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DIAGRAMMATIC THEORY FOR PERIODIC ANDERSON MODEL

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Diagrammatic theory for Periodic Anderson Model has been developed, supposing the Coulomb repulsion of f — localized electrons as a main parameter of the theory. The f electrons are strongly correlated and c — conduction electrons are uncorrelated. Correlation function for f and mass operator for c electrons are determined. The Dyson equation for c and Dyson-type equation for f electrons are formulated for their propagators. The skeleton diagrams are defined for correlation function and thermodynamic functional. The stationary property of renormalized thermodynamic potential about the variation of the mass operator is established. The result is appropriate both for normal and for superconducting state of the system.

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The study of the systems with strongly correlated electrons has become in the last time one of the central problems of condensed matter physics. One of the most important models of strongly correlated electrons is Periodic Anderson Model (PAM) [1].

We will not enlarge upon the most essential stages in the development of this model because there exists a number of consistent reviews [2–7] and books [8, 9] on this field, and we shall use the references to previous our papers.

We consider the simplest form of PAM with a spin degeneration of the level of localized f electrons, a simple energy band of conducting c electrons, Coulomb one-site repulsion U of correlated f electrons with opposite spins and one-site hybridization between both groups of electrons of this system. The Hamiltonian of the system reads:

$$\begin{gathered} H = H_c^0 + H_f^0 + H_{\rm int}, \quad H_c^0 = \sum_{\mathbf{k}\sigma} \epsilon(\mathbf{k}) C_{\mathbf{k}\sigma}^+ C_{\mathbf{k}\sigma}, \\ H_f^0 = \epsilon_f \sum_{i\sigma} n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad H_{\rm int} = \sum_{i\sigma} \left(C_{i\sigma}^+ f_{i\sigma} + f_{i\sigma}^+ C_{i\sigma} \right), \end{gathered} \tag{1}$$

where

$$\epsilon(\mathbf{k}) = \overline{\epsilon}(\mathbf{k}) - \mu, \epsilon_f = \overline{\epsilon}_f - \mu, \quad n_{i\sigma} = f^+_{i\sigma} f_{i\sigma},$$
$$C_{i\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \exp\,(-i\mathbf{k}\mathbf{R_i}) C_{\mathbf{k}\sigma}. \tag{2}$$

Here V is the hybridization amplitude assumed constant. We have indicated with $C^+_{i\sigma}(f^+_{i\sigma})$ the creation operator for an uncorrelated (correlated) electron with spin σ and i lattice site, $n_{i\sigma}$ is the number operator for f electrons, $\epsilon(\mathbf{k})$ is the band energy with momentum $\mathbf{k}$ of conductivity electrons spread on the entire width W of the band, ϵ_f is the energy of localized electrons. Both these energies are evaluated with respect to the chemical potential μ.

In the present paper we develop the thermodynamic perturbation theory for the system in the superconducting state with Hamiltonian (1) under the assumption that the term responsible for hybridization of c and f electrons is a perturbation.

The Hamiltonian H^0_c of the uncorrelated c electrons is diagonal in band representation, whereas the Hamiltonian H^0_f is diagonalized by using Hubbard transfer operators [20].

We use the series expansion for evolution operator:

$$U(\beta) = T \exp\left(-\int\limits_0^\beta H_{\rm int}(\tau)\, d\tau\right) \tag{3}$$

in the interaction representation for electron operators ($a = c, f$):

$$a(x) = \mathrm{e}^{\tau H^0} a(\mathbf{x})\, \mathrm{e}^{-\tau H^0}, \overline{a}(x) = \mathrm{e}^{\tau H^0} a^+(\mathbf{x})\, \mathrm{e}^{-\tau H^0}. \tag{4}$$

Here x means $(\mathbf{x}, \sigma, \tau)$.

We shall denote by $\langle TAB\ldots\rangle_0$ the thermodynamic average with zeroth-order statistical operator of the chronological product of electron operators $(AB\ldots)$. Such averages are calculated independently for c and f operators with using for c electrons the Wick Theorem of weak quantum field theory and by using for f electrons the Generalized Wick Theorem (GWT) proposed by us in papers [10–19] for strongly correlated electron systems.

