

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:

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

where

$$\begin{aligned} \epsilon(\mathbf{k}) &= \bar{\epsilon}(\mathbf{k}) - \mu, \quad \epsilon_f = \bar{\epsilon}_f - \mu, \quad n_{i\sigma} = f_{i\sigma}^+ f_{i\sigma}, \\ C_{i\sigma} &= \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \exp(-i\mathbf{k}\mathbf{R}_i) C_{\mathbf{k}\sigma}. \end{aligned} \quad (2)$$

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

We use the series expansion for evolution operator:

$$U(\beta) = T \exp \left(- \int_0^\beta H_{\text{int}}(\tau) d\tau \right) \quad (3)$$

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

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

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

We shall denote by $\langle TAB \dots \rangle_0$ the thermodynamic average with zeroth-order statistical operator of the chronological product of electron operators $(AB \dots)$. 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],