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ELECTRONIC PROPERTIES OF SOLIDS

Spin-Fluctuation Renormalization of the Temperature of a Superconducting *s*-Phase in Rare-Earth Intermetallides

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Abstract—A theory of the superconducting state with *s*-type symmetry of the order parameter (the transition to this state was observed in recently discovered heavy-fermion skutterudite $LaFe_4P_{12}$) is developed using the periodic Anderson model in the limit of strong electron correlations. Exact representations of Green's functions of the superconducting phase via the normal and anomalous components of the mass and strength operators are obtained. It is shown that an important role in the description of this superconducting phase is played by the anomalous components of the strength operator, which reflect spin-fluctuation processes in the localized subsystem. These components are calculated in the one-loop approximation using the solution of an infinite system of integral equations of self-consistency for the superconducting phase. Numerical calculations show that allowance for the process of scattering on spin fluctuations leads to renormalization of the critical temperature and provides agreement with the experimental data.

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1. INTRODUCTION

The microscopic nature of the superconducting state in compounds with heavy fermions (HFs) is still mysterious in many respects, despite three decades of investigations into this directions (the first HF superconductor $CeCu_2Si_2$ was discovered in 1979 [1]). The main feature of superconductivity in HF compounds is that Cooper pairing takes place in a subsystem of heavy quasi-particles [2] formed as a result of strong correlation involving the magnetic degrees of freedom. The proximity of the domains of the superconducting and antiferromagnetic phases on the phase diagram led to the hypothesis on the important role of spin fluctuations in the mechanism of Cooper instability [3, 4]. This hypothesis agrees well, in particular, with the anisotropic order parameter that is experimentally observed in many HF superconductors.

At present, it has been established that many of the "classical" HF superconductors such as $CeCu_2Si_2$, UBe_{13}, and UPt_3 exhibit superconductivity with *d*-type symmetry of the order parameter (see, e.g., [5, 6]). Unusual properties of this superconducting phase can be theoretically described, irrespective of a particular mechanism of Cooper instability, by the stipulating anisotropic order parameter in the initial assumptions of the theory [7].

On the other hand, experimental investigations of HF skutterudite $LaFe_4P_{12}$ [8], which is a superconductor at $T < T_C = 4.1$ K, led to the conclusion that the *s*-type symmetry of the order parameter in this compound is preferred. More recently, an analogous symmetry type was observed in skutterudite $PrRu_4As_{12}$ [9]. These data stimulated investigations in which the *s*-type symmetry of the order parameter of the superconducting phase was related to the electron–phonon mechanism of Cooper pairing [10]. At the same time, data on the electronic specific heat and magnetic susceptibility of $LaFe_4P_{12}$, which allow this skutterudite to be classified as an HF compound, point to the important role of strong electron correlations. Evidently, these correlations must be manifested in the mechanism by which the superconducting *s*-phase of $LaFe_4P_{12}$ forms. In this context, it is also important to consider the electron mechanism of Cooper instability, which makes it possible to describe the experimentally observed *s*-wave superconductivity under conditions of developed processes of scattering on spin fluctuations in the localized subsystem.

The properties of rare-earth intermetallides with HFs are most frequently described in terms of the periodic Anderson model. Using this model, the methodology of investigations of superconductivity can be subdivided into several directions. One of these is based on the Fermi-liquid description of heavy quasi-particles and the Landau–Ginzburg theory. This approach was successfully applied, in particular, to the construction of the phase diagram of UPt_3 [11]. Another direction in

studying superconductivity in HF systems is related to the application of perturbation theory up to the third order with respect to the on-site Coulomb interaction parameter U [12–14]. Unfortunately, this approach has obviously limited applicability to the systems under consideration, since the U value is not small and this very fact serves as a basis for the HF state formation. Some investigations in this direction were performed using a different perturbative approach that was based on the so-called $1/N$ expansion, where the role of a small parameter is played by the degeneracy N of the rare-earth ion momentum [15].

In studies on the ground-state properties of HF systems as described in terms of the periodic Anderson model, a useful approach is based on the Gutzwiller wave function [16, 17]. In recent years, the dynamic mean field theory has been widely used [18], but this approach is strictly justified only in the limit of infinite dimensionality of space. Finally, the method of slave bosons (SBs) [19] is worth mentioning, which was widely applied in many variants of investigating HF superconductors until recently (see, e.g., [10, 20–22]. An advantage of this approach is the possibility of using the Feynman diagram technique for calculating Green's functions, while the drawback is related to the need for introducing special constraints eliminating the contributions from nonphysical states. The latter circumstance is the source of difficulties encountered in the development of the theory in the SB method. It should be also mentioned that the mean field approximation that is usually employed in the SB method is, strictly speaking, valid only in the case of small concentrations of the slave bosons ($n_{SB} \ll 1$) and, hence, cannot be considered correct states in the regime of mixed valence or in the description of states with HFs.

The present investigation is based on the use of a diagram technique for the Hubbard operators [23, 24], which does not lead to the problem of nonphysical states. In the physical aspect, the complicated character of commutation relations for X-operators is expressed as an additional kinematic interaction [23] underlying Cooper instability [25]. A principally new issue in the proposed theory is the allowance for anomalous components of the strength operator. Expressions obtained for this operator in a one-loop approximation allowed us to take into account the process of dynamic scattering on spin fluctuation in the description of a superconducting phase.

The subsequent presentation is arranged as follows. In Section 2, the periodic Anderson model Hamiltonian is written in the atomic representation for the regime of strong correlations, exact representations of the Matsubara electron Green's functions of the superconducting phase are obtained via the normal and anomalous components of the mass and strength operators of the f-electron Green's functions, and these representations are compared to those obtained using of the SB method. Section 3 is devoted to calculating the contributions of components of the mass and strength operators of the f-electron Green's functions in a one-loop approximation. In Section 4, an expression for the generalized dynamic susceptibility is obtained in the same approximation. Equations for the self-consistent calculation of the critical temperature T_c and the order parameter are considered in Section 5. Section 6 shows the results of self-consistent numerical calculations in a graphical representation. The concluding Section 7 considers the dependence of the critical temperature of superconductivity on the concentration of electrons and the effect of scattering on spin fluctuations on this dependence and points to correlation of the results of self-consistent numerical calculations with experimental values of the critical temperature.

