \) is 3-fold multiple with the residue

\[
\frac{1}{2} \left( \frac{e^{-\beta Z}}{(z + \bar{\delta}_0)(z + \bar{\delta}_1)(z + \bar{\delta}_3)} \right)''_{z = -\bar{\delta}_0}.
\]

(43)

To find all possible multiple poles we consider different values of frequencies using the identity \( 1 = \delta(\omega) + \psi(\omega) \), where \( \psi(\omega) = 1 - \delta(\omega) \). For example we consider the possibility when \( \Omega \) can be equal to zero and \( \omega_1 = \omega_3 \). We have the identity:

\[
1 = (\delta(\Omega) + \psi(\Omega))(\delta(\omega_1 - \omega_3) + \psi(\omega_1 - \omega_3)) = \\
\delta(\Omega)\delta(\omega_1 - \omega_3) + \delta(\Omega)\psi(\omega_1 - \omega_3) + \psi(\Omega)\delta(\omega_1 - \omega_3) + \psi(\Omega)\psi(\omega_1 - \omega_3).
\]

(44)

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

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

\[
Z_0 I^{(1)}_{1324} = \frac{1}{2} \delta(\Omega)\delta(\omega_1 - \omega_3) \left( \frac{e^{-\beta Z}}{(z + \bar{\delta}_0)(z + \bar{\delta}_1)(z + \bar{\delta}_3)} \right)''_{z = -\bar{\delta}_0} + \\
\delta(\Omega)\psi(\omega_1 - \omega_3) \left[ \left( \frac{e^{-\beta Z}}{(z + \bar{\delta}_0)(z + \bar{\delta}_2)(z + \bar{\delta}_3)} \right)'_{z = -\bar{\delta}_0} + \left( \frac{e^{-\beta Z}}{(z + \bar{\delta}_0)^2(z + \bar{\delta}_1)(z + \bar{\delta}_3)} \right)_{z = -\bar{\delta}_2} \right] + \\
\delta(\omega_1 - \omega_3)\psi(\Omega) \left[ \left( \frac{e^{-\beta Z}}{(z + \bar{\delta}_0)(z + \bar{\delta}_1)(z + \bar{\delta}_4)} \right)'_{z = -\bar{\delta}_0} + \left( \frac{e^{-\beta Z}}{(z + \bar{\delta}_0)^2(z + \bar{\delta}_1)(z + \bar{\delta}_3)} \right)_{z = -\bar{\delta}_4} \right] + \\
\psi(\Omega)\psi(\omega_1 - \omega_3) \psi(\omega_2 - \omega_4) \left[ \left( \frac{e^{-\beta Z}}{(z + \bar{\delta}_0)(z + \bar{\delta}_1)(z + \bar{\delta}_3)} \right)_{z = -\bar{\delta}_2} + \left( \frac{e^{-\beta Z}}{(z + \bar{\delta}_0)^2(z + \bar{\delta}_1)(z + \bar{\delta}_3)} \right)_{z = -\bar{\delta}_4} \right] + \\
\left( \frac{e^{-\beta Z}}{(z + \bar{\delta}_0)(z + \bar{\delta}_1)(z + \bar{\delta}_3)(z + \bar{\delta}_4)} \right)_{z = -\bar{\delta}_2} + \left( \frac{e^{-\beta Z}}{(z + \bar{\delta}_0)(z + \bar{\delta}_1)(z + \bar{\delta}_3)(z + \bar{\delta}_4)} \right)_{z = -\bar{\delta}_4}.
\]
The contribution of other poles is negligible. Our next approximation consists in preserving, in the case of low temperature, of the main part of the second derivative \( (43) \) just of the form
\[
\Delta I = \frac{\beta^2 e^{-\beta E_0}}{2Z_0(E_1 - E_0)(E_3 - E_0)}.
\] (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 \(G_2^{(0)\text{irr}}\).