In the superconducting state, unlike the normal one, nontrivial statistical averages of operator products with even total number but inequal number of creation and annihilation electron operators are possible. They realize the Bogoliubov quasi-averages [21] or Gor'kov [22] anomalous Green's functions. To unify the calculation of statistical averages for normal and superconducting phases it is useful to assign an additional quantum number α, called by us charge number [15],

with the values ± 1, which can be added to electron operators according to the rule ($a = c, f$):

$$a^{\alpha}(\mathbf{x}) = \begin{cases} a(\mathbf{x}), & \alpha = 1; \\ a^{+}(\mathbf{x}), & \alpha = -1. \end{cases} \tag{5}$$

In this representation the interaction operator H_{int} becomes:

$$H_{\mathrm{int}} = V \sum_{i\sigma\alpha} \alpha f_{i\sigma}^{-\alpha} C_{i\sigma}^{\alpha}. \tag{6}$$

Obviously, introducing of a new quantum charge number leads to additional summation over its values in all diagram lines and to an additional factor α in the vertices of diagrams.

Now, after such introducing, it is irrelevant whether one deals with creation or annihilation operators. First of all, we shall enumerate the main results of diagrammatic theory obtained in the previous paper [15] necessary to our proving of stationary theorem. Such theorem for uncorrelated many-electron systems in a normal state has been proved by Luttinger and Word [23].

We use the definition of the one-particle Matsubara Green's functions for c and f electrons

$$\begin{aligned} G_{\alpha\alpha'}^{c}(x|x') &= -\left\langle T c^{\alpha}(x) c^{-\alpha'}(x') U(\beta) \right\rangle_0^c, \\ G_{\alpha\alpha'}^{f}(x|x') &= -\left\langle T f^{\alpha}(x) f^{-\alpha'}(x') U(\beta) \right\rangle_0^c, \end{aligned} \tag{7}$$

where index c for $\langle \ldots \rangle_0^c$ means the connection of the diagrams which are taken into account in the right-hand part of definition (7).

The following condition is fulfilled

$$G_{\alpha\alpha'}^{a}(x|x') = -G_{-\alpha',-\alpha}^{a}(x'|x), a = (c, f). \tag{8}$$

In the presence of strong correlations of f electrons, the (GWT) contains additional terms, namely the irreducible one-site many-particle Green's functions or Kubo cumulants of the form ($x = \mathbf{x}, \sigma, \tau$):

$$\begin{aligned} G_n^{(0)ir}[\alpha_1, x_1; \ldots; \alpha_{2n}, x_{2n}] &= \left\langle T f_{x_1}^{\alpha_1} \cdots f_{x_{2n}}^{\alpha_{2n}} \right\rangle_0^{ir} = \\ &= \delta_{\mathbf{x}_1\mathbf{x}_2} \cdots \delta_{\mathbf{x}_1\mathbf{x}_{2n}} \left\langle T f_{\sigma_1}^{\alpha_1}(\tau_1) \cdots f_{\sigma_{2n}}^{\alpha_{2n}}(\tau_{2n}) \right\rangle_0^{ir}. \end{aligned} \tag{9}$$

As a result of applying this theorem we obtain for the renormalized conduction electron propagator the contributions depicted on Fig. 1.

The contributions of perturbation theory for f-electron propagator are depicted on Fig. 2.

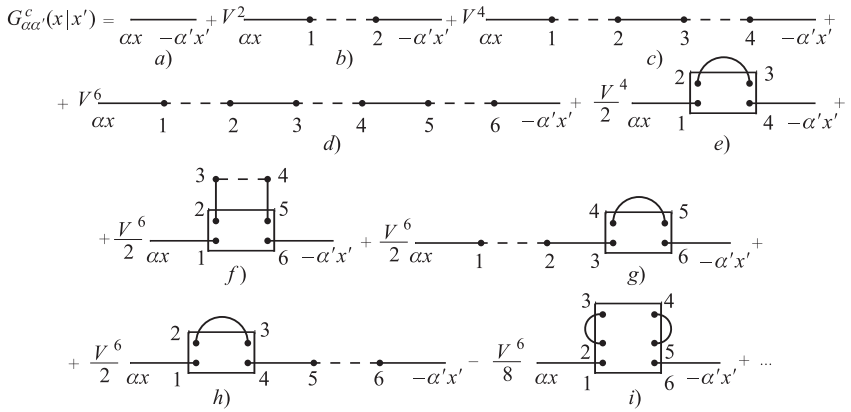

Fig. 1. The first six orders of perturbation theory for conduction electron propagator. The solid and dashed thin lines depict zero order propagators for c and f electrons, correspondingly. The rectangles depict the irreducible Green's functions. The points of diagram are the vertices with α and V contributions