2. HAMILTONIAN OF THE PERIODIC ANDERSON MODEL AND EXACT REPRESENTATIONS OF GREEN'S FUNCTIONS

The Hamiltonian of the periodic Anderson model in the atomic representation in the limit of infinite on-site Coulomb repulsion for two f-electrons can be written as follows

$$H = H_0 + H_{\text{int}}, \tag{1}$$

where

$$\begin{aligned} H_0 &= \sum_{k\sigma} \xi_{k\sigma} c^\dagger_{k\sigma} c_{k\sigma} + \sum_{f\sigma} \tilde{E}_\sigma X^{\sigma\sigma}_f, \\ H_{\text{int}} &= \frac{1}{\sqrt{N}} \sum_{kf\sigma} (V_k e^{-ikf} c^\dagger_{k\sigma} X^{0\sigma}_f + \text{H.c.}). \end{aligned} \tag{2}$$

Here, the first term in H_0 describes the energy $\xi_{k\sigma} = \varepsilon_k - \sigma h - \mu$ (measured relative to the chemical potential μ) of the subsystem of itinerant (collectivized) electrons with the dispersion ε_k in magnetic field h (expressed in energy units); $\sigma = \pm 1/2$ is the electron spin projection; and $c^\dagger_{k\sigma}(c_{k\sigma})$ is the operator of electron creation (annihilation) in the state with quasimomentum k and electron spin projection σ. The second term in H_0 describes the energy of the system of localized f-electrons in the magnetic field, where $\tilde{E}_\sigma = E_0 - \sigma h - \mu$ and E_0 is the bare energy of a localized level. The interaction Hamiltonian H_{int} describes hybridization of the collectivized (band) states and localized states with the intensity characterized by the matrix element V_k and the Hubbard operators are defined on a basis set of single-ion orbitals as $X^{mn} = |m\rangle\langle n|$. For $U = \infty$, this basis set contains two one-electron states $|\uparrow\rangle$, $|\downarrow\rangle$and one vacuum state $|0\rangle$.

In the description of the superconducting phase, we employ two sets of the Matsubara Green's functions. As

is commonly accepted, we introduce the normal Green's functions as

$$\begin{aligned} G_{k\sigma}(\tau-\tau') &= -\langle T_\tau \tilde{c}_{k\sigma}(\tau)\tilde{c}^\dagger_{k\sigma}(\tau')\rangle, \\ \overline{G}_{-k\bar{\sigma}}(\tau-\tau') &= -\langle T_\tau \tilde{c}^\dagger_{-k\bar{\sigma}}(\tau)\tilde{c}_{-k\bar{\sigma}}(\tau')\rangle \end{aligned} \tag{3}$$

and the anomalous Green's functions as

$$\begin{aligned} F_{k\sigma}(\tau-\tau') &= -\langle T_\tau \tilde{c}_{k\sigma}(\tau)\tilde{c}_{-k\bar{\sigma}}(\tau')\rangle, \\ \overline{F}_{k\sigma}(\tau-\tau') &= -\langle T_\tau \tilde{c}^\dagger_{-k\bar{\sigma}}(\tau)\tilde{c}^\dagger_{k\sigma}(\tau')\rangle, \end{aligned} \tag{4}$$

which are constructed using the Fermi operators of secondary quantization for the subsystem of itinerant electrons. In Eqs. (3) and (4), T_τ is the operator of ordering with respect to Matsubara time τ, all operators are used in the Heisenberg representation, and the angle brackets denote thermodynamic averaging with Hamiltonian (1).

Since the structure of Hamiltonian (1) includes the *X*-operators (in addition to the secondary quantization operators), it is also necessary to use the set of Green's functions for localized electrons, which are defined using the Hubbard operators as

$$\begin{aligned} D_{\boldsymbol{\alpha\beta}}(f\tau; g\tau') &= -\langle T_\tau \tilde{X}^{\boldsymbol{\alpha}}_f(\tau)\tilde{X}^{-\boldsymbol{\beta}}_g(\tau')\rangle, \\ \boldsymbol{\alpha}, \boldsymbol{\beta} &= \{(0,\sigma),(\bar{\sigma},0)\}. \end{aligned} \tag{5}$$

In order to determine Green's functions (3)–(5), we use a graphical representation of perturbation theory, which combines the usual Feynman technique [26] and the aforementioned diagram technique for the Hubbard operators [23, 24]. The latter technique has certain special features that are related to the complicated character of the permutation relations for *X*-operators (the result of permutation of two such operators cannot be reduced to a numerical function). This circumstance leads to the appearance of a special class of diagrams called terminal diagrams [23]. The complete set of diagrams constitutes a new structural element called strength operator or (in terms of [24]) the terminal factor.

The diagram representations show that the Green's functions introduced above obey the following relation in the momentum representation:

$$\begin{aligned} \hat{G}_{k\sigma}(i\omega_n) &= \hat{G}^{(0)}_{k\sigma}(i\omega_n) \\ &+ \hat{G}^{(0)}_{k\sigma}(i\omega_n)\hat{V}_k\hat{D}_\sigma(k, i\omega_n)\hat{V}^\dagger_k\hat{G}^{(0)}_{k\sigma}(i\omega_n). \end{aligned} \tag{6}$$

For brevity, we write this equation in the matrix form, where

$$\begin{aligned} \hat{G}_{k\sigma}(i\omega_n) &= \begin{pmatrix} G_{k\sigma}(i\omega_n), & F_{k\sigma}(i\omega_n) \\ \overline{F}_{k\sigma}(i\omega_n), & \overline{G}_{-k,\bar{\sigma}}(i\omega_n) \end{pmatrix}, \\ \hat{D}_\sigma(k, i\omega_n) &= \begin{pmatrix} D_{0\sigma,0\sigma}(k, i\omega_n), & D_{0\sigma,\bar{\sigma}0}(k, i\omega_n) \\ D_{\bar{\sigma}0,0\sigma}(k, i\omega_n), & D_{\bar{\sigma}0,\bar{\sigma}0}(k, i\omega_n) \end{pmatrix}, \end{aligned} \tag{7}$$

$$\begin{aligned} \hat{G}^{(0)}_{k\sigma}(i\omega_n) &= \begin{pmatrix} G^{(0)}_{k\sigma}(i\omega_n), & 0 \\ 0, & \overline{G}^{(0)}_{-k\bar{\sigma}}(i\omega_n) \end{pmatrix}, \\ \hat{V}_k &= \begin{pmatrix} V_k, & 0 \\ 0, & -V^*_{-k} \end{pmatrix}, \end{aligned} \tag{8}$$