After some transformation and summation of different contributions we obtain the main approximation for the correlation function:
\[
G_2^{(0)\text{irr}}[l_1\sigma_1 \omega_1; l_2\sigma_2 \omega_2;l_3\sigma_3 \omega_3; l_4\sigma_4 \omega_4] = \frac{\beta}{6} \delta(\omega_1 + \omega_2 - \omega_3 - \omega_4)p(\omega_1)p(\omega_2) \times
\]
\[
(\beta\delta(\omega_1 - \omega_4)\delta_{l_1l_4}\delta_{l_2l_3}[2\delta_{\sigma_1,-\sigma_4}\delta_{\sigma_2,-\sigma_3}\delta_{\sigma_3,\sigma_4} + \delta_{\sigma_1,\sigma_3}\delta_{\sigma_1,\sigma_4}\delta_{\sigma_2,\sigma_3} - \delta_{\sigma_1,\sigma_4}\delta_{\sigma_2,\sigma_3}\delta_{\sigma_3,-\sigma_1}] -
\]
\[
\beta\delta(\omega_1 - \omega_3)\delta_{l_1l_3}\delta_{l_2l_4}[2\delta_{\sigma_1,-\sigma_3}\delta_{\sigma_2,-\sigma_4}\delta_{\sigma_3,\sigma_4} + \delta_{\sigma_1,\sigma_3}\delta_{\sigma_2,\sigma_4}\delta_{\sigma_3,\sigma_4} - \delta_{\sigma_1,\sigma_3}\delta_{\sigma_2,\sigma_4}\delta_{\sigma_3,-\sigma_1}],
\] (47)
with
\[
p(\omega) = \left(\frac{1}{\omega + E_2 - E_0} - \frac{1}{\omega + E_9 - E_{12}}\right).
\] (48)

5 Mott-Hubbard phase transition

As has been mentioned above, one example of efficient summation of diagrams which determine correlation function \(Z\) and \(\Lambda\) is presented on the Fig. 4. It has the form

![Diagram](attachment:image.png)

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

First of all we shall discuss the approximation with zero order correlation function \(G_2^{(0)\text{irr}}\). Using the result \((47)\) we obtain
\[
\frac{1}{\beta} \sum_{\omega_1} \sum_{l_1\sigma_1} \tilde{G}_2^{(0)\text{irr}}[l\sigma_1 \omega_1; l_1\sigma_1 \omega_1; l'\sigma' \omega]\tilde{G}_2^{(0)\text{irr}}[l_1\sigma_1 \omega_1] = -\frac{1}{2} \delta_{\sigma\sigma'}\delta_{l'l} [p(\omega)]^2 \tilde{G}_{l\sigma}(\omega),
\] (49)

\[
\sum_{l_1\sigma_1 l_2 \sigma_2} \tilde{G}_2^{(0)\text{irr}}[l\sigma_1 \omega_1; l_1\sigma_1 \omega_1; l_2\sigma_2 \omega_1; l'\sigma' \omega]\tilde{G}_2^{(0)\text{irr}}[l_2\sigma_2 l_1\sigma_1 (i\omega_1) G_{l_1\sigma}(i\omega_1)] =
\]
\[
\frac{1}{6} p(\omega)p(\omega_1) \{ \beta \delta(\omega - \omega_1) \delta_{l'l} \sum_{l_1} (2\delta_{\sigma\sigma'} g_{l_1\sigma}(i\omega_1) -
\]
\[
g_{l_1\sigma_1,\sigma_1}(i\omega_1) G_{l_1\sigma}(i\omega_1) + \delta_{\sigma\sigma'} G_{l_1\sigma}(i\omega_1) g_{l_1\sigma_1\sigma}(i\omega_1) G_{l_1\sigma}(i\omega_1) -
\]
\[
-\delta_{\sigma\sigma'} G_{l_1\sigma}(i\omega_1) g_{l_1\sigma l_1 - \sigma}(i\omega_1) G_{l_1\sigma}(i\omega_1)]
\] (50)

