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DIAGRAMMATIC THEORY FOR ANDERSON IMPURITY MODEL

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Москаленко В. А. и др. E17-2008-56

Диаграммный метод для примесной модели Андерсона

Предложена диаграммная теория в окрестности атомного предела в нормальном и сверхпроводящем состояниях для примесной модели Андерсона. Примесные электроны испытывают сильное кулоновское отталкивание между собой.

Новый метод основан на обычной теореме Вика для электронов проводимости и на обобщенной теореме Вика для сильнокоррелированных примесных электронов.

Для среднего значения оператора эволюции доказана теорема о связных диаграммах.

Установлены уравнения типа Дайсона для пропагаторов как электронов проводимости, так и примесных электронов в нормальном и сверхпроводящем состояниях системы.

Исследовано поведение спектральной функции примесных электронов и проанализирована ее структура.

Показано, что термодинамический потенциал этой сильнокоррелированной системы может быть представлен, после введения интегрирования по вспомогательной константе гибридизации, через полный пропагатор проводящих электронов и его массовый оператор. Доказано свойство стационарности этого выражения относительно вариации массового оператора.

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Diagrammatic Theory for Anderson Impurity Model

A diagrammatic theory around atomic limit is proposed for the normal and superconducting states of the Anderson impurity model. The impurity electrons have strong Coulomb repulsion between them. This interaction is the main parameter of the theory. The new method is based on the ordinary Wick theorem for conduction electrons and generalized Wick theorem for strongly correlated impurity electrons.

For the mean value of evolution operator the linked cluster theorem is proved and the Dyson-type equations for one-particle propagators of conduction and impurity electrons in the normal and superconducting states of the system have been established.

The behavior of the impurity electron spectral function has been studied. The structure of the resonances and their properties are analyzed.

We have proved that the thermodynamic potential of this strongly correlated system can be presented, after introduction of special integration by the constant of hybridization strength, as the functional of the full Green function of conduction electrons and its mass operator. The stationary property of this potential related to the changes of the mass operator has been demonstrated as well.

The investigation has been performed at the Bogoliubov Laboratory of Theoretical Physics, JINR.

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1. INTRODUCTION

The study of strongly correlated electron systems becomes in the last decade one of the most active fields of condensed matter physics. One of the important models of strongly correlated electrons is the single-site or impurity model introduced by Anderson [1] in 1961 and discussed intensively in a lot of papers [2–15]. It is a model for a system of free conduction electrons that interact with the system of a local spin, treated as just another electron of d- or f-shell of an impurity atom. The impurity electrons are strongly correlated because of strong Coulomb repulsion and they undergo the exchange and hybridization with conduction electrons. This model has some properties similar to those of Kondo model having more interesting physics [16–18]. It has the application for heavy fermion systems where the local impurity orbital is the f-orbital. Investigations of Anderson impurity model have used intensively the methods and results obtained for Kondo model by Nagaoka [18] and other authors [19, 20]. All the cited papers are based on the method of equations of motion (EOM) for retarded and advanced quantum Green's functions proposed by Bogoliubov and Tiablikov [21] and developed in the papers [22–24].

The first attempt to develop the diagrammatic theory for this problem was realized in the paper [25]. These authors used the expansion by cumulants for averages of products of Hubbard transfer operators and their algebra. With introduction of dynamical mean field theory the interest in Anderson impurity model has increased because infinite-dimensional lattice models can be mapped onto effective impurity models together with a self-consistency condition [26, 27].

The Hamiltonian of the model is written as

$$\begin{aligned} H &= H_0 + H_{\rm int}, \\ H_0 &= H_0^c + H_0^f, \\ H_0^c &= \sum_{\mathbf{k}\sigma} \epsilon(\mathbf{k})\ \mathbf{C}^+_{\mathbf{k}\sigma}\mathbf{C}_{\mathbf{k}\sigma}. \\ H_0^f &= \epsilon_f \sum_{\sigma} f^+_{\sigma} f_{\sigma} + U n^f_{\uparrow} n^f_{\downarrow}, \\ H_{\rm int} &= \frac{1}{\sqrt{N}} \sum_{\mathbf{k}\sigma} \left(V_{\mathbf{k}\sigma} f^+_{\sigma} C_{\mathbf{k}\sigma} + V^*_{\mathbf{k}\sigma} C^+_{\mathbf{k}\sigma} f_{\sigma} \right), \\ n^f_{\sigma} &= f^+_{\sigma} f_{\sigma}, \end{aligned} \tag{1}$$

where $C_{\mathbf{k}\sigma}(C^+_{\mathbf{k}\sigma})$ and $f_\sigma(f^+_\sigma)$ — annihilation (creation) operators of conduction and impurity electrons with spin σ, correspondingly; $\epsilon(\mathbf{k})$ is the kinetic energy of the conduction band state $(\mathbf{k},\sigma)$; ϵ_f is the local energy of f electrons, U is the on-site Coulomb repulsion of the impurity electrons and N is the number of lattice sites. $H_{\rm int}$ is the hybridization interaction between conduction and localized electrons. Summation over $\mathbf{k}$ will be changed to an integral over the energy $\epsilon(\mathbf{k})$ with the density of state $\rho_0(\epsilon)$ of conduction electrons, and the matrix elements will be considered as the function of energy $V(\epsilon)$. Because of the hybridization term of the Hamiltonian down and up spins of conduction electrons come and go in the local orbital and there is no appearance of spin flip process. Thus the important parameters of the Anderson model are the band width W, the conduction density of states $\rho_0(\epsilon)$, the local site energy ϵ_f and the on-site Coulomb interaction U. The electron energies are evaluated from the chemical potential μ of the system: $\epsilon(\mathbf{k}) = \xi(\mathbf{k}) - \mu$, $\epsilon_f = \overline{\epsilon}_f - \mu$. There is also an energy parameter $\Gamma(\epsilon)$ associated with the hybridization term

$$\Gamma(\epsilon) = \frac{\pi}{N}\sum_{\mathbf{k}} V^2_{\mathbf{k}}\delta(\epsilon - \epsilon(\mathbf{k})) = \pi \mathbf{V^2}(\epsilon)\rho_{\mathbf{0}}(\epsilon). \tag{2}$$

This function is assumed to be a constant, independent of energy. The term in the Hamiltonian involving U comes from on-site Coulomb interaction between two impurity electrons. U is far to large to be treated by perturbation theory. It must be included in H_0 which is noninteracting Hamiltonian. The existence of this term invalidates Wick's theorem for local electrons. Therefore, first of all, we formulate the generalized Wick's theorem (GWT) for local electrons, preserving the ordinary Wick theorem for conduction electrons. Our GWT really is the identity which determines the irreducible Green's functions or Kubo cumulants. Such definitions have already been used by us for discussing the properties of one-band Hubbard model [28–30] and for the formulation of the new diagram technique for it [31–34].

In Sec. 2, we start by introducing the finite temperature Green's functions for the conduction and impurity electrons in the interaction representation. We then formulate the generalized Wick theorem and in Secs. 3 and 4 provide explicit examples of diagram calculation for thermodynamical potential and full propagators. The results for symmetrical model are analyzed in Sec. 5 and the spectral function is investigated in Sec. 6. In Sec. 7 the thermodynamic potential of the system is expressed as the functional of the full one-particle propagator of conduction electrons and its mass operator. This expression, obtained only for the normal state of the system, has the stationary property about the changes of the mass operator. In Sec. 8 there are the conclusions.

2. DIAGRAMMATICAL THEORY

The Matsubara renormalized Green's functions of conduction and impurity electrons in interaction representation are defined by

$$\begin{aligned} G(\mathbf{k},\sigma,\tau \mid \mathbf{k}',\sigma,'\tau') &= -\left\langle TC_{\mathbf{k}\sigma}(\tau)\overline{C}_{\mathbf{k}'\sigma'}(\tau')U(\beta)\right\rangle_0^c, \\ g(\sigma,\tau \mid \sigma',\tau') &= -\left\langle Tf_{\sigma}(\tau)\overline{f}_{\sigma'}(\tau')U(\beta)\right\rangle_0^c. \end{aligned} \tag{3}$$

Besides them, there are also anomalous Green's functions defined as

$$\begin{aligned} F(\mathbf{k},\sigma,\tau \mid -\mathbf{k},-\sigma',\tau') &= -\left\langle TC_{\mathbf{k}\sigma}(\tau)C_{-\mathbf{k}'-\sigma'}(\tau')U(\beta)\right\rangle_0^c, \\ \overline{F}(-\mathbf{k},-\sigma,\tau \mid \mathbf{k}',\sigma',\tau') &= -\left\langle T\overline{C}_{-\mathbf{k}-\sigma}(\tau)\overline{C}_{\mathbf{k}'\sigma'}(\tau')U(\beta)\right\rangle_0^c, \\ f(\sigma,\tau \mid -\sigma',\tau') &= -\left\langle Tf_{\sigma}(\tau)f_{-\sigma'}(\tau')U(\beta)\right\rangle_0^c, \\ \overline{f}(-\sigma,\tau \mid \sigma',\tau') &= -\left\langle T\overline{f}_{-\sigma}(\tau)\overline{f}_{\sigma'}(\tau')U(\beta)\right\rangle_0^c, \end{aligned} \tag{4}$$

if the system is in superconducting state. Here τ and τ' stand for imaginary time with $0 < \tau < \beta$, β — inverse temperature and T is the chronological ordering operator. The evolution operator $U(\beta)$ is given by

$$\begin{aligned} U(\beta) = T\exp\left(-\int_0^\beta H_{\rm int}(\tau)d\tau\right) = \\ = \sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\int_0^\beta d\tau_1 ... \int_0^\beta d\tau_n T(H_{\rm int}(\tau_1)...H_{\rm int}(\tau_n)). \end{aligned} \tag{5}$$

The statistical averaging is carried out in (3) and (4) with respect to the zero-order density matrix of the conduction and impurity electrons

$$\frac{e^{-\beta H_0}}{Tre^{-\beta H_0}} = \frac{e^{-\beta H_0^c}}{Tre^{-\beta H_0^c}} \times \frac{e^{-\beta H_0^f}}{Tre^{-\beta H_0^f}}. \tag{6}$$

The thermodynamic perturbation theory in $H_{\rm int}$ requires an adequate generalization for calculation of the statistical averages of the T-products of localized f-electron operators. This necessity appears since f electrons are not free. The Hamiltonian H_0 can be diagonalized by using the algebra of Hubbard [28–30] transfer operators $\chi^{mn} = |m><n|$ when the $\mid m >$ with $m = -1,0,1,2$ enumerates four states of the impurity atom: $\mid 0 >$ is the empty or vacuum state with energy $E_0 = 0$, the $\mid 1 >$ and $\mid -1 >$ or $|\uparrow>$ and $|\downarrow>$ are the states with one particle with energy $E_\sigma = \epsilon_f$ and spin $\sigma = \pm 1$ and the state $\mid 2 >= |\uparrow\downarrow>$

contains two f electrons with opposite spins and the energy $E_2 = U + 2\epsilon_f$. By using the relation

$$f_\sigma = \chi^{0\sigma} + \sigma\chi^{\overline{\sigma}2}, \tag{7}$$

we obtain the diagonalized form of the impurity Hamiltonian

$$H_0^f = \sum_{n=-1}^{2} E_n \chi^{nn}, \qquad \sum_{n=-1}^{2} \chi^{nn} = 1. \tag{8}$$

In zero order approximation, when we neglect the process of hybridization of the conduction and impurity electrons, the corresponding Green's functions have the form ($\omega \equiv \omega_n = (2n+1)\pi/\beta$)

$$\begin{aligned} G^0_{\sigma\sigma'}(\mathbf{k},\mathbf{k}' \mid \mathbf{i}\omega) &= \delta_{\sigma\sigma'}\delta_{\mathbf{k}\mathbf{k}'}\frac{1}{i\omega - \epsilon(\mathbf{k})}, \\ g^0_{\sigma\sigma'} = \delta_{\sigma\sigma'} g^0_\sigma(i\omega) &= \frac{1-n_{\overline{\sigma}}}{\lambda_\sigma(i\omega)} + \frac{n_{\overline{\sigma}}}{\overline{\lambda}_{\overline{\sigma}}(i\omega)}, \end{aligned} \tag{9}$$

where ($\overline{\sigma} = -\sigma$)

$$\begin{aligned} \lambda_\sigma(i\omega) &= i\omega + E_0 - E_\sigma, \\ \overline{\lambda}_{\overline{\sigma}}(i\omega) &= i\omega + E_{\overline{\sigma}} - E_2, \\ Z_0 &= e^{-\beta E_0} + e^{-\beta E_\sigma} + e^{-\beta E_{\overline{\sigma}}} + e^{-\beta E_2}, \\ n_{\overline{\sigma}} &= \frac{e^{-\beta E_{\overline{\sigma}}} + e^{-\beta E_2}}{Z_0}, \\ 1 - n_{\overline{\sigma}} &= \frac{e^{-\beta E_0} + e^{-\beta E_\sigma}}{Z_0}. \end{aligned}$$