$$\begin{aligned} G^{(0)}_{k\sigma}(i\omega_n) &= \frac{1}{i\omega_n - \xi_{k\sigma}}, \\ \overline{G}^{(0)}_{-k\bar{\sigma}}(i\omega_n) &= \frac{1}{i\omega_n + \xi_{-k\bar{\sigma}}}, \end{aligned} \tag{9}$$

and take into account that, in writing the average of the *T*-ordered product

$$\langle T_\tau X^\alpha_f(\tau) X^{-\beta}_f(\tau') H_{\rm int}(\tau_1) H_{\rm int}(\tau_2)\ldots H_{\rm int}(\tau_n)\rangle,$$

the pairing of *c*-operators is performed independently of the pairing of *X*-operators. The pairing of operator $c_{k\sigma}(\tau_l)$ from $H_{\rm int}(\tau_l)$ with operator $c^\dagger_{k\sigma}(\tau_m)$ from $H_{\rm int}(\tau_m)$ yields the following operator:

$$|V_k|^2 G^{(0)}_{k\sigma}(\tau_l - \tau_m)\exp[ik(l-m)]X^{\sigma 0}_l(\tau_l)X^{0\sigma}_m(\tau_m), \tag{10}$$

which describes the process of localized electron hopping from site *m* to site *l*. In this respect, the new operator is analogous to the operator of kinetic energy in the Wannier representation, while the difference is that a shift appears in the Matsubara time between the events of electron annihilation on site *m* and its production on site *l*. In the Hubbard model, these events take place simultaneously. Despite this difference, the problem of determining the Green's functions of the *f*-electrons formally reduces to an analogous problem for the Hubbard model in the regime of strong correlations, in which the role of a hopping integral t_k is played by the quantity $\tilde{t}_\sigma(k, i\omega_n) = |V_k|^2 G^{(0)}_{k\sigma}(i\omega_n)$. It should be noted that, for the nonsuperconducting phase, such equivalence was established for the first time by the method of generating functional [27]. The dependence of the effective hopping integral $\tilde{t}_\sigma(k, i\omega_n)$ on the Matsubara frequency is determined by the aforementioned time shift between the events of electron annihilation and production (an analogous situation is revealed by the analysis of electron–phonon interaction [26]). Once the Green's functions of the localized subsystem are found, those of *c*-electrons are obtained by substituting $\hat{D}_\sigma(k, i\omega_n)$ into Eq. (6).

The presence of terminal diagrams results in the fact that $\hat{D}_\sigma(k, i\omega_n)$ in the (k, ω_n) representation can be expressed via the function

$$\hat{\mathcal{G}}_\sigma(k, i\omega_n) = \begin{pmatrix} \mathcal{G}_{0\sigma,0\sigma}(k, i\omega_n), & \mathcal{G}_{0\sigma,\bar{\sigma}0}(k, i\omega_n) \\ \mathcal{G}_{\bar{\sigma}0,0\sigma}(k, i\omega_n), & \mathcal{G}_{\bar{\sigma}0,\bar{\sigma}0}(k, i\omega_n) \end{pmatrix} \quad (11)$$

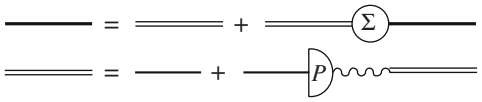
and the strength operator

$$\hat{P}_\sigma(k, i\omega_n) = \begin{pmatrix} P_{0\sigma,0\sigma}(k, i\omega_n), & P_{0\sigma,\bar{\sigma}0}(k, i\omega_n) \\ P_{\bar{\sigma}0,0\sigma}(k, i\omega_n), & P_{\bar{\sigma}0,\bar{\sigma}0}(k, i\omega_n) \end{pmatrix} \quad (12)$$

as follows:

$$\hat{D}_\sigma(k, i\omega_n) = \hat{\mathcal{G}}_\sigma(k, i\omega_n)\hat{P}_\sigma(k, i\omega_n).$$

It should be emphasized that, in addition to the normal components, there are nonzero anomalous components $P_{0\sigma,\bar{\sigma}0}(k, i\omega_n)$ and $P_{\bar{\sigma}0,0\sigma}(k, i\omega_n)$. In graphical form, the system of equations for determining function (11) can be presented as follows:



(13)

where thick solid line corresponds to $\hat{\mathcal{G}}_\sigma(k, i\omega_n)$, the encircled Σ symbol corresponds to the mass operator

$$\hat{\Sigma}_\sigma(k, i\omega_n) = \begin{pmatrix} \Sigma_{0\sigma,0\sigma}(k, i\omega_n), & \Sigma_{0\sigma,\bar{\sigma}0}(k, i\omega_n) \\ \Sigma_{\bar{\sigma}0,0\sigma}(k, i\omega_n), & \Sigma_{\bar{\sigma}0,\bar{\sigma}0}(k, i\omega_n) \end{pmatrix}, \quad (14)$$

symbol P in semicircle corresponds to the strength operator, the double line corresponds to the function

$$\hat{\mathcal{G}}^{(0)}_\sigma(k, i\omega_n) = \begin{pmatrix} \mathcal{G}^{(0)}_{0\sigma,0\sigma}(k, i\omega_n), & \mathcal{G}^{(0)}_{0\sigma,\bar{\sigma}0}(k, i\omega_n) \\ \mathcal{G}^{(0)}_{\bar{\sigma}0,0\sigma}(k, i\omega_n), & \mathcal{G}^{(0)}_{\bar{\sigma}0,\bar{\sigma}0}(k, i\omega_n) \end{pmatrix}, \quad (15)$$

the thin solid line corresponds to the diagonal matrix of local propagators

$$\hat{g}_\sigma(i\omega_n) = \begin{pmatrix} (i\omega_n - \tilde{E}_\sigma)^{-1}, & 0 \\ 0, & (i\omega_n + \tilde{E}_{\bar{\sigma}})^{-1} \end{pmatrix}, \quad (16)$$

and the wavy line corresponds to the effective interaction matrix

$$\hat{t}_\sigma(k, i\omega_n) = \hat{V}_k\hat{G}^{(0)}_{k\sigma}(i\omega_n)\hat{V}^\dagger_k = \begin{pmatrix} |V_k|^2(i\omega_n - \xi_{k\sigma})^{-1}, & 0 \\ 0, & |V_{-k}|^2(i\omega_n + \xi_{-k\bar{\sigma}})^{-1} \end{pmatrix}. \quad (17)$$