\[
-\beta \delta(\omega \omega_1) [2\delta_{\sigma\sigma'} G_{l_1\sigma}(i\omega_1) g_{l_1\sigma l_1 - \sigma}(i\omega_1) G_{l_1\sigma}(i\omega_1) +
\]
\[
+\delta_{\sigma\sigma'} G_{l_1\sigma}(i\omega_1) g_{l_1\sigma l_1 - \sigma}(i\omega_1) G_{l_1\sigma}(i\omega_1) - \delta_{\sigma\sigma'} G_{l_1\sigma}(i\omega_1) g_{l_1\sigma l_1 - \sigma}(i\omega_1) G_{l_1\sigma}(i\omega_1)]\}. \]
We keep the terms which preserve the spin and have the form $\delta_{\sigma\sigma}$, and omit the terms with spin-flipp of the form $\delta_{\sigma',-\sigma}$ and also omit the terms which are reciprocally subtracted and differ only by the sign of spin. We take into account that the function $G^{(0)}(i\omega)$ doesn’t depend of spin index and

$$
\sum_{\sigma_1} \sigma_1 \sigma G^{(0)}_{1\sigma_1}(i\omega) = 0.
$$

As a result of such simplifications we obtain

$$
\sum_{l_1\sigma_1 l_2 \sigma_2} \tilde{G}^{(0)rr}_{l_1 l_2}(\omega \sigma_1; l_1 \sigma_1 \omega_1 | l_2 \sigma_2 \omega_2; \tau' \tau \omega) G^{(0)}_{l_2 \sigma_2}(\omega \sigma) g_{l_2 \sigma_2 l_1 \sigma_1}(\omega \sigma_1) G^{(0)}_{l_1 \sigma_1}(\omega \sigma_1) = -\frac{1}{2} \beta \delta(\omega - \omega_1) p(\omega) p(\omega_1) \delta_{\sigma \sigma'} G^{(0)}_{l \sigma}(\omega_1) g_{l \sigma \sigma'}(\omega_1) G^{(0)}_{l \sigma'}(\omega_1),
$$

with the following realizations

$$
\Lambda_{l \sigma \sigma'}(\omega) = \delta_{l \tau} \delta_{\sigma \sigma'} [m_l(\omega) + \frac{p^2(\omega)}{2} G^{(0)}_{l \sigma}(\omega)] + \frac{p^2(\omega)}{2} G^{(0)}_{l \sigma}(\omega) G^{(0)}_{l \sigma'}(\omega) g_{l \sigma \sigma'}(\omega),
$$

where

$$
\Lambda_{11}(\omega) = m_1(\omega) + \frac{p^2(\omega)}{2} G^{(0)}_{1 \sigma}(\omega), \quad \Lambda_{22}(\omega) = m_2(\omega) + \frac{p^2(\omega)}{2} G^{(0)}_{2 \sigma}(\omega), \quad \Lambda_{12}(\omega) = \frac{p^2(\omega)}{2} G^{(0)}_{1 \sigma} G^{(0)}_{2 \sigma}(\omega) g_{12}(\omega).
$$

We take into account the Dyson type equation

$$
g_{11}(\omega) = \frac{\Lambda_{11}(\omega) - G^{(0)}_{2 \sigma}(\omega) \Lambda_{12}(\omega) \Lambda_{12}(\omega) - \Lambda_{12}(\omega) \Lambda_{21}(\omega)}{d(\omega)}, \quad g_{12}(\omega) = \frac{\Lambda_{12}(\omega)}{d(\omega)},
$$

$$
d(\omega) = (1 - \Lambda_{11}(\omega) G^{(0)}_{1 \sigma}(\omega))(1 - \Lambda_{22}(\omega) G^{(0)}_{2 \sigma}(\omega)) - G^{(0)}_{1 \sigma}(\omega) G^{(0)}_{2 \sigma}(\omega) \Lambda_{12}(\omega) \Lambda_{21}(\omega)).
$$