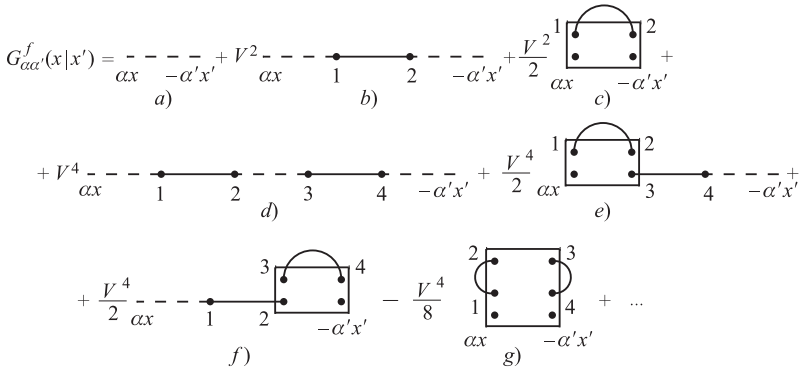

Fig. 2. The contributions of the first four orders of perturbation theory for the f-electron propagator

The sum of all strong connected diagrams for f electron belong to the correlation function which is denoted by us as $\Lambda_{\alpha\alpha'}(x|x')$ function. The quantity $\Lambda_{\alpha\alpha'}(x|x')$ is defined by the equation

$$\Lambda_{\alpha\alpha'}(x|x') = G^{f(0)}_{\alpha\alpha'}(x|x') + Z_{\alpha\alpha'}(x|x'), \tag{10}$$

where the function $Z_{\alpha\alpha'}(x|x')$ contains the contribution of strongly connected diagram based on the irreducible many-particle Green's functions.

The strong connected part of the c-electron propagator without the external lines is determined by us as a mass operator for uncorrelated electrons. This quantity is denoted as $\Sigma_{\alpha\alpha'}(x|x')$.

A simple relation exists between these two functions:

$$\Sigma_{\alpha\alpha'}(x|x') = V^2 \alpha\alpha' \Lambda_{\alpha\alpha'}(x|x'). \tag{11}$$

The analysis of the propagator diagrams permits us to formulate the following Dyson equation for uncorrelated electron propagator:

$$G^c_{\alpha\alpha'}(x|x') = G^{c(0)}_{\alpha\alpha'}(x|x') + \sum_{\alpha_1\alpha_2}\sum_{12} G^{c(0)}_{\alpha\alpha_1}(x|1)\Sigma_{\alpha_1\alpha_2}(1|2)G^c_{\alpha_2\alpha'}(2|x'). \tag{12}$$

At the same time we can formulate the Dyson-type equation for correlated electron propagator G^f:

$$G^f_{\alpha\alpha'}(x|x') = \Lambda_{\alpha\alpha'}(x|x') + \\ + V^2 \sum_{\alpha_1\alpha_2}\sum_{12} \alpha_1\alpha_2 \Lambda_{\alpha\alpha_1}(x|1) G^{c(0)}_{\alpha_1\alpha_2}(1|2) G^f_{\alpha_2\alpha'}(2|x'). \tag{13}$$

On Fig. 3 the skeleton diagrams for the correlation function $\Lambda_{\alpha\alpha'}(x|x')$ are depicted.

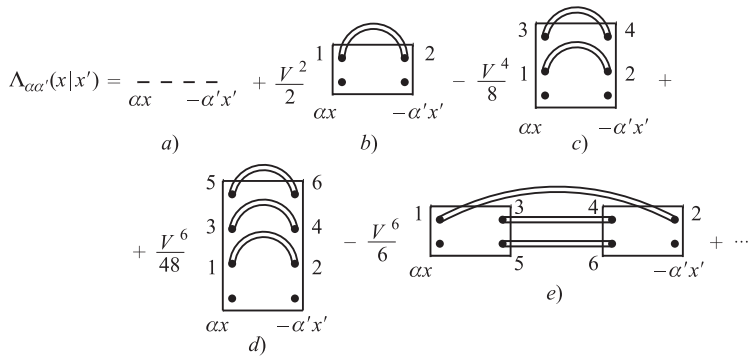

Fig. 3. The skeleton diagrams for correlation function $\Lambda_{\alpha\alpha'}(x|x')$. The thin dashed line is zero-order f-electron Green's function. The rectangles depict the many-particle irreducible Green's function. The double solid lines depict the renormalized conduction electron Green's function $G^c_{\alpha\alpha'}(x|x')$

The transition of the diagram contribution from superconducting version to the normal one is realized by the condition of equality to zero of the sums of all α indices of every dynamical quantity.