In the analytical form, Eqs. (13) are written as follows:

$$\begin{aligned} \hat{\mathcal{G}}_\sigma(k, i\omega_n) &= \hat{\mathcal{G}}^{(0)}_\sigma(k, i\omega_n) \\ &+ \hat{\mathcal{G}}^{(0)}_\sigma(k, i\omega_n)\hat{\Sigma}_\sigma(k, i\omega_n)\hat{\mathcal{G}}_\sigma(k, i\omega_n), \\ \hat{\mathcal{G}}^{(0)}_\sigma(k, i\omega_n) &= \hat{g}_\sigma(i\omega_n) \\ &+ \hat{g}_\sigma(i\omega_n)\hat{P}_\sigma(k, i\omega_n)\hat{t}_\sigma(k, i\omega_n)\hat{\mathcal{G}}^{(0)}_\sigma(k, i\omega_n). \end{aligned} \quad (18)$$

Excluding $\hat{\mathcal{G}}^{(0)}_\sigma(k, i\omega_n)$ from these relations, we arrive at an exact matrix representation that relates function (11) to the mass and strength operators:

$$\begin{aligned} \hat{\mathcal{G}}_\sigma(k, i\omega_n) &= [\hat{g}^{-1}_\sigma(i\omega_n) \\ &- \hat{P}_\sigma(k, i\omega_n)\hat{t}_\sigma(k, i\omega_n) - \hat{\Sigma}_\sigma(k, i\omega_n)]^{-1}. \end{aligned} \quad (19)$$

Writing the components separately, we obtain

$$\begin{aligned} \mathcal{G}_{0\sigma,0\sigma}(k, i\omega_n) &= [i\omega_n + \tilde{E}_{\bar{\sigma}} - P_{\bar{\sigma}0,\bar{\sigma}0}(k, i\omega_n)|V_{-k}|^2 \\ &\times \overline{G}^{(0)}_{-k\bar{\sigma}}(i\omega_n) - \Sigma_{\bar{\sigma}0,\bar{\sigma}0}(k, i\omega_n)] \\ &\times [\det_\sigma(k, i\omega_n)]^{-1}, \end{aligned} \quad (20)$$

$$\begin{aligned} \mathcal{G}_{0\sigma,\bar{\sigma}0}(k, i\omega_n) &= [P_{0\sigma,\bar{\sigma}0}(k, i\omega_n)|V_{-k}|^2\overline{G}^{(0)}_{-k\bar{\sigma}}(i\omega_n) \\ &+ \Sigma_{0\sigma,\bar{\sigma}0}(k, i\omega_n)][\det_\sigma(k, i\omega_n)]^{-1}, \end{aligned} \quad (21)$$

$$\begin{aligned} \mathcal{G}_{\bar{\sigma}0,0\sigma}(k, i\omega_n) &= [P_{\bar{\sigma}0,0\sigma}(k, i\omega_n)|V_k|^2G^{(0)}_{k\sigma}(i\omega_n) \\ &+ \Sigma_{\bar{\sigma}0,0\sigma}(k, i\omega_n)][\det_\sigma(k, i\omega_n)]^{-1}, \end{aligned} \quad (22)$$

$$\begin{aligned} \mathcal{G}_{\bar{\sigma}0,\bar{\sigma}0}(k, i\omega_n) &= [i\omega_n - \tilde{E}_\sigma - P_{0\sigma,0\sigma}(k, i\omega_n) \\ &\times |V_k|^2G^{(0)}_{k\sigma}(i\omega_n) - \Sigma_{0\sigma,0\sigma}(k, i\omega_n)] \\ &\times [\det_\sigma(k, i\omega_n)]^{-1}, \end{aligned} \quad (23)$$

where

$$\begin{aligned} \det_\sigma(k, i\omega_n) &= [i\omega_n - \tilde{E}_\sigma - P_{0\sigma,0\sigma}(k, i\omega_n) \\ &\times |V_k|^2G^{(0)}_{k\sigma}(i\omega_n) - \Sigma_{0\sigma,0\sigma}(k, i\omega_n)] \\ &\times [i\omega_n + \tilde{E}_{\bar{\sigma}} - P_{\bar{\sigma}0,\bar{\sigma}0}(k, i\omega_n) \\ &\times |V_{-k}|^2\overline{G}^{(0)}_{-k\bar{\sigma}}(i\omega_n) - \Sigma_{\bar{\sigma}0,\bar{\sigma}0}(k, i\omega_n)] \\ &- [P_{0\sigma,\bar{\sigma}0}(k, i\omega_n)|V_{-k}|^2\overline{G}^{(0)}_{-k\bar{\sigma}}(i\omega_n) \\ &+ \Sigma_{0\sigma,\bar{\sigma}0}(k, i\omega_n)] \\ &\times [P_{\bar{\sigma}0,0\sigma}(k, i\omega_n)|V_k|^2G^{(0)}_{k\sigma}(i\omega_n) \\ &+ \Sigma_{\bar{\sigma}0,0\sigma}(k, i\omega_n)]. \end{aligned} \quad (24)$$

Equations (20)–(24) give exact representations of the normal and anomalous Green's functions of the localized f-electrons in the superconducting phase via

the normal and anomalous components of the mass and strength operators. These equations, together with Eq. (6), also determine the exact representation of the normal and anomalous Green's functions of itinerant electrons via the same (*f*-electron) mass and strength operators. The further use of these equations implies the choice of a particular approximation, with the explicit calculation of the mass and strength operators.