For the higher orders in the perturbation expansion, in the case of f electrons, we use the identity which corresponds to our generalized Wick's theorem (GWT) for the normal state of the system:

$$\begin{aligned} \left\langle T f_1 f_2 \overline{f}_3 \overline{f}_4 \right\rangle_0 = \left\langle T f_1 \overline{f}_4 \right\rangle_0 \left\langle T f_2 \overline{f}_3 \right\rangle_0 - \\ - \left\langle T f_1 \overline{f}_3 \right\rangle_0 \left\langle T f_2 \overline{f}_4 \right\rangle_0 + \left\langle T f_1 f_2 \overline{f}_3 \overline{f}_4 \right\rangle_0^{\mathrm{ir}} \end{aligned} \tag{10}$$

or

$$g_2^0(1,2|3,4) \quad = \quad g^0(1|4)g^0(2|3) - g^0(1|3)g^0(2|4) + g_2^{(0)\mathrm{ir}}(1,2|3,4), \tag{11}$$

where n stands for (σ_n, τ_n). The generalization for more complicate averages of type $g_n^0(1,...,n \mid n+1,...,2n) = (-1)^n \left\langle T f_1 ... f_n \overline{f}_{n+1} ... \overline{f}_{2n} \right\rangle_0$ is straightforward, namely the right-hand part of this quantity will contain $n!$ term of ordinary

Wick type (chain diagrams) and also the different products of irreducible functions with the same total number of operators. The full irreducible function in $g_n^0(1,...,n|n+1,...,2n)$ also appears. For example, $g_3^0(123|456)$ contains the contribution of $3!=6$ terms of ordinary Wick kind, then appear 9 terms of the form $g^0(1|4)g_2^{(0)\mathrm{ir}}(23|56)$ and the last term is $g_3^{(0)\mathrm{ir}}(123|456)$. The total number of terms is 16. In the case of $g_4^0(1234|5678)$ there are $4!=24$ terms of ordinary Wick kind, the 72 terms of the type $g^0(1|5)g^0(2|6)g_2^{(0)\mathrm{ir}}(34|78)$, then 18 terms of type $g_2^{(0)\mathrm{ir}}(12|56)g_2^{(0)\mathrm{ir}}(34|78)$, then 16 terms of the form $g^0(1|5)g_3^{(0)\mathrm{ir}}(234|678)$ and finally one form $g_4^{(0)\mathrm{ir}}(1234|5678)$. The total number of terms is 131. The signs of all these contributions can be easy determined by commutation rules. Thus the definition of the irreducible Green's functions or Kubo cumulants comes naturally from our GWT. In the absence of Coulomb repulsion U all these irreducible functions are equal to zero. When $U\neq 0$ they contain all the spin, charge and pairing fluctuations produced by the strong correlations. These definitions are the simplification of that ones for Hubbard and other lattice models. The calculation of the simplest irreducible functions, for example $g_2^{(0)\mathrm{ir}}(12|34)$, is rather cumbersome but straightforward. It is necessary to find the values of chronological averages for $4!=24$ different orders of τ_1,τ_2,τ_3 and τ_4 times and then to determine their Fourier representation

$$g_2^{(0)\mathrm{ir}}[\sigma_1,\tau_1;\sigma_2,\tau_2|\sigma_3,\tau_3;\sigma_4,\tau_4]=$$
$$=\frac{1}{\beta^4}\sum_{\omega_1\omega_2\omega_3\omega_4}\exp(-i\omega_1\tau_1-i\omega_2\tau_2+i\omega_3\tau_3+i\omega_4\tau_4)\times$$
$$\times\, g_2^{(0)\mathrm{ir}}[\sigma_1,i\omega_1;\sigma_2,i\omega_2|\sigma_3,i\omega_3;\sigma_4,i\omega_4]. \quad (12)$$

The Fourier representation conserves the frequencies

$$g_2^{(0)\mathrm{ir}}[\sigma_1,i\omega_1;\sigma_2,i\omega_2|\sigma_3,i\omega_3;\sigma_4,i\omega_4]=\beta\delta(\omega_1+\omega_2-\omega_3-\omega_4)\times$$
$$\times\,\widetilde{g}_2^{(0)\mathrm{ir}}[\sigma_1,i\omega_1;\sigma_2,i\omega_2|\sigma_3,i\omega_3;\sigma_4,i\omega_1+i\omega_2-i\omega_3]. \quad (13)$$

There is also the spin conservation $\sigma_1+\sigma_2=\sigma_3+\sigma_4$. Thus we have the rules to deal with chronological averages of thermodynamic perturbation theory.

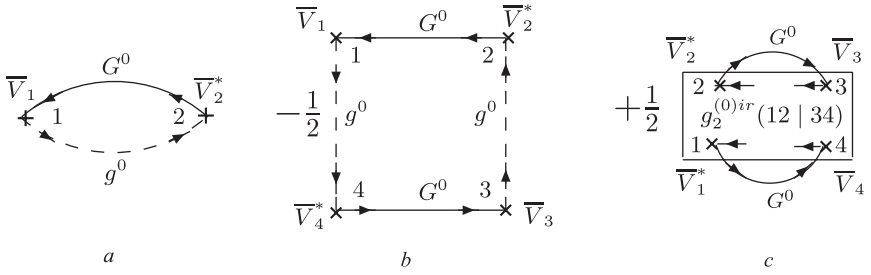
3. THERMODYNAMIC POTENTIAL

First of all, we can determine the thermodynamic potential F of the system

$$\begin{aligned} F&=F_0-\frac{1}{\beta}\ln\langle U(\beta)\rangle_0\,,\\ F_0&=-\frac{1}{\beta}\ln Z_0-\frac{2}{\beta}\sum_{\mathbf{k}}\ln\left[1+\exp\left(-\beta\epsilon(\mathbf{k})\right)\right], \end{aligned} \quad (14)$$

where Z_0 is the partition function of the free impurity atom, and the other term is the contribution from conduction electrons. The diagrams which determine the thermodynamic potential have not the external lines and are named vacuum.

In Fig. 1 the simplest vacuum connected diagrams of the normal state are shown. In the diagrams we shall depict the process of hybridization of C and f electrons. The zero order propagators of conduction and impurity electrons are represented by their solid and dashed lines, correspondingly. These lines connect the crosses which depict the impurity states. To crosses are attached two arrows, one of which is ingoing and the other one is outgoing. They depict the annihilation and creation operators, correspondingly. The index n means (σ_n, τ_n) for impurity and $(\mathbf{k_n}, \sigma_\mathbf{n}, \tau_\mathbf{n})$ — for conduction electrons. The rectangles with $2n$ crosses depict the irreducible $g_n^{(0)\mathrm{ir}}$ Green's functions of f electrons.



a *b* *c*

Fig. 1. The simplest connected vacuum diagrams in normal state. The diagram a) is of the second and b), c) of the fourth order of the theory. Here $\overline{V}_n = V_n/\sqrt{N}$

Besides the vacuum diagrams of the fourth order shown in Fig. 1, b and Fig. 1, c, there is also one disconnected diagram composed from two diagrams of Fig. 1, a type and containing additional factor $1/2!$. Such a situation is repeated in high order of perturbation theory and permits us to formulate linked cluster theorem. It has the form

$$\langle U(\beta)\rangle_0 = \exp\,\langle U(\beta)\rangle_0^c\,, \tag{15}$$

where $\langle U(\beta)\rangle_0^c$ contains only connected diagrams and is equal to zero when hybridization is absent. If we admit the existence of the pairing mechanism of conduction electrons, thanks the hybridization, the pairing mechanism appears also for impurity electrons. This mechanism results in appearance of the anomalous propagators of both kinds of electrons.

Figure 2 shows some of the simplest connected anomalous vacuum diagrams. The anomalous propagators are depicted by the thin (solid and dashed) lines with two opposite directions at the end of them.

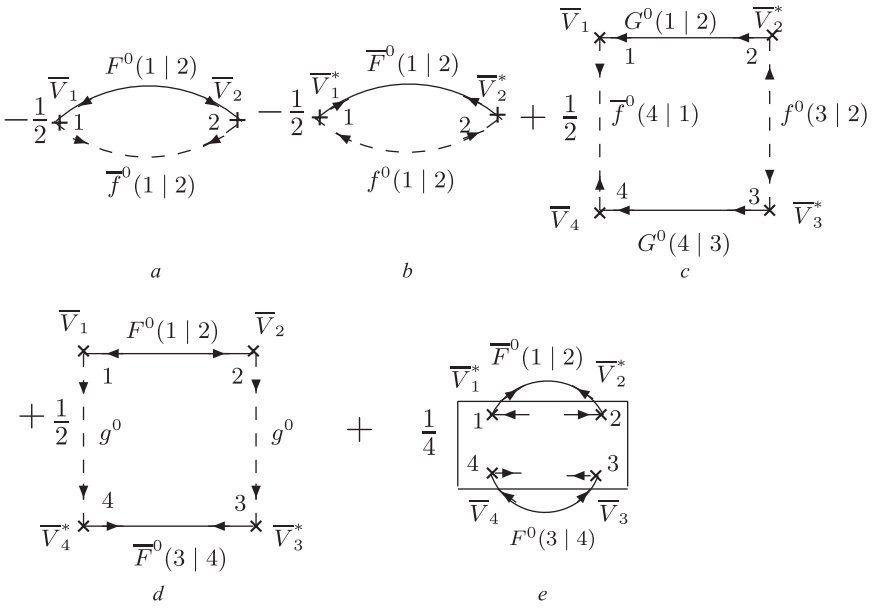


Fig. 2. The simplest vacuum anomalous diagrams. The diagrams a) and b) are of the second and c), d) and e) of the fourth order of perturbation theory

4. RENORMALIZED PROPAGATORS

Now we shall consider the diagrammatical analysis of the perturbation series for renormalized propagators (3) and (4). The simplest contributions to such series are represented in Figs. 3–6. All such diagrams contain two external points with attached arrows determined by the arguments of Green's functions and their kind. At the inner points of diagrams is supposed summation on $\sigma_n, \mathbf{k_n}$, and integration on τ_n.

In the same second order approximation of perturbation theory the diagrams for impurity electron propagators contain new diagrammatical elements namely the irreducible two particle Green's functions. These functions can also be normal or anomalous. The process of their renormalization will be not considered by us, supposing the necessity of renormalization only for the propagators.

In Fig. 5 the diagrams for impurity electron normal propagator are shown.

The last two irreducible Green's functions of Fig. 5 are anomalous because they contain nonequal number of annihilation and creation f operators enumerated in the left and right parts about the vertical bare, correspondingly. Thanks the summation of the infinite series diagrams, the renormalized normal and anomalous

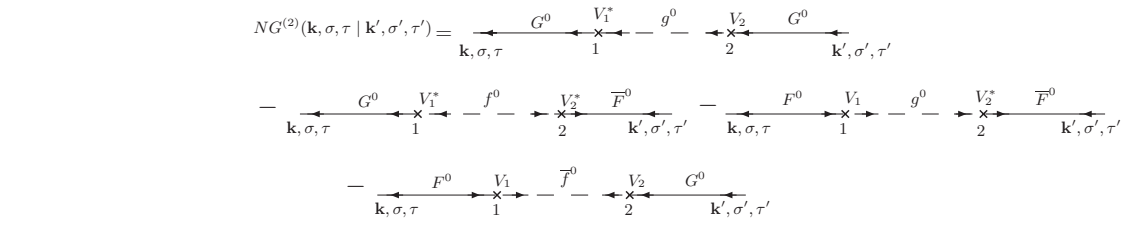


Fig. 3. The second order perturbation theory contribution for conduction electron normal propagator

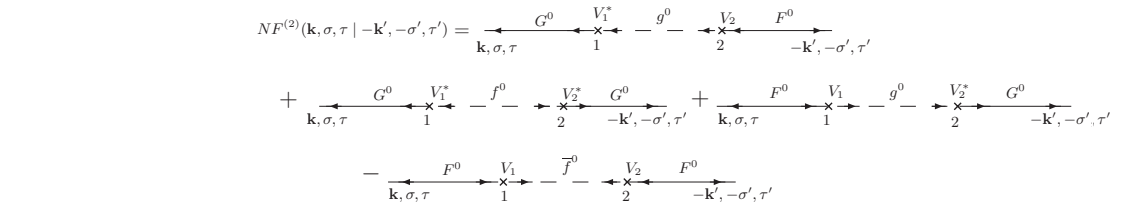


Fig. 4. The second order perturbation theory contribution for conduction electron anomalous propagator

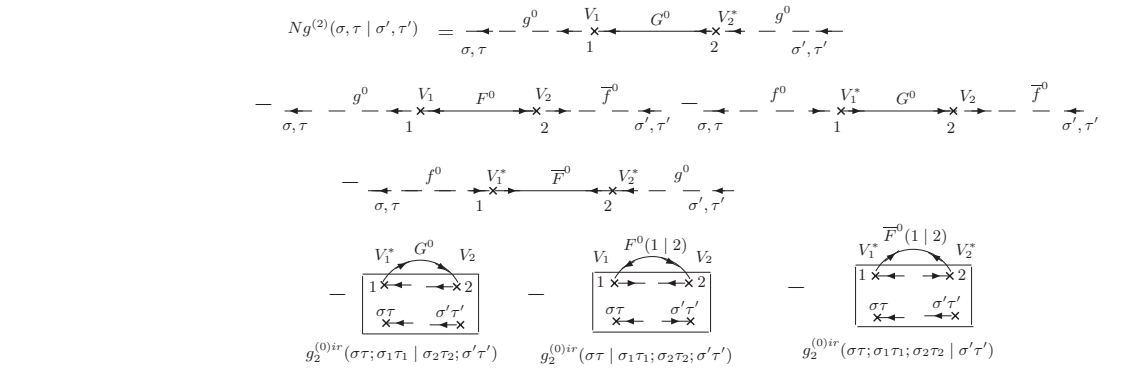


Fig. 5. The second order perturbation contribution for the impurity electron normal propagator

propagators appear, and now it is necessary to put equal to zero the source of electron pairs and simultaneously the bare f^0 and $\overline{f}^0$ together with anomalous irreducible Green's functions. The corresponding contributions to the anomalous impurity electron function $f_{\sigma\sigma'}(\tau-\tau')$ are depicted in Fig. 6.