We make some generalization by considering function $m(\omega)$ dependent on orbital quantum number $l$ even if it is really not. The function $g_{22}$ 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

$$
\Lambda_{11}(\omega) = m_1(\omega), \quad g_{11}(\omega) = -\frac{1}{G^{(0)}_{1 \sigma}(\omega)},
$$

$$
\Lambda_{22}(\omega) = \frac{1}{G^{(0)}_{2 \sigma}(\omega)}, \quad g_{22}(\omega) = -\frac{1}{G^{(0)}_{2 \sigma}(\omega)} \left(1 + \frac{m_2(\omega) G^{(0)}_{2 \sigma}(\omega) - 1}{\frac{p^2(\omega)}{2} (G^{(0)}_{2 \sigma}(\omega))^2}\right),
$$

$$
\Lambda_{12}(\omega) = \Lambda_{21}(\omega) = \pm \frac{ip(\omega)}{\sqrt{2}}, \quad g_{12}(\omega) = \pm \frac{i\sqrt{2}}{p(\omega) G^{(0)}_{1 \sigma}(\omega) G^{(0)}_{2 \sigma}(\omega)},
$$

with the condition that

$$
\frac{1}{G^{(0)}_{1 \sigma}(\omega)} - m_1(\omega) = \frac{1}{G^{(0)}_{2 \sigma}(\omega)} - m_2(\omega)
$$

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

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

$$
\rho_{ll}(E) = -2Im g_{ll}(E + i\delta).
$$
For example intraorbital contribution has a form

\[ \rho_{11}(E) = -\frac{2 Im G_1^{(0)}(E + i\delta)}{(Re G_1^{(0)})^2 + (Im G_1^{(0)})^2}, \]  

(59)

where

\[ Im G_1^{(0)}(E + i\delta) = -\pi \rho_0(E)|V_1|^2. \]  

(60)

The quantity \( \rho_{11}(E) \) differs from zero thanks the existence of the matrix element of hybridization and of the zero order density of states \( \rho_0(E) \). For \( E = 0 \) \( \rho_0(0) \) is positive and state of the system is metallic.

Interorbital contribution to the phase transition is determined by the value

\[ \rho_{12}(E) = -Im g_{12}(E + i\delta) = \frac{2(E + \Delta E_1)(\Delta E_2 - E)}{Im G_1^{(0)}(0)Im G_2^{(0)}(0)(\Delta E_1 + \Delta E_2)}, \]  

(61)

where

\[ \Delta E_1 = E_2 - E_9 > 0, \quad \Delta E_2 = E_{12} - E_9 > 0. \]

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

For these energy values the state of the system is metallic. The appearance of spectral weight et the Fermi level is considered as a definition of Mott transition.

### 6 Conclusions

Diagram approach for investigation the properties of twofold degenerate Anderson impurity model has been elaborated.

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

Perturbation theory around the atomic limit has been developed and Matsubara Green’s functions as in normal and in superconducting states has been defined.

Dyson-type equations for these functions have been established for both states but detailed solutions were discussed only for normal state supposing additional investigation in the next paper.

Because the main elements of our diagram technique are the irreducible Green’s functions we have undertaken the determination of simplest two-particle irreducible Green’s function and determined its dependence of the spin and orbital quantum numbers. This quantity has been determined only in the low temperature limit.

Having this quantity and summing some class of diagrams we have obtained the \( \Lambda_{\alpha\lambda\tau\sigma} \) correlation function.

We found two solutions for the renormalized Green’s functions of the \( d-\) electrons and determined the spectral weight.

### Acknowledgment

Two of authors (V.M, L.D) would like to express their sincere thanks to Dr. S. Cojocaru for frequent valuable discussions and comments.
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