Let us analyze the structure of the representation for the normal phase, assuming that the anomalous components of the mass and strength operators are zero and Eq. (20) takes the following form:

$$\mathcal{G}_{0\sigma,\,0\sigma}(k, i\omega_n) = [i\omega_n - \tilde{E}_\sigma - \Sigma_{0\sigma,\,0\sigma}(k, i\omega_n) - P_{0\sigma,\,0\sigma}(k, i\omega_n)|V_k|^2 G^{(0)}_{k\sigma}(i\omega_n)]^{-1}. \quad (25)$$

Using the explicit form of the *c*-electron propagator $G^{(0)}_{k\sigma}(i\omega_n)$, we obtain the following expression for the Green's functions of localized electrons:

$$D_{0\sigma,\,0\sigma}(k, i\omega_n) = (i\omega_n - \xi_{k\sigma})P_{0\sigma,\,0\sigma}(k, i\omega_n) \times \{(i\omega_n - \xi_{k\sigma})[i\omega_n - \tilde{E}_\sigma - \Sigma_{0\sigma,\,0\sigma}(k, i\omega_n)] - P_{0\sigma,\,0\sigma}(k, i\omega_n)|V_k|^2\}^{-1}. \quad (26)$$

The equation with an analogous structure for the normal component of the Green's functions of *f*-electrons in a nonsuperconducting phase was obtained previously [27] using the generation functional method. Substituting expression (26) into the equation

$$G_{k\sigma}(i\omega_n) = G^{(0)}_{k\sigma}(i\omega_n) + (G^{(0)}_{k\sigma}(i\omega_n))^2|V_k|^2 D_{0\sigma,\,0\sigma}(k, i\omega_n), \quad (27)$$

derived from matrix relation (6), we obtain the exact representation of the Green's functions of itinerant electrons in the normal phase:

$$G_{k\sigma}(i\omega_n) = [i\omega_n - \tilde{E}_\sigma - \Sigma_{0\sigma,\,0\sigma}(k, i\omega_n)] \times \{(i\omega_n - \xi_{k\sigma})[i\omega_n - \tilde{E}_\sigma - \Sigma_{0\sigma,\,0\sigma}(k, i\omega_n)] - P_{0\sigma,\,0\sigma}(k, i\omega_n)|V_k|^2\}^{-1}. \quad (28)$$

Let us compare the exact representations (26) and (28) to those obtained within the framework of the method of slave bosons (most popular until recently in the HF superconductor theory), which can be written as follows:

$$D^{SB}_{k\sigma}(i\omega_n) = (i\omega_n - \xi_{k\sigma}) \times [(i\omega_n - \xi_{k\sigma})(i\omega_n - \tilde{E}_\sigma - \lambda) - (1 - n_f)|V_k|^2]^{-1}, \quad (29)$$

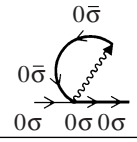
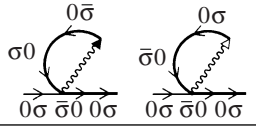
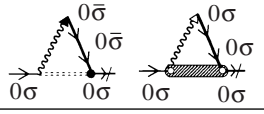
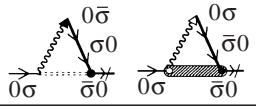
$$G^{SB}_{k\sigma}(i\omega_n) = (i\omega_n - \tilde{E}_\sigma - \lambda) \times [(i\omega_n - \xi_{k\sigma})(i\omega_n - \tilde{E}_\sigma - \lambda) - (1 - n_f)|V_k|^2]^{-1}. \quad (30)$$

Here, λ is the Lagrange renormalization factor determined from the condition $n_{SB} = 1 - n_f$, where n_{SB} is the SB concentration. The comparison of Eqs. (28) and (30) shows that the mass operator $\Sigma_{0\sigma,\,0\sigma}$ of the exact representation corresponds to factor λ in the SB description, while the strength operator corresponds to the slave boson concentration:

$$\Sigma_{0\sigma,\,0\sigma}(k, i\omega_n) \longrightarrow \lambda, \quad P_{0\sigma,\,0\sigma}(k, i\omega_n) \longrightarrow n_{SB} = 1 - n_f. \quad (31)$$

Adopting this correspondence, we note that the exact representation (26) differs from approximate (29) by the factor $P_{0\sigma,\,0\sigma}(k, i\omega_n)$ entering into the numerator. Since the established correspondence implies that factor $P_{0\sigma,\,0\sigma}(k, i\omega_n) = 1 - n_f$, the difference between the two representations is small provided that $n_f \ll 1$. From this it follows that the domain of applicability of the mean field theory of slave bosons is restricted to small concentrations of localized electrons ($n_f \ll 1$) and, hence, the use of this theory in the HF regime is not correct. In the absence of the aforementioned renormalization factor in the numerator, application of the SB approach to description of the localized electrons in the Kondo regime ($n_f \longrightarrow 1$) significantly distorts the spectral intensity and absolute values of thermodynamic means. In concluding this comparative analysis, it should be noted that, in view of the dependence of the mass and strength operators on the Matsubara frequency, the actual renormalizations will be different on various energy scales. Evidently, this circumstance is ignored in the methodology of slave bosons, at least in the first approximation.

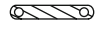
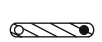
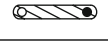
Table 1. One-loop diagrams for the mass and force operators

$\Sigma_{0\sigma,\,0\sigma}$	
$\Sigma_{0\sigma,\,\bar{\sigma}0}$	
$\delta P_{0\sigma,\,0\sigma}$	
$P_{0\sigma,\,\bar{\sigma}0}$	

3. ONE-LOOP APPROXIMATION FOR THE MASS AND STRENGTH OPERATORS IN A SUPERCONDUCTING PHASE

Self-consistent equations for calculating parameters of the superconducting phase will be derived in a one-loop approximation. The diagrams determining contri-

Table 2. Graphical elements of diagrams and the corresponding functions

	$g_{0\sigma}(i\omega_n)$		$\mathcal{G}_{0\sigma,\,0\sigma}(k, i\omega_n)$
	$D_{\bar{\sigma}\sigma,\,\bar{\sigma}\sigma}(k, i\omega_n)$		$\mathcal{G}_{\bar{\sigma}0,\,0\sigma}(k, i\omega_n)$
	$\lvert V_k\rvert^2 G^{(0)}_{k\sigma}(i\omega_n)$		$D^{(\mathrm{irr})}_{\sigma\sigma,\,\sigma\sigma}(k, i\omega_n)$
	$\lvert V_k\rvert^2 G^{(0)}_{k\bar{\sigma}}(i\omega_n)$		$D^{(\mathrm{irr})}_{\sigma\sigma,\,\bar{\sigma}\bar{\sigma}}(k, i\omega_n)$

butions to the mass and strength operators in this approximation are presented in Table 1. These diagrams were obtained using the topological continuity principle [28] supplemented by the principle that the Fermi-like Hubbard operators are superior to Bose-like operators [24]. There is one diagram for a normal component of the mass operator, and two diagrams for all other components. The normal component of the strength operator in the loopless approximation is nonzero and is expressed as $1 - N_\sigma$, where N_σ is the probability of occupation of the f-level by an electron with the spin projection σ. Denoting the one-loop correction to this value by $\delta P_{0\sigma,\,0\sigma}$, we have $P_{0\sigma,\,0\sigma} = 1 - N_{\bar{\sigma}} + \delta P_{0\sigma,\,0\sigma}$.