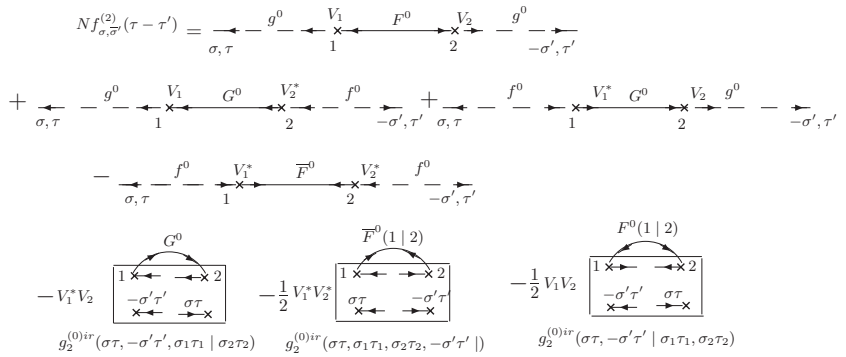


Fig. 6. Anomalous impurity electron Green's function in the second order perturbation theory

The final equations for the renormalized functions are more convenient to write down in the Fourier representation

$$\begin{aligned} G(\mathbf{k},\sigma,\tau|\mathbf{k}',\sigma',\tau') &= \frac{1}{\beta}\sum_{\omega} G_{\sigma\sigma'}(\mathbf{k},\mathbf{k}'|\,\mathbf{i}\omega)\,\exp\left[-\mathbf{i}\omega(\tau-\tau')\right], \\ F(\mathbf{k},\sigma,\tau|-\mathbf{k}',-\sigma',\tau') &= \frac{1}{\beta}\sum_{\omega} F_{\sigma\overline{\sigma}'}(\mathbf{k},-\mathbf{k}'|\,\mathbf{i}\omega)\exp\left[-\mathbf{i}\omega(\tau-\tau')\right]. \end{aligned}$$

The complete equations for the conduction electron propagators have the form:

$$\begin{aligned} G_{\sigma\sigma'}(\mathbf{k},\mathbf{k}'|\,\mathbf{i}\omega) &= \delta_{\mathbf{k}\mathbf{k}'}\delta_{\sigma\sigma'}\mathbf{G}^{\mathbf{0}}_{\sigma}(\mathbf{k}|\,\mathbf{i}\omega)+ \\ &+\frac{V^*_{\mathbf{k}}V_{\mathbf{k}'}}{N}(G^0_{\sigma}(\mathbf{k}|\mathbf{i}\omega)\mathbf{g}_{\sigma\sigma'}(\mathbf{i}\omega)\mathbf{G}^{\mathbf{0}}_{\sigma'}(\mathbf{k}'|\mathbf{i}\omega)- \\ -G^0_{\sigma}(\mathbf{k}|\mathbf{i}\omega)\mathbf{f}_{\sigma\overline{\sigma}'}(\mathbf{i}\omega)\overline{\mathbf{F}}^{\mathbf{0}}_{\overline{\sigma}'\sigma'}(-\mathbf{k}'|\mathbf{i}\omega)) &- \mathbf{F}^{\mathbf{0}}_{\sigma\overline{\sigma}}(\mathbf{k}|\mathbf{i}\omega)\mathbf{g}_{\overline{\sigma}'\overline{\sigma}}(-\mathbf{i}\omega)\overline{\mathbf{F}}^{\mathbf{0}}_{\overline{\sigma}'\sigma'}(-\mathbf{k}|\mathbf{i}\omega)- \\ &- F^0_{\sigma\overline{\sigma}}(\mathbf{k}|\mathbf{i}\omega)\overline{\mathbf{f}}_{\overline{\sigma}\sigma'}(\mathbf{i}\omega)\mathbf{G}^{\mathbf{0}}_{\sigma'}(\mathbf{k}'|\mathbf{i}\omega)), \quad (16) \end{aligned}$$

$$F_{\sigma\overline{\sigma}'}(\mathbf{k},-\mathbf{k}'|\,\mathrm{i}\omega)=\mathbf{F^0}_{\sigma\overline{\sigma}}(\mathbf{k}|\,\mathrm{i}\omega)\delta_{\mathbf{k}\mathbf{k}'}\delta_{\sigma\sigma'}+$$
$$+\frac{V^*_{\mathbf{k}}V_{\mathbf{k}'}}{N}(G^0_\sigma(\mathbf{k}|\mathrm{i}\omega)\mathbf{g}_{\sigma\sigma'}(\mathrm{i}\omega)\mathbf{F^0}_{\sigma'\overline{\sigma}'}(\mathbf{k}'|\mathrm{i}\omega)+$$
$$+G^0_\sigma(\mathbf{k}|\mathrm{i}\omega)\mathbf{f}_{\sigma\overline{\sigma}'}(\mathrm{i}\omega)\mathbf{G^0}_{\overline{\sigma}'}(-\mathbf{k}'|-\mathrm{i}\omega)+\mathbf{F^0}_{\sigma\overline{\sigma}}(\mathbf{k}|\mathrm{i}\omega)\mathbf{g}_{\overline{\sigma}'\overline{\sigma}}(-\mathrm{i}\omega)\mathbf{G^0}_{\overline{\sigma}'}(-\mathbf{k}'|-\mathrm{i}\omega)-$$
$$-F^0_{\sigma\overline{\sigma}}(\mathbf{k}|\mathrm{i}\omega)\overline{\mathbf{f}}_{\overline{\sigma}\sigma'}(\mathrm{i}\omega)\mathbf{F^0}_{\sigma'\overline{\sigma}'}(\mathbf{k}'|\mathrm{i}\omega)). \quad (17)$$

These renormalized propagators are expressed through the full propagators g, f and $\overline{f}$ of impurity electrons.

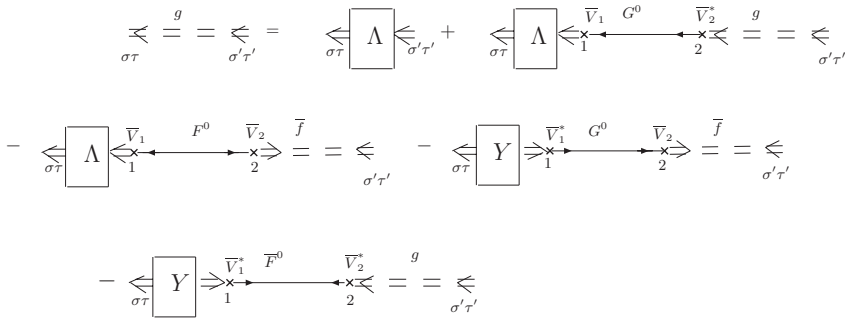


Fig. 7. Dyson-type equation for the normal propagator of impurity electrons. Double dashed lines depict full electron propagators. The arrows on them distinguish the normal and anomalous ones. The squares with attached arrows depict the correlated functions. On double repeated indices 1 and 2 is supposed summation by σ_n and $\mathbf{k_n}$ and integration by τ_n

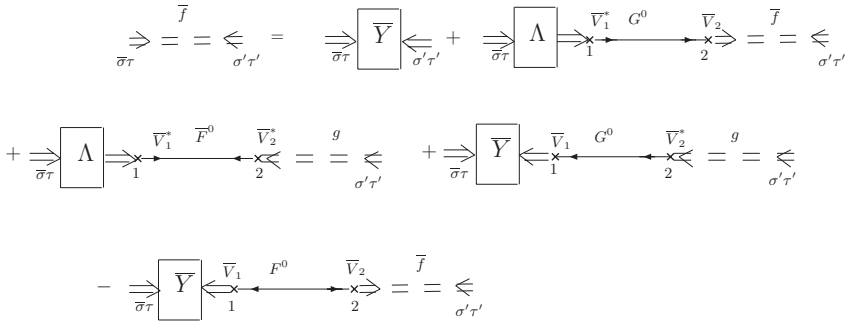


Fig. 8. Dyson-type equation for one of anomalous Green's functions of f electrons

Now it is necessary to obtain the corresponding equations for the full impurity electron propagators. Because the subsystem of f electrons is strongly correlated we have to introduce the correlation functions $Z_{\sigma\sigma'}, Y_{\sigma\overline{\sigma}'}$ and $\overline{Y}_{\overline{\sigma}\sigma'}$ which are represented by strong connected diagrams with irreducible Green's functions [31–35]. The process of renormalization of f-electron propagators is shown in Figs. 7 and 8, where the double dashed lines depict the full f-electron functions and the rectangles represent the correlation functions $\Lambda_{\sigma\sigma'} = g^0_{\sigma\sigma'} + Z_{\sigma\sigma'}$, $Y_{\sigma\sigma'}$ and $\overline{Y}_{\overline{\sigma}\sigma}$. The second equation we shall depict for anomalous propagator $\overline{f}$ of the impurity electrons (see Fig. 8).

In both these equations the bare conduction electron propagators $G^0_\sigma(\mathbf{k}|\mathbf{i}\omega)$, $F^0_{\sigma\overline{\sigma}}(\mathbf{k}|\mathbf{i}\omega)$ and $\overline{F}^0_{\overline{\sigma}\sigma}(-\mathbf{k}|\mathbf{i}\omega)$ play the role of mass operators for the f-electron propagators. It is easy to see that these functions participate in above equations being averaged on the Brillouin cell with matrix elements of hybridization. Therefore we define the new quantities:

$$\frac{1}{N}\sum_{\mathbf{k_1}\mathbf{k_2}} V^*_{\mathbf{k_2}} V_{\mathbf{k_1}} G^0(\mathbf{k_1},\sigma_1,\tau_1|\mathbf{k_2},\sigma_2,\tau_2) =$$

$$= \frac{1}{N}\sum_{\mathbf{k_1}} |V_{\mathbf{k_1}}|^2 G^0_{\sigma_1\sigma_2}(\mathbf{k}|\tau_1-\tau_2) \equiv \delta_{\sigma_1\sigma_2}\mathbf{G^0_{\sigma_1}}(\tau_1-\tau_2),$$

$$\frac{1}{N}\sum_{\mathbf{k_1}\mathbf{k_2}} V^*_{\mathbf{k_1}} V^*_{\mathbf{k_2}} \overline{F}^0(\mathbf{k_1},\overline{\sigma}_1,\tau_1|\mathbf{k_2},\sigma_2,\tau_2) =$$

$$= \frac{1}{N}\sum_{\mathbf{k_1}} |V_{\mathbf{k_1}}|^2 \overline{F}^0_{\overline{\sigma}_1\sigma_2}(-\mathbf{k_1}|\tau_1-\tau_2) \equiv \delta_{\sigma_1\sigma_2}\mathbf{\overline{F}^0_{\overline{\sigma}_1\sigma_1}}(\tau_1-\tau_2),$$

$$\frac{1}{N}\sum_{\mathbf{k_1}\mathbf{k_2}} V_{\mathbf{k_1}} V_{\mathbf{k_2}} F^0(\mathbf{k_1},\sigma_1,\tau_1|\mathbf{k_2},\overline{\sigma}_2,\tau_2) =$$

$$= \frac{1}{N}\sum_{\mathbf{k_1}} |V_{\mathbf{k_1}}|^2 F^0_{\sigma_1\overline{\sigma}_2}(\mathbf{k_1}|\tau_1-\tau_2) \equiv \delta_{\sigma_1\sigma_2}\mathbf{F^0_{\sigma_1\overline{\sigma}_1}}(\tau_1-\tau_2). \quad (18)$$