After discussion of the propagators properties, we shall proceed to the main part of our paper and investigate the properties of evolution operator average.

By using the perturbation theory, we have obtained for the connected part of evolution operator average, the contributions depicted in Fig. 4.

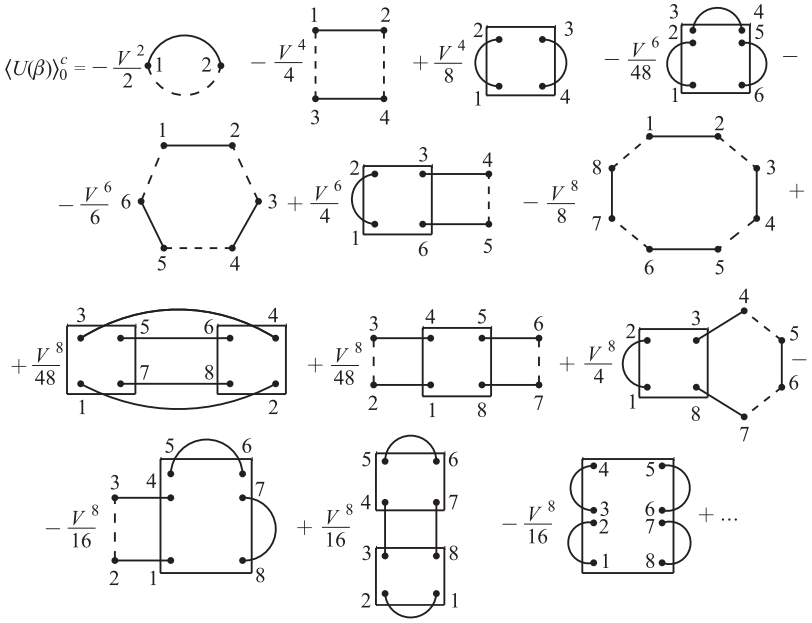

Fig. 4. Vacuum diagrams of first eight orders of perturbation theory in superconducting state

Vacuum diagrams in superconducting and normal states contain the factor $1/n$, where n is the order of perturbation theory in which given diagram appears. This factor makes difficult the investigation of this contributions. In order to remove this coefficient, it is necessary to use the trick of integration by constant of interaction V.

On the base of series expansions for renormalized propagators of the conduction c electrons (see Fig. 1), localized f electrons (see Fig. 2), and definition of the correlation function $\Lambda_{\alpha\alpha'}(x|x')$, we can prove that the contribution in every order of perturbation theory can be presented as the product of some contribution from G^c and some one from Λ. If the contribution of G^c is of n_1 order of perturbation theory and the contribution of Λ is of n_2 order, then the order of $\langle U(\beta)\rangle_0^c$ is equal to n with the condition $n_1+n_2+2=n$ which must be satisfied. There are different possibilities to satisfy this condition and all of them must be taken into account.

The integrand of the evolution operator average can be presented as a product of $\lambda^2 G^c \Lambda$ of the form

$$\langle U(\beta)\rangle_0^c = -\int_0^V \frac{d\lambda}{\lambda} \sum_{\alpha\alpha'} \sum_{xx'} \alpha\alpha' \lambda^2 G^c_{\alpha\alpha'}(x|x'|\lambda) \Lambda\alpha'\alpha(x'|x|\lambda) =$$

$$= -\int_0^V \frac{d\lambda}{\lambda} \sum_{\alpha\alpha'} \sum_{xx'} G^c_{\alpha\alpha'}(x|x'|\lambda) \Sigma\alpha'\alpha(x'|x|\lambda) = -\int_0^V \frac{d\lambda}{\lambda} \operatorname{Tr}\left(\hat{G}^c(\lambda)\hat{\Sigma}^c(\lambda)\right), \quad (14)$$

where the operators $\hat{G}^c(\lambda)$ and $\hat{\Sigma}^c(\lambda)$ have the matrix elements $G^c_{\alpha\alpha'}(x|x'|\lambda)$ and $\Sigma\alpha\alpha'(x|x'|\lambda)$, correspondingly. Index λ underlines that these quantities depend of the auxiliary constant of integration λ.