Table 2 presents separate graphical elements of the diagrams and the corresponding functions, where the double-dash line with a black circle corresponds to the Fourier transform of the transverse quasi-spin Green's function

$$D_{\bar{\sigma}\sigma,\,\bar{\sigma}\sigma}(f\tau;\, g\tau') = -\langle T_\tau \tilde{X}^{\bar{\sigma}\sigma}_f(\tau)\tilde{X}^{\sigma\bar{\sigma}}_g(\tau')\rangle \qquad (32)$$

and cross-hatched regions corresponds to the Fourier transform of the irreducible Green's function

$$D^{(\mathrm{irr})}_{\sigma\sigma,\,ss}(f\tau;\, g\tau') = -\langle T_\tau \Delta\tilde{X}^{\bar{\sigma}\bar{\sigma}}_f(\tau)\Delta\tilde{X}^{\bar{s}\bar{s}}_g(\tau')\rangle \qquad (33)$$

of the quasi-Bose diagonal Hubbard operators, where $\Delta X = X - \langle X\rangle$. For $s = \sigma$, this irreducible Green's function corresponds to the region with two open circles, and for $s = \bar{\sigma}$, this function corresponds to the region with one open and one black circle. The condition of irreducibility implies the absence of split graphs (see, e.g., [29]) in the diagrams of Green's functions (33). The other functions presented in Table 2 are as defined above. Using the rules of the diagram technique for Hubbard operators and the data of Tables 1 and 2, we can write the following analytical expressions for the normal and anomalous components of the mass and strength operators:

$$\Sigma_{0\sigma,\,0\sigma} = -\frac{T}{N}\sum_{q,\,\omega_m} \lvert V_q\rvert^2 G^{(0)}_{q,\,\bar{\sigma}}(i\omega_m)\mathcal{G}_{0\bar{\sigma},\,0\bar{\sigma}}(q, i\omega_m), \qquad (34)$$

$$\Sigma_{0\sigma,\,\bar{\sigma}0} = \frac{T}{N}\sum_{q,\,\omega_m} \lvert V_q\rvert^2 \times [G^{(0)}_{q,\,\bar{\sigma}}(i\omega_m)\mathcal{G}_{0\bar{\sigma},\,\sigma0}(q, i\omega_m) - G^{(0)}_{q,\,\sigma}(i\omega_m)\mathcal{G}_{0\sigma,\,\bar{\sigma}0}(q, i\omega_m)], \qquad (35)$$

$$\delta P_{0\sigma,\,0\sigma}(k, i\omega_n) = -\frac{T}{N}\sum_{q,\,\omega_m} \lvert V_q\rvert^2 \times [G^{(0)}_{q,\,\bar{\sigma}}(i\omega_m)\mathcal{G}_{0\bar{\sigma},\,0\bar{\sigma}}(q, i\omega_m)D_{\bar{\sigma}\sigma,\,\bar{\sigma}\sigma}(k-q, i\omega_n - i\omega_m) + G^{(0)}_{q,\,\sigma}(i\omega_m)\mathcal{G}_{0\sigma,\,0\sigma}(q, i\omega_m) \times D^{(\mathrm{irr})}_{\sigma\sigma,\,\sigma\sigma}(k-q, i\omega_n - i\omega_m)], \qquad (36)$$

$$P_{0\sigma,\,\bar{\sigma}0}(k, i\omega_n) = -\frac{T}{N}\sum_{q,\,\omega_m} \lvert V_q\rvert^2 \times [G^{(0)}_{q,\,\bar{\sigma}}(i\omega_m)\mathcal{G}_{0\bar{\sigma},\,\sigma0}(q, i\omega_m)D_{\bar{\sigma}\sigma,\,\bar{\sigma}\sigma}(k-q, i\omega_n - i\omega_m) + G^{(0)}_{q,\,\sigma}(i\omega_m)\mathcal{G}_{0\sigma,\,\bar{\sigma}0}(q, i\omega_m) \times D^{(\mathrm{irr})}_{\sigma\sigma,\,\bar{\sigma}\bar{\sigma}}(k-q, i\omega_n - i\omega_m)]. \qquad (37)$$

As can be seen, the mass operator components in the one-loop approximation are independent of the quasi-momentum k and frequency ω_n, and the mass operator obeys the relation $\Sigma_{0\sigma,\,\bar{\sigma}0} = -\Sigma_{0\bar{\sigma},\,\sigma0}$. Expressions (36) and (37) for the strength operator components contain the Fourier transforms of the quasi-spin Green's function (32) and the irreducible Green's function [33]. Thus, the scattering on spin fluctuations influences, via the strength operator, the mechanism of Cooper instability in HF systems.

Applying representation (21) to expressions (35) and (37), we obtain a closed system of integral equations for determining the anomalous components of the mass and strength operators of the superconducting phase. Taking into account that the magnetic field in this phase is absent, the system of equations for $\Sigma_{12} = \Sigma_{0\uparrow,\,\downarrow0}$ and $2P(k, i\omega_n) = P_{0\uparrow,\,\downarrow0}(k, i\omega_n) - P_{0\downarrow,\,\uparrow0}(k, i\omega_n)$ can be written as follows:

$$\Sigma_{12} = -\frac{2T}{N}\sum_{q,\,\omega_m} \lvert V_q\rvert^2 G^{(0)}_q(i\omega_m) \times \frac{\lvert V_q\rvert^2 \bar{G}^{(0)}_q(i\omega_m)P(q, i\omega_m) + \Sigma_{12}}{\det(q, i\omega_m)}, \qquad (38)$$

$$P(k, i\omega_n) = \frac{T}{N}\sum_{q,\,\omega_m} \lvert V_q\rvert^2 G^{(0)}_q(i\omega_m) \times \chi^{(-)}_C(k-q, i\omega_n - i\omega_m) \times \frac{\lvert V_q\rvert^2 \bar{G}^{(0)}_q(i\omega_m)P(q, i\omega_m) + \Sigma_{12}}{\det(q, i\omega_m)}. \qquad (39)$$