These definitions give us the possibility to simplify the structure of equations for the f-electron propagators. By using these average bare propagators G^0_σ, $F^0_{\sigma\overline{\sigma}}$ and $\overline{F}^0_{\overline{\sigma}\sigma}$ and the Fourier representation for τ-variables we obtain

$$g_\sigma(i\omega) = \frac{\Lambda_\sigma(i\omega) \; - \; G^0_{\overline{\sigma}}(-i\omega)[\Lambda_\sigma(i\omega)\Lambda_{\overline{\sigma}}(-i\omega) \; + \; Y_{\sigma\overline{\sigma}}(i\omega)\overline{Y}_{\overline{\sigma}\sigma}(i\omega)]}{d_\sigma(i\omega)}, \quad (19)$$

$$\overline{f}_{\overline{\sigma}\sigma}(i\omega) =$$

$$= \frac{\overline{Y}_{\overline{\sigma}\sigma}(i\omega) \; + \; \overline{F}^0_{\overline{\sigma}\sigma}(i\omega)(\Lambda_\sigma(i\omega)\Lambda_{\overline{\sigma}}(-i\omega) \; + \; Y_{\sigma\overline{\sigma}}(i\omega)\overline{Y}_{\overline{\sigma}\sigma}(i\omega))}{d_\sigma(i\omega)}, \quad (20)$$

$$f_{\sigma\overline{\sigma}}(i\omega) = \\ = \frac{\{Y_{\sigma\overline{\sigma}}(i\omega) \ + \ F^0_{\sigma\overline{\sigma}}(i\omega)[(\Lambda_\sigma(i\omega)\Lambda_{\overline{\sigma}}(-i\omega) \ + \ Y_{\sigma\overline{\sigma}}(i\omega)\overline{Y}_{\overline{\sigma}\sigma}(i\omega)]\}}{d_\sigma(i\omega)}, \quad (21)$$

$$d_\sigma(i\omega) = (1 - \Lambda_\sigma(i\omega)G^0_\sigma(i\omega))(1 - \Lambda_{\overline{\sigma}}(-i\omega)G^0_{\overline{\sigma}}(-i\omega)) + \overline{Y}_{\overline{\sigma}\sigma}(i\omega)F^0_{\sigma\overline{\sigma}}(i\omega) + \\ + Y_{\sigma\overline{\sigma}}(i\omega)\overline{F}^0_{\overline{\sigma}\sigma}(i\omega) + \overline{F}^0_{\overline{\sigma}\sigma}(i\omega)F^0_{\sigma\overline{\sigma}}(i\omega)[Y_{\sigma\overline{\sigma}}(i\omega)\overline{Y}_{\overline{\sigma}\sigma}(i\omega) + \Lambda_\sigma(i\omega)\Lambda_{\overline{\sigma}}(-i\omega)] + \\ + G^0_{\overline{\sigma}}(-i\omega)G^0_\sigma(i\omega)Y_{\sigma\overline{\sigma}}(i\omega)\overline{Y}_{\overline{\sigma}\sigma}(i\omega). \quad (22)$$

In the previous part of the paper we supposed the existence of pairing potential of conduction electrons with order parameter Δ and with the bare propagators:

$$\begin{aligned} G^0_\sigma(\mathbf{k}|\mathbf{i}\omega) &= \frac{i\omega \ + \ \epsilon(\mathbf{k})}{(i\omega)^2 - E^2(\mathbf{k})}; \\ F^0_{\sigma\overline{\sigma}}(\mathbf{k}|\mathbf{i}\omega) = \overline{\mathbf{F}}^{\mathbf{0}}_{\overline{\sigma}\sigma}(-\mathbf{k}|\mathbf{i}\omega) &= \frac{\Delta}{(i\omega)^2 - \ E^2(\mathbf{k})}; \\ E(\mathbf{k}) &= \sqrt{\epsilon^2(\mathbf{k}) + \mathbf{\Delta^2}}. \end{aligned} \quad (23)$$

Now we shall discuss the case when the pairing potential is absent and the superconducting state appears simultaneously with both subsystems as a consequence of the broken symmetry and phase transition. In this more simple case the renormalized conduction electron propagators have the form

$$G_{\sigma\sigma'}(\mathbf{k}, \mathbf{k}'|\mathbf{i}\omega) = \\ = \delta_{\mathbf{k}\mathbf{k}'}\delta_{\sigma\sigma'}G^0_\sigma(\mathbf{k}|\mathbf{i}\omega) + \frac{\mathbf{V}^*_{\mathbf{k}}\mathbf{V}_{\mathbf{k}'}}{\mathbf{N}}\mathbf{G}^{\mathbf{0}}_\sigma(\mathbf{k}|\mathbf{i}\omega)\mathbf{g}_{\sigma\sigma'}(\mathbf{i}\omega)\mathbf{G}^{\mathbf{0}}_{\sigma'}(\mathbf{k}'|\mathbf{i}\omega), \quad (24)$$

$$F_{\sigma\overline{\sigma}'}(\mathbf{k}, -\mathbf{k}|\mathbf{i}\omega) = \frac{\mathbf{V}^*_{\mathbf{k}}\mathbf{V}_{\mathbf{k}}}{\mathbf{N}}\mathbf{G}^{\mathbf{0}}_\sigma(\mathbf{k}|\mathbf{i}\omega)\mathbf{f}_{\sigma\overline{\sigma}'}(\mathbf{i}\omega)\mathbf{G}^{\mathbf{0}}_{\overline{\sigma}'}(-\mathbf{k}| - \mathbf{i}\omega), \quad (25)$$

$$G^0_\sigma(\mathbf{k}|\mathbf{i}\omega) = (\mathbf{i}\omega - \epsilon(\mathbf{k}))^{-\mathbf{1}}. \quad (26)$$

The renormalized propagators of impurity electron in this case are:

$$g_\sigma(i\omega) = \\ = \frac{\Lambda_\sigma(i\omega) \ - \ G^0_{\overline{\sigma}}(-i\omega)[\Lambda_\sigma(i\omega)\Lambda_{\overline{\sigma}}(-i\omega) \ + \ Y_{\sigma\overline{\sigma}}(i\omega)\overline{Y}_{\overline{\sigma}\sigma}(i\omega)]}{d_\sigma(i\omega)}, \quad (27)$$

$$\overline{f}_{\overline{\sigma}\sigma}(i\omega) = \frac{\overline{Y}_{\overline{\sigma}\sigma}(i\omega)}{d_\sigma(i\omega)}; \qquad f_{\sigma\overline{\sigma}}(i\omega) = \frac{Y_{\sigma\overline{\sigma}}(i\omega)}{d_\sigma(i\omega)}, \quad (28)$$

$$d_\sigma(i\omega) = (1 - \Lambda_\sigma(i\omega)G^0_\sigma(i\omega))(1 - \Lambda_{\overline{\sigma}}(-i\omega)G^0_{\overline{\sigma}}(-i\omega)) + \\ + G_{\overline{\sigma}}(-i\omega)G^0_\sigma(i\omega)Y_{\sigma\overline{\sigma}}(i\omega)\overline{Y}_{\overline{\sigma}\sigma}(i\omega). \quad (29)$$

Equation (24) has been established many years ago in the paper of Anderson [1] by using the equations of motion of conduction electron operators. In this equation the propagator $g_\sigma(i\omega)$ has the role of t-matrix for non-spin-flip scattering. By setting $\mathbf{k} = \mathbf{k}'$ in $G_\sigma(\mathbf{k}, \mathbf{k}'|\mathbf{i}\omega)$

$$G_\sigma(\mathbf{k}, \mathbf{k}|\mathbf{i}\omega) = \frac{\mathbf{1}}{\mathbf{i}\omega - \epsilon(\mathbf{k})} + \frac{|\mathbf{V_k}|^\mathbf{2}\mathbf{g}_\sigma(\mathbf{i}\omega)}{\mathbf{N}(\mathbf{i}\omega - \epsilon(\mathbf{k}))^\mathbf{2}} \quad (30)$$

and considering the Lehmann spectral representation it is possible to conclude that the discontinuity of $g_\sigma(E)$ across the real axis is pure imaginary [8]

$$g_\sigma(E + i\delta) = [g_\sigma(E - i\delta)]^*. \quad (31)$$

Green's function $g_\sigma(i\omega)$ has been known till now in approximate form as a result of special decoupling mechanism used for equations of motion of quantum Green's functions. As is known, in such a decoupling approximation some combinations of operators are taken off the average value of product of operators and are replaced by their average values. After that truncation the Green's functions of low order remain. This approximation has been proposed by Bogoliubov, Tiablikov, Zubarev and Tserkovnikov [21–24] and used by other authors [2–14,18]. The hybridization of conduction and impurity electrons causes the appearance of mixed Green's functions:

$$\begin{aligned} G_m(\mathbf{k}, \sigma, \tau|\sigma', \tau') &= -\left\langle TC_{\mathbf{k}\sigma}(\tau)\overline{f}_{\sigma'}(\tau')U(\beta)\right\rangle_0^c, \\ F_m(\mathbf{k}, \sigma, \tau|\overline{\sigma}', \tau') &= -\left\langle TC_{\mathbf{k}\sigma}(\tau)f_{\overline{\sigma}'}(\tau')U(\beta)\right\rangle_0^c, \\ \overline{F}_m(-\mathbf{k}, \overline{\sigma}, \tau|\sigma', \tau') &= -\left\langle T\overline{C}_{-\mathbf{k}\overline{\sigma}}(\tau)\overline{f}_{\sigma'}(\tau')U(\beta)\right\rangle_0^c, \end{aligned} \quad (32)$$

and also

$$\begin{aligned} G^m(\sigma, \tau|\mathbf{k}, \sigma', \tau') &= -\left\langle Tf_\sigma(\tau)\overline{C}_{\mathbf{k}\sigma'}(\tau')U(\beta)\right\rangle_0^c, \\ F^m(\sigma, \tau|-\mathbf{k}, \overline{\sigma}', \tau') &= -\left\langle Tf_\sigma(\tau)C_{-\mathbf{k}\overline{\sigma}'}(\tau')U(\beta)\right\rangle_0^c, \\ \overline{F}^m(\overline{\sigma}, \tau|\mathbf{k}, \sigma', \tau') &= -\left\langle T\overline{f}_{\overline{\sigma}}(\tau)\overline{C}_{\mathbf{k}\sigma'}(\tau')U(\beta)\right\rangle_0^c. \end{aligned} \quad (33)$$

Let $G_{m\sigma\sigma'}(\mathbf{k}|\mathbf{i}\omega)$, $F_{m\sigma\overline{\sigma}'}(\mathbf{k}|\mathbf{i}\omega)$ and $F_{m\overline{\sigma}\sigma'}(\mathbf{k}|\mathbf{i}\omega)$ be the Fourier representation of the first group of Green's functions and $G^m_{\sigma\sigma'}(\mathbf{k}|\mathbf{i}\omega)$, $F^m_{\sigma\overline{\sigma}'}(-\mathbf{k}|\mathbf{i}\omega)$ and $\overline{F}^m_{\overline{\sigma}\sigma'}(\mathbf{k}|\mathbf{i}\omega)$ of the second group.

In the presence of superconducting pairing of conduction electrons we obtain the following results:

$$\begin{aligned} G_{m\sigma\sigma'}(\mathbf{k}|\mathbf{i}\omega) &= \frac{V_{\mathbf{k}}^*}{\sqrt{N}}\left[G_{\sigma}^0(\mathbf{k}|\mathbf{i}\omega)\mathbf{g}_{\sigma\sigma'}(\mathbf{i}\omega) - \mathbf{F}^{\mathbf{0}}_{\sigma\overline{\sigma}}(\mathbf{k}|\mathbf{i}\omega)\overline{\mathbf{f}}_{\overline{\sigma}\sigma'}(\mathbf{i}\omega)\right], \\ F_{m\sigma\overline{\sigma}'}(\mathbf{k}|\mathbf{i}\omega) &= \frac{V_{\mathbf{k}}^*}{\sqrt{N}}\left[G_{\sigma}^0(\mathbf{k}|\mathbf{i}\omega)\mathbf{f}_{\sigma\sigma'}(\mathbf{i}\omega) + \mathbf{F}^{\mathbf{0}}_{\sigma\overline{\sigma}'}(\mathbf{k}|\mathbf{i}\omega)\mathbf{g}_{\overline{\sigma}'\overline{\sigma}}(-\mathbf{i}\omega)\right], \quad (34) \\ \overline{F}_{m\overline{\sigma}\sigma'}(-\mathbf{k}|\mathbf{i}\omega) &= \frac{V_{\mathbf{k}}^*}{\sqrt{N}}\left[G_{\overline{\sigma}}^0(-\mathbf{k}|-\mathbf{i}\omega)\overline{\mathbf{f}}_{\overline{\sigma}\sigma'}(\mathbf{i}\omega) + \overline{\mathbf{F}}^{\mathbf{0}}_{\overline{\sigma}\sigma}(-\mathbf{k}|\mathbf{i}\omega)\mathbf{g}_{\sigma\sigma'}(\mathbf{i}\omega)\right]. \end{aligned}$$

For the second group of mixed propagators we have

$$\begin{aligned} G^m_{\sigma\sigma'}(\mathbf{k}|\mathbf{i}\omega) &= \frac{V_{\mathbf{k}}}{\sqrt{N}}\left[g_{\sigma\sigma'}(i\omega)G^0_{\sigma'}(\mathbf{k}|\mathbf{i}\omega) - \mathbf{f}_{\sigma\overline{\sigma}'}(\mathbf{i}\omega)\overline{\mathbf{F}}^{\mathbf{0}}_{\overline{\sigma}'\sigma'}(-\mathbf{k}|\mathbf{i}\omega)\right], \\ F^m_{\sigma\overline{\sigma}'}(-\mathbf{k}|\mathbf{i}\omega) &= \frac{V_{\mathbf{k}}}{\sqrt{N}}\left[g_{\sigma\sigma'}(i\omega)F^0_{\sigma'\overline{\sigma}'}(\mathbf{k}|\mathbf{i}\omega) + \mathbf{f}_{\sigma\overline{\sigma}'}(\mathbf{i}\omega)\mathbf{G}^{\mathbf{0}}_{\overline{\sigma}'}(-\mathbf{k}|\mathbf{i}\omega)\right], \quad (35) \\ \overline{F}^m_{\overline{\sigma}\sigma'}(\mathbf{k}|\mathbf{i}\omega) &= \frac{V_{\mathbf{k}}}{\sqrt{N}}\left[\overline{f}_{\overline{\sigma}\sigma'}(i\omega)G^0_{\sigma'}(\mathbf{k}|\mathbf{i}\omega) + \mathbf{g}_{\overline{\sigma}\sigma'}(-\mathbf{i}\omega)\overline{\mathbf{F}}^{\mathbf{0}}_{\overline{\sigma}'\sigma'}(-\mathbf{k}|\mathbf{i}\omega)\right]. \end{aligned}$$