Therefore the thermodynamic potential of our system F is equal to

$$F = F_0 + \frac{1}{\beta} \int_0^V \frac{d\lambda}{\lambda} \operatorname{Tr}\left[\hat{G}^c(\lambda)\hat{\Sigma}^c(\lambda)\right]. \quad (15)$$

This expression for renormalized thermodynamic potential of the strongly correlated system contains additional integration over the integration strength λ and because of this is awkward. Equation (15) generalizes the result of Luttinger and Ward [23] proved for noncorrelated many-electron system in normal state.

Our generalization has been obtained for the case of strong correlations of special kind which contains one uncorrelated subsystem and one strongly correlated, and we admit also the existence of superconductivity in both of them.

Luttinger and Ward have proved the possibility of transforming this expression into much more convenient formula without such integration. For that they used a special functional constricted from skeleton diagrams, the lines of which are the renormalized electron Green's functions. We shall use the skeleton diagrams of strongly correlated system, which differ essentially from Luttinger and Ward [23] case, and transform equation (15) to more convenient form.

In our strong correlated case we introduce the following functional:

$$Y = -\frac{1}{2\beta} \operatorname{Tr}\left\{\ln\left(\hat{G}^{c(0)}\hat{\Sigma} - 1\right) + \hat{G}^c\hat{\Sigma}\right\} + Y', \quad (16)$$

which is the generalization of the Luttinger–Ward [23] equation just for the strongly correlated systems.

As a result of our investigation, we obtain the stationarity property of the functional Y:

$$\frac{\delta Y}{\delta\Sigma(y, y')} = 0. \quad (17)$$

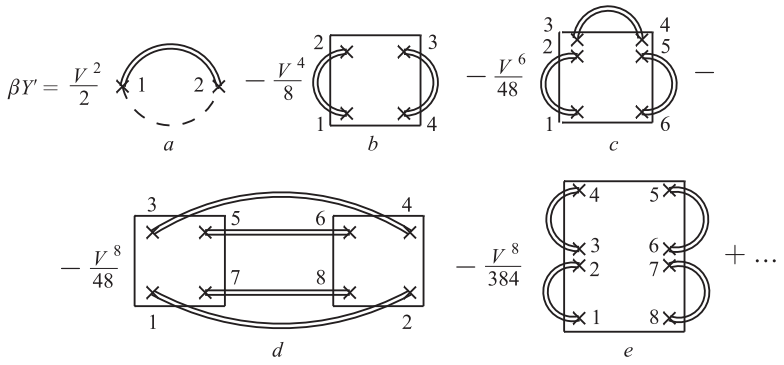

Fig. 5. Skeleton diagrams for functional Y'

Now we shall discuss the derivative over interaction constant V of functional Y. We shall take into account the stationarity Y about $\hat{\Sigma}$ and $\hat{G}^c$ and equation (12). We obtain:

$$V\frac{dY}{dV} = V\frac{\partial Y}{\partial V}\bigg|_{\Sigma} + V\frac{\delta Y}{\delta \Sigma}\frac{\partial \Sigma}{\partial V} = V\frac{\partial Y'}{\partial V}\bigg|_{\Sigma} = \frac{\mathrm{Tr}\,(\hat{\Sigma}\hat{G}^c)}{\beta}. \tag{18}$$

From equation (15) we have:

$$V\frac{dF}{dV} = \frac{\mathrm{Tr}\,(\hat{G}^c\hat{\Sigma})}{\beta}, \tag{19}$$

and as a consequence we establish

$$V\frac{dF}{dV} = V\frac{dY}{dV}, \tag{20}$$

with the solution

$$F = Y + \mathrm{const}.$$

This constant is F_0. Therefore

$$F = F_0 + Y,$$

with the stationary property

$$\frac{\delta F}{\delta \Sigma(x, x')} = 0, \tag{21}$$

both in superconducting and in normal states.

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