The passage to the symmetrized combination for P is advantageous in that the longitudinal and transverse quasi-spin Green's functions enter into the equation in an additive manner so that

$$\begin{aligned}\chi_C^{(-)}(k, i\omega_n) &= D_\perp(k, i\omega_n) + D_\parallel(k, i\omega_n)\\ -\frac{1}{4}C(k, i\omega_n) &= 3D_\parallel(k, i\omega_n) - \frac{1}{4}C(k, i\omega_n).\end{aligned} \tag{40}$$

In introducing the longitudinal quasi-spin Green's function $D_\parallel(k, i\omega_n)$ and the Green's function of charge fluctuations $C(k, i\omega_n)$, we took into account the completeness condition, according to which $X_f^{00} + X_f^{\sigma\sigma} + X_f^{\bar\sigma\bar\sigma} = 1$, and the operator identity $X_f^{\sigma\sigma} = \hat N_f/2 + 2\sigma S_f^z$, where $\sigma = \pm 1/2$ and $\hat N_f = X_f^{\uparrow\uparrow} + X_f^{\downarrow\downarrow}$. With allowance for these relations, the Fourier transforms of irreducible Green's functions [33] can be written as follows:

$$\begin{aligned}D^{(\mathrm{irr})}_{\sigma\sigma,\sigma\sigma}(k, i\omega_n) &= \frac{1}{4}C(k, i\omega_n) + D_\parallel(k, i\omega_n),\\ D^{(\mathrm{irr})}_{\sigma\sigma,\bar\sigma\bar\sigma}(k, i\omega_n) &= \frac{1}{4}C(k, i\omega_n) - D_\parallel(k, i\omega_n).\end{aligned} \tag{41}$$

where $C(k, i\omega_n)$, $D_\parallel(k, i\omega_n)$, and $D_\perp(k, i\omega_n)$ are expressed by the expansions

$$-\langle T_\tau \Delta\tilde{\hat N}_f(\tau)\Delta\tilde{\hat N}_g(\tau')\rangle = \frac{T}{N} \tag{42}$$

$$\times \sum_{k, i\omega_m} \exp[ik(f-g) - i\omega_m(\tau-\tau')]C(k, i\omega_m),$$

$$-\langle T_\tau \tilde S_f^z(\tau)\tilde S_g^z(\tau')\rangle = \frac{T}{N} \tag{43}$$

$$\times \sum_{k, i\omega_m} \exp[ik(f-g) - i\omega_m(\tau-\tau')]D_\parallel(k, i\omega_m),$$

$$-\langle T_\tau X_f^{\bar\sigma\sigma}(\tau)X_g^{\sigma\bar\sigma}(\tau')\rangle = \frac{T}{N} \tag{44}$$

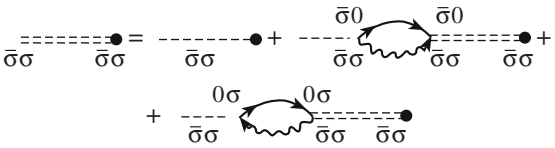
$$\times \sum_{k, i\omega_m} \exp[ik(f-g) - i\omega_m(\tau-\tau')]D_\perp(k, i\omega_m),$$

under the condition that $h = 0$. In writing the last equation, we took into account that, for $h = 0$, the quasi-spin Green's functions are spherically symmetric, so that $D_\perp(k, i\omega_n) = 2D_\parallel(k, i\omega_n)$.

4. QUASI-SPIN GREEN'S FUNCTIONS IN THE ONE-LOOP APPROXIMATION

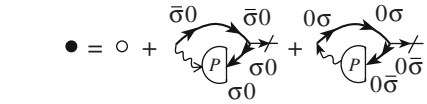
For the subsequent consideration of system of self-consistent equations (38), it is necessary to calculate $\chi_C^{(-)}(q, i\omega_m)$. The characteristic energies of charge fluctuations in most cases significantly exceed the energies of spin fluctuations. For this reason, the contribution of charge fluctuations is smaller than that of spin fluctuations and can be ignored.

In the one-loop approximation, the graphic equation for the transverse quasi-spin Green's function is as follows:



(45)

where the black circle corresponds to the quasi-spin strength operator $P_{\bar\sigma\sigma,\bar\sigma\sigma}(q, i\omega_m)$ defined as



(46)

Here, the open circle corresponds to the zero-order contribution $(N_{\bar\sigma} - N_\sigma)$, and the next two elements represent the one-loop corrections $\delta P_{\bar\sigma\sigma,\bar\sigma\sigma}(q, i\omega_m)$. In Eq. (45), the thick wavy element corresponds to the effective interaction obeying the following equation:

(47)

where symbol P in the semicircle again denotes the f-electron strength operator $P_{0\sigma,0\sigma}(q, i\omega_m)$. Using the rules of the diagram technique for the Hubbard operators, we can write Eq. (45) in the analytical form as

$$\begin{aligned}D_{\bar\sigma\sigma,\bar\sigma\sigma}(k, i\omega_m) &= g^{(0)}_{\bar\sigma\sigma}(i\omega_m)P_{\bar\sigma\sigma,\bar\sigma\sigma}(k, i\omega_m)\\ &+ g^{(0)}_{\bar\sigma\sigma}(i\omega_m)\Sigma_{\bar\sigma\sigma,\bar\sigma\sigma}(k, i\omega_m)D_{\bar\sigma\sigma,\bar\sigma\sigma}(k, i\omega_m).\end{aligned} \tag{48}$$

Taking into account the relation $g^{(0)}_{\bar\sigma\sigma}(i\omega_m) = 1/(i\omega_m + 2\sigma h)$ for a quasi-spin propagator, this equation can be rewritten as follows:

$$D_{\bar\sigma\sigma,\bar\sigma\sigma}(k, i\omega_m) = \frac{P_{\bar\sigma\sigma,\bar\sigma\sigma}(k, i\omega_m)}{i\omega_m + 2\sigma h - \Sigma_{\bar\sigma\sigma,\bar\sigma\sigma}(k, i\omega_m)}. \tag{49}$$