Now we multiply the system of operators (33) by $V_{\mathbf{k}}^*/\sqrt{N}$, and after summing over $\mathbf{k}$, use the definitions (18) and supposing the paramagnetic phase of the system. Then we obtain

$$G^m_{\sigma}(i\omega) = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} V_{\mathbf{k}}^* G^m_{\sigma}(\mathbf{k}|\mathbf{i}\omega) = \mathbf{g}_{\sigma}(\mathbf{i}\omega)\mathbf{G}^{\mathbf{0}}_{\sigma}(\mathbf{i}\omega) - \mathbf{f}_{\sigma\overline{\sigma}'}(\mathbf{i}\omega)\overline{\mathbf{F}}^{\mathbf{0}}_{\overline{\sigma}\sigma}(\mathbf{i}\omega),$$

$$F^m_{\sigma\overline{\sigma}}(i\omega) = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} V_{\mathbf{k}}^* F^m_{\sigma\overline{\sigma}}(-\mathbf{k}|\mathbf{i}\omega) = \\ = g_{\sigma}(i\omega)F^0_{\sigma\overline{\sigma}}(i\omega) + f_{\sigma\overline{\sigma}}(i\omega)G^0_{\overline{\sigma}}(-i\omega), \quad (36)$$

$$\overline{F}^m_{\overline{\sigma}\sigma}(i\omega) = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} V_{\mathbf{k}}^* \overline{F}^m_{\overline{\sigma}\sigma}(\mathbf{k}|\mathbf{i}\omega) = \mathbf{g}_{\overline{\sigma}}(-\mathbf{i}\omega)\overline{\mathbf{F}}^{\mathbf{0}}_{\overline{\sigma}\sigma}(\mathbf{i}\omega) + \overline{\mathbf{f}}_{\overline{\sigma}\sigma}(\mathbf{i}\omega)\mathbf{G}^{\mathbf{0}}_{\sigma}(\mathbf{i}\omega).$$

When the superconducting state is established in the both f and c subsystems, simultaneously, and the bare anomalous Green's functions of conduction electrons are equal to zero, the above equations become more simple:

$$\begin{aligned} G^m_{\sigma}(i\omega) &= g_{\sigma}(i\omega)G^0_{\sigma}(i\omega), \\ F^m_{\sigma\overline{\sigma}}(i\omega) &= f_{\sigma\overline{\sigma}}(i\omega)G^0_{\overline{\sigma}}(-i\omega), \quad (37) \\ \overline{F}^m_{\overline{\sigma}\sigma}(i\omega) &= \overline{f}_{\overline{\sigma}\sigma}(i\omega)G^0_{\sigma}(i\omega). \end{aligned}$$

For the second group of mixed functions in the same conditions we obtain

$$\begin{aligned} G_{m\sigma}(i\omega) &= G^0_\sigma(i\omega) g_\sigma(i\omega), \\ F_{m\sigma\overline{\sigma}}(i\omega) &= G^0_\sigma(i\omega) f_{\sigma\overline{\sigma}}(i\omega), \\ \overline{F}_{m\overline{\sigma}\sigma}(i\omega) &= G^0_{\overline{\sigma}}(-i\omega) \overline{f}_{\overline{\sigma}\sigma}(i\omega). \end{aligned} \tag{38}$$

Further we shall restrict ourselves only to consider the case of a paramagnetic system in the normal state. The equations for corresponding Green's functions of conduction and impurity electrons became:

$$\begin{aligned} G_\sigma(\mathbf{k},\mathbf{k}'|\mathbf{i}\omega) &= \delta_{\mathbf{k}\mathbf{k}'} G^0_\sigma(\mathbf{k}|\mathbf{i}\omega) + \frac{\mathbf{V_k V^*_{k'}}}{\mathbf{N}} \mathbf{G^0_\sigma}(\mathbf{k}|\mathbf{i}\omega) \mathbf{g}_\sigma(\mathbf{i}\omega) \mathbf{G^0_\sigma}(\mathbf{k}'|\mathbf{i}\omega), \\ g_\sigma(i\omega) &= \frac{\Lambda_\sigma(i\omega)}{1 - \Lambda_\sigma(i\omega) G^0_\sigma(i\omega)}, \quad \Lambda_\sigma(i\omega) = g^0_\sigma(i\omega) + Z_\sigma(i\omega), \end{aligned} \tag{39}$$

where

$$G^0_\sigma(i\omega) = \frac{1}{N} \sum_{\mathbf{k}} |V_\mathbf{k}|^2 G^0_\sigma(\mathbf{k}|\mathbf{i}\omega) = \int \mathbf{d}\epsilon \frac{\mathbf{V^2}(\epsilon)\rho_\mathbf{0}(\epsilon)}{\mathbf{i}\omega - \epsilon}.$$

Here $\rho_0(\epsilon)$ is the density of states of the bare conduction band and matrix element of hybridization $V_\mathbf{k}$ is supposed to be dependent on the energy. Equations (39) are exact, but for correlation function $Z_\sigma(i\omega)$ doesn't exist an exact Dyson-type equation and only approximate expressions can be available (see Fig. 9 in this paper). The diagrams of Fig. 10, b type are omitted in this investigation. Our main approximation comes to the summation of the ladder diagrams which will be enough to obtain the leading contributions of the spin and charge fluctuations. This approximation has used only the simplest irreducible Green's function $g_2^{(0)\mathrm{ir}}$ which is iterated many times. It has the form:

$$\begin{aligned} Z_{\sigma\sigma'}(\tau - \tau') = -\sum_{\mathbf{k_1 k_2} \sigma_1 \sigma_2} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 g_2^{(0)\mathrm{ir}}[\sigma, \tau; \sigma_1, \tau_1 | \sigma_2, \tau_2; \sigma', \tau'] \\ \frac{1}{N} V^*_{\mathbf{k_1}} V_{\mathbf{k_2}} G_{\sigma_2\sigma_1}(\mathbf{k_2}, \tau_\mathbf{2} | \mathbf{k_1}, \tau_\mathbf{1}), \end{aligned} \tag{40}$$

or in Fourier representation

$$\begin{aligned} Z_{\sigma\sigma'}(i\omega) = -\frac{1}{\beta} \sum_{\omega_1} \sum_{\sigma_1\sigma_2} \sum_{\mathbf{k_1 k_2}} \widetilde{g}_2^{(0)\mathrm{ir}}[\sigma, i\omega; \sigma_1, i\omega_1 | \sigma_2, i\omega_1; \sigma', i\omega] \\ \frac{1}{N} V^*_{\mathbf{k_1}} V_{\mathbf{k_2}} G_{\sigma_2\sigma_1}(\mathbf{k_1}, \mathbf{k_2} | \mathbf{i}\omega_\mathbf{1}). \end{aligned} \tag{41}$$

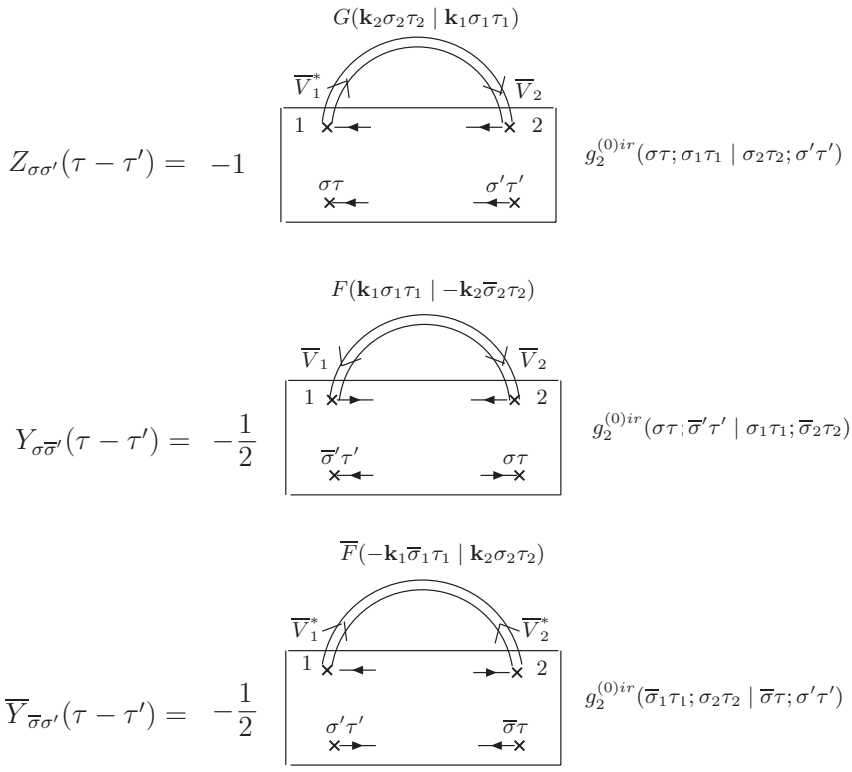


Fig. 9. Schematic representation of the main approximations for the correlated functions. The solid double lines with arrows depict the renormalized one-particle Green's functions of conduction electrons. The rectangles depict the irreducible Green's functions of impurity electrons

Here we take into account the conservation law of the frequencies:

$$g_2^{(0)\mathrm{ir}}[\sigma, i\omega; \sigma_1, i\omega_1|\sigma_1, i\omega_1; \sigma', i\omega'] = \\ = \beta\delta(\omega-\omega')\widetilde{g}_2^{(0)\mathrm{ir}}[\sigma, i\omega; \sigma_1, i\omega_1|\sigma_2, i\omega_1; \sigma', i\omega]. \quad (42)$$

In paramagnetic phase we have more simple equation ($\sigma' = \sigma$):

$$Z_\sigma(i\omega) = -\frac{1}{\beta}\sum_{\omega_1}\sum_{\sigma_1}\widetilde{g}_2^{(0)\mathrm{ir}}[\sigma, i\omega; \sigma_1, i\omega_1|\sigma_1, i\omega_1; \sigma, i\omega]G_{\sigma_1}(i\omega_1), \quad (43)$$

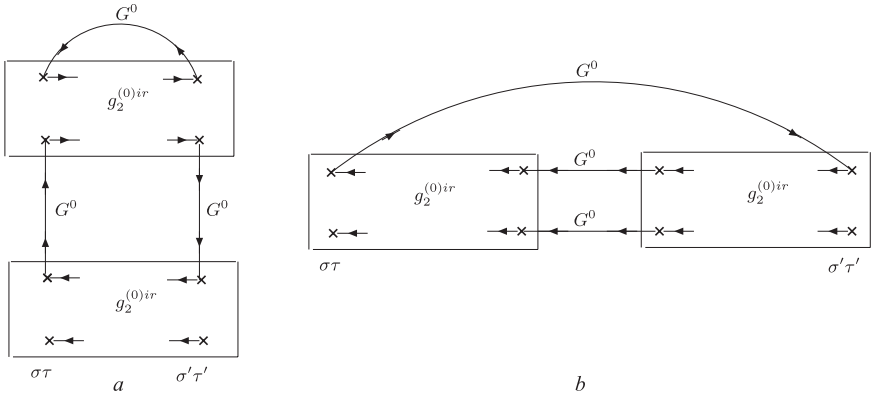


Fig. 10. Examples of the simplest ladder diagram for g function

where

$$G_\sigma(i\omega) = \frac{1}{N}\sum_{\mathbf{k_1}\mathbf{k_2}} V^*_{\mathbf{k_1}} V_{\mathbf{k_2}} G_\sigma(\mathbf{k_1}, \mathbf{k_2}|\mathbf{i}\omega). \tag{44}$$

On the base of equations (9) and (39) the last function (44) can be presented in the form:

$$G_\sigma(i\omega) = G^0_\sigma(i\omega) + [G^0_\sigma(i\omega)]^2 g_\sigma(i\omega) = \frac{G^0_\sigma(i\omega)}{1 - \Lambda_\sigma(i\omega) G^0_\sigma(i\omega)}. \tag{45}$$

By using the definition (39) of correlation function of normal state $\Lambda_\sigma(i\omega)$ and approximation (43) for function $Z_\sigma(i\omega)$, we obtain the final integral equation for Λ_σ:

$$\Lambda_\sigma(i\omega) = g^{(0)}_\sigma(i\omega) - \frac{1}{\beta}\sum_{\omega_1}\sum_{\sigma_1} \widetilde{g}^{(0)\mathrm{ir}}_2 [\sigma, i\omega; \sigma_1, i\omega_1|\sigma_1, i\omega_1; \sigma, i\omega] \frac{G^0_{\sigma_1}(i\omega_1)}{1 - \Lambda_{\sigma_1}(i\omega_1) G^0_{\sigma_1}(i\omega_1)}. \tag{46}$$

In the following Section of this paper we shall discuss the simplest case of symmetric impurity Anderson model with the condition $2\epsilon_f + U = 0$.

5. SYMMETRIC MODEL

In the simplest case of symmetric impurity Anderson model when $\epsilon_f = -U/2 < 0$ and $\epsilon_f + U = U/2 > 0$ we have more simple equations:

$$\begin{aligned} g^0_\sigma(i\omega) &= \frac{i\omega}{(i\omega)^2 - (U/2)^2}, \\ Z_0 &= 2(1 + \exp(-\beta\epsilon_f)) = 2(1 + \exp(\beta U/2)), \\ n_\sigma &= 1/2, \end{aligned} \tag{47}$$

and the antisymmetry property of zero order impurity Green's function $g^0_\sigma(-i\omega) = -g^0_\sigma(i\omega)$ takes place.

Additionally we assume the evenness of the matrix element $V(\epsilon)$ and of the bare density of state $\rho_0(\epsilon)$. In this case the function $G^0_\sigma(i\omega)$ is also antisymmetric $G^0_\sigma(-i\omega) = -G^0_\sigma(i\omega)$.

Thanks to these antisymmetry properties, we may look for an antisymmetric solution

$$\Lambda_\sigma(-i\omega) = -\Lambda_\sigma(i\omega) \tag{48}$$

of equation (46). Analytical continuation of these functions have the property of oddness of their real parts and evenness of imaginary parts

$$\begin{aligned} g^0_\sigma(E + i\delta) &= -g^0_\sigma(-E - i\delta), \\ G^0_\sigma(E + i\delta) &= -G^0_\sigma(-E - i\delta), \\ \Lambda^0_\sigma(E + i\delta) &= -\Lambda^0_\sigma(-E - i\delta), \end{aligned} \tag{49}$$

where

$$\begin{aligned} G^0_\sigma(E + i\delta) &= I(E) - i\Gamma(E), \\ I(E) &= P\int \frac{|V(\epsilon)|^2 \rho_0(\epsilon) d\epsilon}{E - \epsilon}, \\ \Gamma(E) &= \pi |V(E)|^2 \rho_0(E). \end{aligned} \tag{50}$$

$I(E)$ is the principal part of the integral. This function is antisymmetric. $\Gamma(E)$ is the band width of the virtual level and an even function of energy. The symmetric impurity Anderson model has the advantage to be of a simple form for the irreducible two particles Green's functions in different spin and frequency channels. In this special case we have [31, 32]

$$\widetilde{g}_2^{(0)\mathrm{ir}}[\sigma, i\omega; \sigma, i\omega_1 | \sigma, i\omega_1; \sigma, i\omega] = \frac{\beta(U/2)^2(1 - \delta\omega\omega_1)}{[(i\omega)^2 - (U/2)^2][(i\omega_1)^2 - (U/2)^2]}, \tag{51}$$

$$\widetilde{g}_2^{(0)\mathrm{ir}}[\sigma, i\omega; \overline{\sigma}, i\omega_1 | \overline{\sigma}, i\omega_1; \sigma, i\omega] =$$
$$= \frac{U}{2}\left\{\frac{\beta U}{2}\frac{(1-\exp(\beta U/2))}{(1+\exp(\beta U/2))[\omega^2+(U/2)^2][\omega_1^2+(U/2)^2]} - \right.$$
$$- \frac{\beta U\delta(\omega-\omega_1)\exp(\beta U/2)}{(1+\exp(\beta U/2))[\omega^2+(U/2)^2][\omega_1^2+(U/2)^2]} +$$
$$+ \frac{\beta U\delta(\omega+\omega_1)}{(1+\exp(\beta U/2))[\omega^2+(U/2)^2][\omega_1^2+(U/2)^2]} -$$
$$- \frac{2}{[\omega^2+(U/2)^2][\omega_1^2+(U/2)^2]} + 4(U/2)^2$$
$$\left[\frac{1}{[\omega^2+(U/2)^2][\omega_1^2+(U/2)^2]^2} + \right.$$
$$\left.\left. + \frac{1}{[\omega^2+(U/2)^2]^2[\omega_1^2+(U/2)^2]}\right]\right\}. \quad (52)$$

Now we come back to equation (46) and note that thanks the antisymmetry property (48) of $\Lambda_\sigma(i\omega)$ only those terms of equations (51) and (52) which contain Kronecker δ-symbols give the nonzero contribution in the right-hand part of it.

The result of summation has the form:

$$\Lambda_\sigma(i\omega) = \frac{i\omega}{(i\omega)^2-(U/2)^2} + \frac{3(U/2)^2}{[(i\omega)^2-(U/2)^2]^2}\frac{G_\sigma^0(i\omega)}{[1-\Lambda_\sigma(i\omega)G_\sigma^0(i\omega)]}. \quad (53)$$

We notice that the scattering channel with opposite spins (52) gives in equation (53) the twise contribution in comparison with parallel spin channel (51) and both of them are added together giving the factor 3 in the right-hand part of equation (53). There are two solutions of equation (53) and we take that of them which has the correct asymptotic behavior $\lambda_\sigma(i\omega) \to \frac{1}{i\omega}$ when $|\omega|$ tends to infinity. This solution has the form:

$$\Lambda_\sigma(i\omega) = \frac{1}{2G_\sigma^0(i\omega)[(i\omega)^2-(U/2)^2]}\left\{[(i\omega)^2-(U/2)^2+i\omega G_\sigma^0(i\omega)] - \right.$$
$$\left. -[(i\omega)^2-(U/2)^2-i\omega G_\sigma^0(i\omega)]\sqrt{1-12Q(i\omega)}\right\}, \quad (54)$$

where

$$Q(i\omega) = \left(\frac{(U/2)G_\sigma^0(i\omega)}{(i\omega)^2-(U/2)^2-i\omega G_\sigma^0(i\omega)}\right)^2. \quad (55)$$

We have used that branch of square root which gives one when $Q(i\omega)$ tends to zero. On the basis of equations (39) we obtain the renormalized impurity electron

propagator

$$g(i\omega) = \\ = \frac{2[g^0(i\omega)[G^0(i\omega)]^{-1} + 3Q(i\omega)(g^0(i\omega) - [G^0(i\omega)]^{-1})^2]}{[[G^0(i\omega)]^{-1} - g^0(i\omega)][1 + \sqrt{1 - 12Q(i\omega)} + 6Q(i\omega)(g^0(i\omega)G^0(i\omega) - 1)]}. \quad (56)$$

In the last equations the spin index σ is omitted because it is not significant. Equation (56) has been obtained by taking into account the spin and charge fluctuations contained in the correlation function $Z_\sigma(i\omega)$.

The spectral function of the impurity electrons is equal to

$$A_f(E) = -2Img(E + i\delta), \quad (57)$$

where $g(E + i\delta)$ with $\delta = +0$ is the analytical continuation of the Matsubara to retarded Green's function. In absence of the correlation function $Z_\sigma(i\omega)$ instead of equation (56) a more simple form appears

$$g^I_\sigma(i\omega) = \frac{g^0_\sigma(i\omega)}{1 - g^0_\sigma(i\omega)G^0_\sigma(i\omega)} = \frac{1}{[g^0_\sigma(i\omega)]^{-1} - G^0_\sigma(i\omega)}, \quad (58)$$

which can be named as Hubbard I approximation. This equation contains the zero order Green's function $g^0(i\omega)$ determined by equation (47) and averaged by hybridization conduction electron function $G^0_\sigma(i\omega)$ of equation (50).

Analytical continuation of equation (58) gives

$$g^I_\sigma(E + i\delta) = \frac{1}{E - (U/2)^2E^{-1} - I(E) + i\Gamma(E)}. \quad (59)$$

We shall compare our renormalized spectral function (57) with more simple bare quantity $A^0_f(E)$:

$$A^0_f(E) = -2Img^0(E + i\delta) = \\ 2\pi\delta(E - (U/2)^2E^{-1}) = \pi\left(\delta(E - \frac{U}{2}) + \delta(E + \frac{U}{2})\right), \quad (60)$$

and the value $A^I_f(E)$ obtained in Hubbard I approximation:

$$A^I_f(E) = -2Img^I(E + i\delta) = \frac{2\Gamma(E)}{(E - (U/2)^2E^{-1} - I(E))^2 + \Gamma^2(E)}. \quad (61)$$

Here the odd $I(E)$ and even $\Gamma(E)$ functions are determined by equation (50). Two resonances of equation (60) situated at energies $E = \pm\frac{U}{2}$ have not the

width. After some interactions taken into account by Hubbard I approximation a new spectral function (61) appears. It has two resonances with shifted values of energies $E = \pm E_0$ determined by the presence of function $I(E)$:

$$E_0 - \frac{(U/2)^2}{E_0} - I(E_0) = 0. \tag{62}$$

These resonances are broadened by the presence of the function $\Gamma(E)$, which is the width of the virtual level. This function $\Gamma(E)$ determines the height and width of both resonances. Near the new values of resonance energies $\pm E_0$ we can approximate (61) with more simple Lorentzian forms:

$$\frac{2\Gamma}{\psi^2(E \mp E_0)^2 + \Gamma^2}, \tag{63}$$

where

$$\psi = 1 + \left(\frac{U}{2E_0}\right)^2 - I'(E_0), \tag{64}$$

and E_0 is determined by equation (62).

Both approximations (60) and (61) give the zero value of spectral functions on the Fermi surface, where $E = 0$. The correctness of the result has to be verified by the sum rule

$$\int_{-\infty}^{\infty} A_f(E)dE = 2\pi. \tag{65}$$

Equation (60) fulfils this condition. If we omit for the simplicity function $I(E)$ in equation (61) we can verify also the fulfillment of this condition for equation (61), but not for its approximations (63), because the parameter ψ is not equal to two. Some details connected with the choice of the density states can be found in Appendix.

In the next Section we use equations (55) and (56) to obtain more complete spectral function of impurity electrons and to verify the existence of the resonance at zero energy.

6. RENORMALIZED SPECTRAL FUNCTION

Analytical continuation of equations (55) and (56) which are necessary to calculate the spectral function have the form

$$g(E+i\delta) = [[G^0(E+i\delta)]^{-1} - g^0(E+i\delta)]^{-1} \times$$
$$\times \frac{2[g^0(E+i\delta)[G^0(E+i\delta)]^{-1} + 3Q(E+i\delta)(g^0(E+i\delta) - [G^0(E+i\delta)]^{-1})^2]}{\left[1 + \sqrt{1 - 12Q(E+i\delta)} + 6Q(E+i\delta)(g^0(E+i\delta)G^0(E+i\delta) - 1)\right]}, \tag{66}$$

$$Q(E+i\delta)=\left(\frac{UG^0(E+i\delta)/2}{E^2-(U/2)^2-EG^0(E+i\delta)}\right)^2. \qquad (67)$$

First of all, we shall analyze the behavior of the renormalized Green's function on the Fermi surface for $E=0$. Near the value of the energy $E=0$ we can approximate the quantity $Q(E+i\delta)$ by the expression

$$Q(E+i\delta)\mid_{E=0}=-\left(\frac{2\Gamma(0)}{U}\right)^2, \qquad (68)$$

and supposing the smallness of the parameter $2\Gamma/U$ we can approximate equation (66) by more simple one:

$$g(E+i\delta)\simeq\frac{6Q(E+i\delta)}{G^0(E+i\delta)[1+\sqrt{1-12Q(E+i\delta)}-6Q(E+i\delta)]}. \qquad (69)$$

For little values of energy we have

$$g(E+i\delta) \simeq \frac{6\left(2\Gamma/U\right)^2}{\Gamma^2(E)+E^2I'(0)^2}\frac{\left[-EI'(0)+i(\Gamma(E)+I'(0)^2E^2/\Gamma(0))\right]}{\left[1+\sqrt{1+12\left(2\Gamma/U\right)^2}+6\left(2\Gamma/U\right)^2\right]}.$$

The spectral function of impurity electrons in the region of little values of energy E is different from zero and has the form

$$A_f(E) \simeq \frac{12\left(2\Gamma/U\right)^2/\Gamma(0)}{\left[1+6\left(2\Gamma/U\right)^2+\sqrt{1+12\left(2\Gamma/U\right)^2}\right]}. \qquad (70)$$

In Appendix the values of the quantity $I'(0)$ equal to $4\rho(0)V^2(0)/W$ or $\pi V^2(0)\rho(0)/D$ for two different models of density of states are cited. The result (70) differs essentially from the zero value obtained in such more simple approximations for $A_f(E)$ as $A_f^0(E)$ and $A_f^I(E)$. Thus we have established the existence of two resonances at energies $E=\pm E_0$ determined by (62) and the peculiarity $E=0$. We can find the corrections to the spectral function $A_f(E)$ at two resonances $E=\pm E_0$. With this end in view, we determine the quantity Q for $E=E_0$

$$Q(E+i\delta)=-\left(I(E_0)-i\Gamma(E_0)\right)^2\left(\frac{U}{2E_0\Gamma(E_0)}\right)^2,$$

where we suppose that the value E_0 is inside the edges of the band width. After some calculations made with the supposition that the quantities $I(E_0)/\Gamma(E_0)$ and $UI(E_0)/2E_0\Gamma(E_0)$ are large and superior in number to one, we obtain

$$A_f(E_0)=\frac{1}{\sqrt{3}\left(1+3(U/2E_0)^2\right)}\frac{4E_0}{UI(E_0)}.$$

This quantity essentially differs from the value $A_f^I(E_0) = 2/\Gamma(E_0)$ being considerable less. Thus the process of renormalization of the impurity electron propagator results in the appearance of the peculiarity at $E = 0$ and to diminution of two resonances situated at $E = \pm E_0$.

The full spectral function can be calculated on the basis of equations (66) and (67). In Fig. 11 the results of numerical investigation of the full spectral function are presented for different values of theory parameters. For comparison in this figure the result obtained in Hubbard I approximation is also presented. As can be seen from Fig. 11, there are two sharp resonance peaks near the energies $E = \pm E_0$ and smooth behavior near $E = 0$. The distance between peaks is determined by parameter U and the height and width of peaks are determined by parameter Γ.

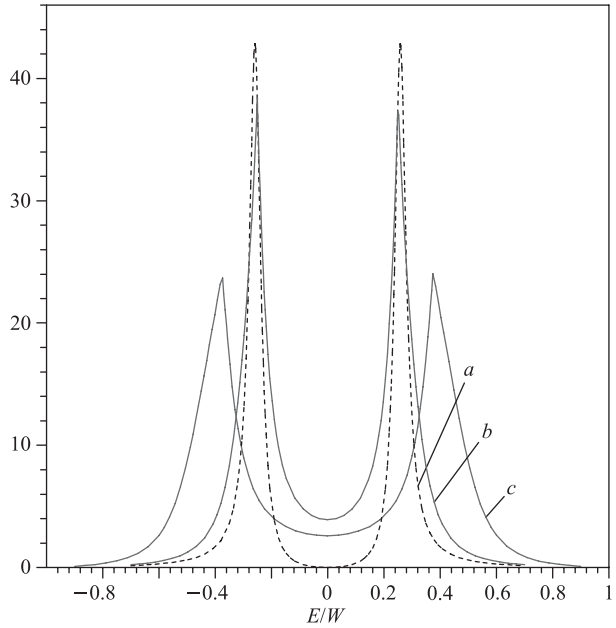


Fig. 11. Spectral function $A_f(E) \times W$ for different values of the theory parameters as function of energy E/W in the Hubbard I approximation (case a) and in our ladder approximation (cases b and c). In the cases a and b: $U = 1\,\mathrm{eV}$, $W = 2\,\mathrm{eV}$, $\Gamma = 0.1\,\mathrm{eV}$ and in case c: $U = 1.5\,\mathrm{eV}$, $W = 2\,\mathrm{eV}$, $\Gamma = 0.15\,\mathrm{eV}$

7. THE STATIONARY PROPERTY OF THERMODYNAMIC POTENTIAL IN THE NORMAL STATE

The full one-particle Matsubara Green's functions of conduction and localized electrons in interaction representation are defined in Sec. 2.

In this Section we define the local operator for conduction electrons in the form

$$b_\sigma = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} V_{\mathbf{k}} C_{\mathbf{k}\sigma}. \tag{71}$$

The corresponding full conduction electron Green's function has the form

$$G_{\sigma\sigma'}(\tau - \tau') = -\left\langle T b_\sigma(\tau) \overline{b}_{\sigma'}(\tau') U(\beta) \right\rangle_0^c, \tag{72}$$

where $U(\beta)$ is the evolution operator (5).

Because the matrix element of hybridization $V_{\mathbf{k}}$ is absorbed by local operator b_σ it is convenient to introduce a new parameter λ, which will be associated to each vertex of the diagrams. In such a way the order of perturbation theory will be determined by λ and not by the matrix element $V_{\mathbf{k}}$ of hybridization which can be present even in zero order Green's function. In the last stage of the calculation λ will be put equal to one.

In zero order of perturbation theory the Fourier representation for the conduction electrons is determined by the formulae

$$\begin{aligned} G^0_{\sigma\sigma'}(i\omega) &= \delta_{\sigma\sigma'} G^0_\sigma(i\omega), \\ G^0_\sigma(i\omega) &= \frac{1}{N} \sum_{\mathbf{k}} \frac{|V_{\mathbf{k}}|^2}{i\omega - \epsilon(\mathbf{k})}. \end{aligned} \tag{73}$$

The presence in the definition of zero order Green's function G^0_σ of the square of matrix element of hybridization is the consequence of our equation (71) but not of the perturbation. The thermodynamical perturbation theory gives us in the normal state the results for one-particle Green's functions presented in Figs. 12 and 13. The double solid and dashed lines depict the renormalized and the thin lines the bar propagators of conduction and impurity electrons. The lines connect the crosses which depict the impurity states. To crosses are attached two arrows one of which is ingoing and the other one is outgoing. They depict the annihilation and creation of the electrons, correspondingly. The crosses are the vertices of the diagrams and a λ multiplier is attached to each of them. The index n means (σ_n, τ_n). The summation on the index σ_n and the integration on the τ_n are intended. The rectangles with $2n$ indices and crosses depict the irreducible $g_n^{(0)\mathrm{ir}}[1, ..., n \mid n+1, ..., 2n]$ Green's functions. The sign of diagrams is determined by the parity (even or odd) of the permutation of the Fermi operators

necessary to obtain the diagram. Using Feynman's rules, it is possible to establish the next equation for the diagrams shown in Fig. 12:

$$G_{\sigma\sigma'}(\tau-\tau^{'}|\lambda)=G^{0}_{\sigma\sigma'}(\tau-\tau^{'})+ \sum_{\sigma_1\sigma_2}\int\limits_0^\beta d\tau_1\int\limits_0^\beta d\tau_2 G^{0}_{\sigma\sigma_1}(\tau-\tau_1)\lambda g_{\sigma_1\sigma_2}(\tau_1-\tau_2|\lambda)\lambda G^{0}_{\sigma_2\sigma'}(\tau_2-\tau^{'}). \quad (74)$$

On the basis of the diagrams depicted in Fig. 13, it is possible to establish the following Dyson-type equation for $g_{\sigma\sigma'}$:

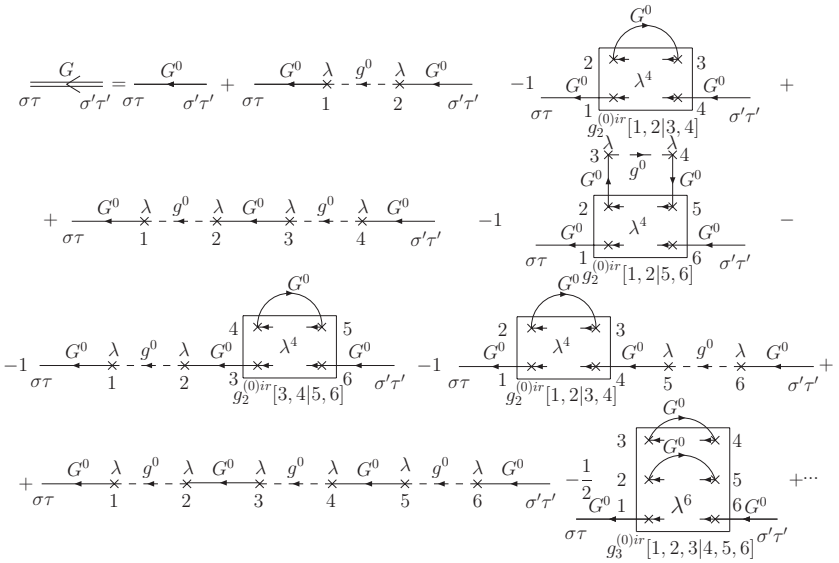


Fig. 12. Diagrams of the first six orders of perturbation theory for the conduction electron propagator. The thin solid lines represent the conduction electron propagator and dashed lines — the impurity electron propagators of zero order. Double line represents the full propagator

$$g_{\sigma\sigma'}(\tau-\tau^{'}|\lambda)=\Lambda_{\sigma\sigma'}(\tau-\tau^{'}|\lambda)+ \sum_{\sigma_1\sigma_2}\int\limits_0^\beta d\tau_1\int\limits_0^\beta d\tau_2 \Lambda_{\sigma\sigma_1}(\tau-\tau_1)\lambda G^{0}_{\sigma_1\sigma_2}(\tau_1-\tau_2)\lambda g_{\sigma_2\sigma'}(\tau_2-\tau^{'}), \quad (75)$$

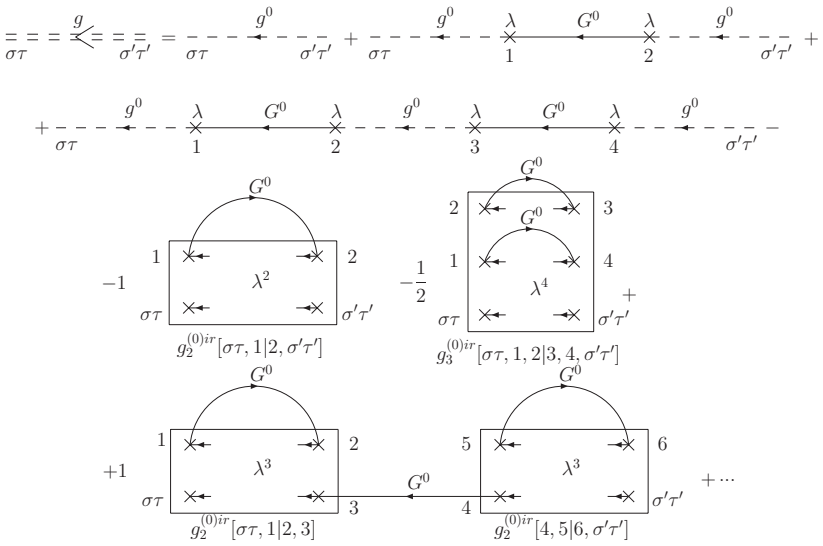


Fig. 13. Some diagrams for impurity electron propagator $g_{\sigma\sigma'}(\tau - \tau')$. The last three diagrams contain the correlation contributions. Two of them are strong connected and the last one is weak connected

where

$$\Lambda_{\sigma\sigma'}(\tau - \tau^{'}|\lambda) = g^0_{\sigma\sigma'}(\tau - \tau^{'}) + Z_{\sigma\sigma'}(\tau - \tau^{'}|\lambda). \tag{76}$$

Here $Z_{\sigma\sigma'}$ is the new correlation function which contains an infinite sum of the irreducible Green's functions. As was underlined above, this function contains all spin, charge and pairing fluctuations and is the main element of our diagram technique.

Diagram representation of the correlation function $\Lambda_{\sigma\sigma'}(\tau - \tau^{'}|\lambda)$ is depicted in Fig. 14.

The series expansion of the full propagator $G_{\sigma\sigma'}(\tau - \tau')$ can give us more detailed representation of this quantity.

By using the Fourier representation of Matsubara functions on the base of equations (74) and (75), we have

$$G_\sigma(i\omega|\lambda) = \frac{G^0_\sigma(i\omega)}{1 - \Lambda_\sigma(i\omega|\lambda)G^0_\sigma(i\omega)\lambda^2}, \tag{77}$$

$$g_\sigma(i\omega|\lambda) = \frac{\Lambda_\sigma(i\omega|\lambda)}{1 - \Lambda_\sigma(i\omega|\lambda)G^0_\sigma(i\omega)\lambda^2}. \tag{78}$$

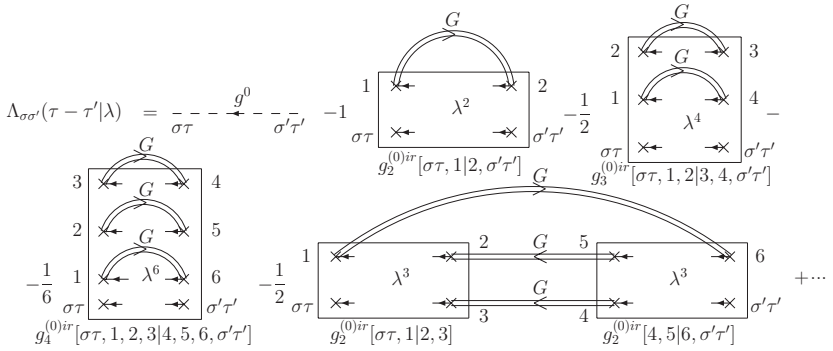


Fig. 14. Diagram representation of the correlation function $\Lambda_{\sigma\sigma'}$. Double solid lines depict the renormalized conduction electron propagators $G_{\sigma\sigma'}(\tau-\tau^{'}|\lambda)$. The arguments of irreducible functions are supposed arranged in the clock wise direction

Equation (77) for conduction electron propagator is the Dyson one with mass operator determined by the correlation function of impurity electrons:

$$\Sigma_\sigma(i\omega|\lambda)=\lambda^2\Lambda_\sigma(i\omega|\lambda). \tag{79}$$

When λ is equal to one these quantities coincide.

Equation (78) for impurity electrons is of Dyson type and coincides, for $\lambda=1$, with other equations obtained for strongly correlated electrons [31–35]. In equations (77), (78) the parameter λ can be taken equal to one and can be omitted.

The thermodynamic potential of our strongly correlated system are defined in Sec. 3

In Fig. 15 some of the simplest vacuum diagrams in the normal phase of the system are depicted. The first three diagrams are of chain type and are originated from the ordinary Wick contributions. The last three diagrams contain the correlation functions and are determined by the new contributions of GWT. The factor $\frac{1}{n}$, where n is the perturbation theory order, present in these diagrams makes it difficult to carry out the summation over n. As is usual in such cases [36], we employ a trick, that of integrating over the interacting strength λ. The result of this procedure is depicted in Fig. 16. Now we shall use the diagrams of the conduction electron propagator G_σ depicted in Fig. 12 and these of Λ_σ from Fig. 14 to combine them in such a way to obtain the vacuum diagrams of Fig. 16. Either diagrams of Fig. 16 of the n order of perturbation theory can be considered as the product of the contribution of order n_1 from G_σ and of the contribution of order n_2 from Λ_σ with the condition that $n_1+n_2=n$. There are in general case different possibilities to arrange such a contribution and the number of these

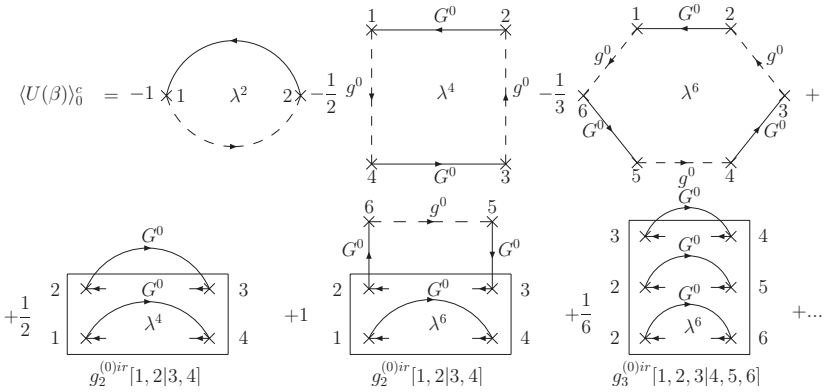


Fig. 15. Connected vacuum diagrams of the second, fourth and sixth orders of perturbation theory

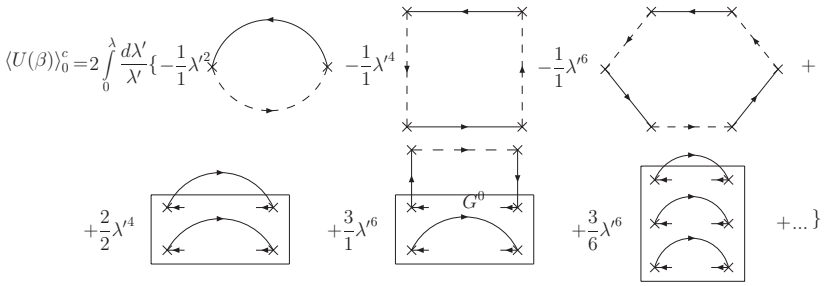


Fig. 16. The result of integration over the interacting strength of the vacuum diagrams

possibilities is determined by the numerator of the fraction before the diagrams of Fig. 16. The denominator of this fraction is determined from Fig. 15. Therefore, we obtain

$$\langle U(\beta)\rangle_0^c = (-2)\sum_{\sigma_1\sigma_2}\int\limits_0^\beta d\tau_1\int\limits_0^\beta d\tau_2\int\limits_0^\lambda \frac{d\lambda'}{\lambda'}G_{\sigma_1\sigma_2}(\tau_1-\tau_2|\lambda')\Sigma_{\sigma_2\sigma_1}(\tau_2-\tau_1|\lambda') =$$

$$= (-2)\sum_{\sigma}\sum_{\omega}\int\limits_0^\lambda \frac{d\lambda'}{\lambda'}G_{\sigma}(i\omega|\lambda')\Sigma_{\sigma}(i\omega|\lambda'). \quad (80)$$

The thermodynamical potential becomes equal to

$$F = F_0 + \frac{2}{\beta}\sum_{\sigma}\sum_{\omega}\int_0^{\lambda}\frac{d\lambda'}{\lambda'}G_{\sigma}(i\omega|\lambda')\Sigma_{\sigma}(i\omega|\lambda'). \quad (81)$$

From this equation we obtain

$$\lambda\frac{\partial F}{\partial\lambda} = \frac{2}{\beta}\sum_{\sigma}\sum_{\omega}G_{\sigma}(i\omega|\lambda)\Sigma_{\sigma}(i\omega|\lambda). \quad (82)$$

Expression (81) for thermodynamical potential contains additional integration over the interaction strength λ and is awkward because of it. As was proved for non-correlated many-electron system by Luttinger and Ward [36], this expression can be transformed into a much more convenient formula.

We consider the following expression:

$$Y = -\frac{1}{\beta}\sum_{\sigma}\sum_{\omega}\exp(i\omega 0^+)\{\ln[G^0_{\sigma}(i\omega)\Sigma_{\sigma}(i\omega|\lambda) - 1] + G_{\sigma}(i\omega|\lambda)\Sigma_{\sigma}(i\omega|\lambda)\} + Y', \quad (83)$$

which is the generalization of the Luttinger–Ward equation for strongly correlated systems. Here Y' is the sum of closed linked skeleton diagrams with full G_{σ} function as a contribution of conduction electron lines.

In Fig. 17 some of simplest skeleton diagrams are depicted. These diagrams depend on the interaction strength λ not only through the factors in front of each diagram but also through the full Green's function $G_{\sigma}(i\omega|\lambda)$.

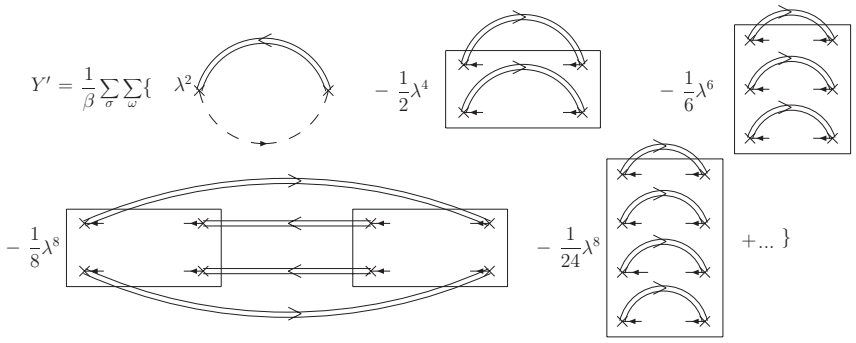


Fig. 17. Closed linked skeleton diagrams. The double solid lines correspond to full propagators $G_{\sigma}(i\omega|\lambda)$ of conduction electrons. The rectangles correspond to the correlation functions of the correlated electrons

From equations (77), (79) and (83) we obtain

$$\frac{\partial Y}{\partial \Sigma_\sigma(i\omega|\lambda)} = -\frac{1}{\beta}\Sigma_\sigma(i\omega|\lambda)\ G^2_\sigma(i\omega|\lambda) + \frac{\partial Y'}{\partial \Sigma_\sigma(i\omega|\lambda)}, \tag{84}$$

where, from Figs. 14, 17 and definition (79), it follows that

$$\frac{\partial Y'}{\partial G_\sigma(i\omega|\lambda)} = \frac{\lambda^2}{\beta}\Lambda_\sigma(i\omega|\lambda) = \frac{\Sigma_\sigma(i\omega|\lambda)}{\beta}. \tag{85}$$

As a result, we obtain the stationary property with respect to changes of the mass operator:

$$\frac{\partial Y}{\partial \Sigma_\sigma(i\omega|\lambda)} = 0. \tag{86}$$

Now we shall find the quantity $\dfrac{\partial Y}{\partial \lambda}$. By the stationary property of Y we can ignore the dependence of Σ_σ and G_σ on λ and take into account only the explicit dependence of λ in Y', depicted in Fig. 17. From this figure it is easy to obtain

$$\lambda\frac{\partial Y}{\partial \lambda}\ |_\Sigma = \lambda\frac{\partial Y'}{\partial \lambda}\ |_\Sigma = \frac{2}{\beta}\sum_\sigma\sum_\omega G_\sigma(i\omega|\lambda)\Sigma_\sigma(i\omega|\lambda). \tag{87}$$

From equations (82) and (87) we obtain

$$\lambda\frac{\partial F}{\partial \lambda} = \lambda\frac{\partial Y}{\partial \lambda}. \tag{88}$$

The consequence of this equation is the solution

$$F(\lambda) = Y(\lambda) + \text{const}. \tag{89}$$

For $\lambda = 0$, we have $Y(0) = 0$ and $F(o) = F_0$. Therefore, $\text{const} = F_0$.

The final result has the form

$$F = F_0 + Y. \tag{90}$$

8. CONCLUSIONS

We discuss the Anderson impurity model and take into account the strong electronic correlations of the impurity electrons by elaborating the suitable diagram technique. We have established a linked cluster theorem derived from a generalized Wick theorem and then we have derived the expression for the renormalized propagators, both for normal and anomalous conduction and the

impurity electrons. The impurity full propagator is expressed via a correlation function $Z_\sigma(i\omega)$.

The special approximation for the correlation function $Z_\sigma(i\omega)$ has been obtained which gives the possibility to close the system of equations and to find the solution for renormalized function $g_\sigma(i\omega)$. This Matsubara Green's function has been continued analytically to obtain the retarded one. Spectral function of impurity electrons for the symmetric model is obtained, and the structure of resonances and their properties are analyzed. Two of the resonances of this function at $E = \pm E_0$ (Fig. 11), correspond to the energies of quantum transitions of single-site impurity, and the smooth behavior was found at the energy $E = 0$. The details of the spectral function renormalization are based on the properties of real $I(E)$ and imaginary $\Gamma(E)$ parts of function $G^0_\sigma(i\omega)$, which is the conduction band electron Green function averaged by the hybridization interaction. The values of these functions and the values of energies $\pm E_0$ are discussed in Appendix. In particular, we have shown that going beyond the Hubbard I approximation, some spectral weight is transferred from the resonances $E = \pm E_0$ to energy $E = 0$. The peculiarity at $E = 0$ is the novel result of our analysis, and although our approximation does not yet yield the resonance at zero energy, could be relevant to understand some physical properties of realistic systems, e.g., spin susceptibility, and the magnetotransport of dilute magnetic alloys or quantum dots.

The thermodynamic potential of a strongly correlated system described by the Anderson impurity model has been calculated in the normal phase. Within our diagrammatic technique we first obtained an exact expression for the thermodynamic potential as a product of the full propagator G_σ of the conduction electrons and its mass operator Σ_σ, then a Luttinger–Ward-type [48] of identity based on the stationary property of the potential was established. The expression for the thermodynamic potential so obtained could be very useful to calculate in a systematic way all thermodynamic quantities (e.g., specific heat) of strongly correlated electron systems.

Appendix

SIMPLE EXAMPLES OF DENSITY OF STATE

We can demonstrate some simple examples of the choice of the density of states and of the corresponding functions $I(E)$ and $\Gamma(E)$. For simplicity the energy dependence of the matrix element of hybridization $V(\epsilon)$ is supposed smooth and can be neglected. One example of density of states has been proposed in the paper [3]. In this paper the following equations are used:

$$\begin{gathered}\rho_0(\epsilon) = \rho_0(0)\left(1 - (\epsilon/W)^2\right), \qquad |\epsilon| < W, \\ I(\epsilon) = \rho_0(0)V^2(0)[2\epsilon/W + \left(\epsilon^2/W^2 - 1\right)\ln\left|(\epsilon - W)/(\epsilon + W)\right|, \qquad \text{(A.1)} \\ \Gamma(\epsilon) = \pi V^2(\epsilon)\rho_0(\epsilon).\end{gathered}$$

where $2W$ is the conduction band width. For little value of energy we have $I(\epsilon) = I'(0)\epsilon$ with

$$I'(0) = 4\rho_0(0)V^2(0)/W, \tag{A.2}$$

and for $E \to \pm\infty$ function $I(E)$ tends to zero as $1/E$. In the case $(A1)$ equation (62) takes the form $(x_0 = E_0/W)$:

$$x_0 - a^2/x_0 - b\varphi(x_0) = 0, \tag{A.3}$$

where

$$\varphi(x) = 2x + (x^2 - 1)\ln\left|\frac{x-1}{x+1}\right|;$$
$$a = U/2W; \qquad b = \rho(0)V^2/W.$$

We note that the functions $\rho_0(\epsilon)$ and $\Gamma(\epsilon)$ exist only inside the edges of the conduction electron band $|E| < W$ whereas the function $I(\epsilon)$ and the solution of equation $(A2)$ can exist also for $|E| > W$. Therefore we have to find the solution of $(A2)$ with $x < 1$ and consider the conditions for the values of parameters a and b compatible with this requirement.

Another simple example of the density of state is one with Lorentzian shape [16]

$$\rho_0(\epsilon) = 2D/(E^2 + D^2), \tag{A.4}$$

with chemical potential placed at the $\epsilon = 0$. This choice has the advantage of not introducing band edges. It has the parameter D as an effective band width:

$$\begin{aligned} I(E) &= 2\pi V^2(0)E/(E^2 + D^2), \\ \Gamma(E) &= \pi\rho_0(0)V^2(0) = 2\pi V^2(0)/D. \end{aligned} \tag{A.5}$$

In this case instead of equation $(A3)$ we have other values of parameters a and b and other form of function $\varphi(x)$:

$$\begin{aligned} x - a^2/x - bx/(1 + x^2) = 0, \\ a = U/2D; \;\; b = 2\pi V^2(0)/D^2. \end{aligned} \tag{A.6}$$

Equation $(A6)$ has two solutions $\pm x_0$ with

$$x_0 = \left[\sqrt{(1 - a^2 + b)^2 + 4a^2} + a^2 + b - 1\right]^{1/2}/\sqrt{2}. \tag{A.7}$$

The value of parameter $I'(0)$ is equal to $2\pi V^2(0)/D^2 = \pi V^2(0)\rho_0(0)/D$.

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