Here, the spin mass operator $\Sigma_{\bar\sigma\sigma,\bar\sigma\sigma}(k, i\omega_m)$ that represents contributions due to the two loops in the right-hand part of Eq. (45) is expressed as

$$\begin{aligned}\Sigma_{\bar\sigma\sigma,\bar\sigma\sigma}(k, i\omega_m) &= -\frac{T}{N}\sum_{q,\omega_n} t_\sigma(q, i\omega_n)\\ &\times [1 + t_\sigma(q, i\omega_n)D_{0\sigma,0\sigma}(q, i\omega_n)]G_{\bar\sigma 0,\bar\sigma 0}(k-q, i\omega_{m-n})\\ &- \frac{T}{N}\sum_{q,\omega_n} t_{\bar\sigma}(q, i\omega_n)[1 + t_{\bar\sigma}(q, i\omega_n)D_{0\bar\sigma,0\bar\sigma}(q, i\omega_n)]\\ &\times G_{0\sigma,0\sigma}(k+q, i\omega_{m+n}).\end{aligned} \tag{50}$$

For the strength operator $P_{\bar{\sigma}\sigma,\,\bar{\sigma}\sigma}(k, i\omega_m)$ determined by Eq. (46), the rules of the diagram technique for the Hubbard operators yield the following analytical expression:

$$P_{\bar{\sigma}\sigma,\,\bar{\sigma}\sigma}(k, i\omega_m) = (N_{\bar{\sigma}} - N_\sigma) + \frac{T}{N}\sum_{q,\,\omega_n}[t_\sigma(q+k, i\omega_{n+m})P_{0\sigma,\,0\sigma}(q+k, i\omega_{n+m}) - t_{\bar{\sigma}}(q, i\omega_n)P_{0\bar{\sigma},\,0\bar{\sigma}}(q, i\omega_n)] \times G_{0\sigma,\,0\sigma}(q+k, i\omega_{n+m})G_{0\bar{\sigma},\,0\bar{\sigma}}(q, i\omega_n). \quad (51)$$

Formulas (49)–(51), together with the system of self-consistency equations derived in Section 3 and the representations of quasi-spin Green's functions, it is possible to study in a self-consistent manner the conditions under which the superconducting phase exists in the system under consideration.

5. SELF-CONSISTENCY EQUATIONS AT THE POINT OF TRANSITION

Since the quasi-spin Green's functions enter only into the one-loop correction to the strength operator, we can solve the self-consistency equations with the assumed accuracy using some simplifying assumptions. First, in calculating the quasi-spin mass operator $\Sigma_{\bar{\sigma}\sigma,\,\bar{\sigma}\sigma}(k, i\omega_m)$, the electron Green's functions can be taken in the loopless approximation. This allows summation over Matsubara frequencies in Eq. (50) to be performed in an analytical form that yields

$$\Sigma_{\bar{\sigma}\sigma,\,\bar{\sigma}\sigma}(k, i\omega_m) = \frac{1}{N}\sum_q\sum_\alpha \alpha\left\{ f(\tilde{E}^\alpha_{q\sigma})\frac{|V_q|^2(\tilde{E}^\alpha_{q\sigma} - \tilde{\varepsilon}_{f\sigma})(-i\omega_m + \tilde{E}^\alpha_{q\sigma} - \xi_{q-k,\,\bar{\sigma}}) - |V_{q-k}|^2(\tilde{E}^\alpha_{q\sigma} - \xi_{q\sigma})(-i\omega_m + \tilde{E}^\alpha_{q\sigma} - \tilde{\sigma}_{f\bar{\sigma}})}{\nu_{q\sigma}(-i\omega_m + \tilde{E}^\alpha_{q\sigma} - \tilde{E}^{\bar{\alpha}}_{q-k,\,\bar{\sigma}})(-i\omega_m + \tilde{E}^\alpha_{q\sigma} - \tilde{E}^\alpha_{q-k,\,\bar{\sigma}})} - f(\tilde{E}^\alpha_{q\bar{\sigma}})\frac{|V_q|^2(\tilde{E}^\alpha_{q\bar{\sigma}} - \tilde{\varepsilon}_{f\bar{\sigma}})(i\omega_m + \tilde{E}^\alpha_{q\bar{\sigma}} - \xi_{q-k,\,\sigma}) - |V_{q-k}|^2(\tilde{E}^\alpha_{q\bar{\sigma}} - \xi_{q\bar{\sigma}})(i\omega_m + \tilde{E}^\alpha_{q\bar{\sigma}} - \tilde{\varepsilon}_{f\sigma})}{\nu_{q\bar{\sigma}}(i\omega_m + \tilde{E}^\alpha_{q\bar{\sigma}} - \tilde{E}^{\bar{\alpha}}_{q-k,\,\sigma})(i\omega_m + \tilde{E}^\alpha_{q\bar{\sigma}} - \tilde{E}^\alpha_{q-k,\,\sigma})}\right\}, \quad (52)$$

where $f(x) = [\exp(x/T) + 1]^{-1}$ is the Fermi–Dirac function and $\tilde{\varepsilon}_{f\sigma} = E_\sigma + \Sigma_{0\sigma,\,0\sigma} - \mu$ is the energy of a localized electron level. Note that, in calculating the transverse Green's functions, the magnetic field is considered to be nonzero and the limit $h \longrightarrow 0$ is taken only at the final stage. The one-particle mixon spectrum is given by the following expression:

$$\tilde{E}^\alpha_{k\sigma} = \frac{\xi_{k\sigma} + \tilde{\varepsilon}_{f\sigma}}{2} + \frac{\alpha}{2}\nu_{k\sigma},$$

where

$$\nu_{k\sigma} = \sqrt{(\xi_{k\sigma} - \tilde{\varepsilon}_{f\sigma})^2 + 4(1 - N_{\bar{\sigma}})|V_k|^2}, \quad \alpha = \pm 1. \quad (53)$$

The summation over Matsubara frequencies in Eq. (51) yields the following expression for the strength operator:

$$P_{\bar{\sigma}\sigma,\,\bar{\sigma}\sigma}(k, i\omega_m) = -\frac{4}{3}\frac{\sigma\chi_0 n_f^2}{(2-n_f)^2}h + R_\sigma(k, i\omega_m), \quad (54)$$

where

$$R_\sigma(k, i\omega_m) = (i\omega_m + 2\sigma h + \Sigma_{0\bar{\sigma},\,0\bar{\sigma}} - \Sigma_{0\sigma,\,0\sigma}) \times \frac{1}{N}\sum_q\sum_\alpha \alpha\left\{ f(\tilde{E}^\alpha_{q,\,\sigma})\frac{(-i\omega_m + \tilde{E}^\alpha_{q\sigma} - \xi_{q+k,\,\bar{\sigma}})(\tilde{E}^\alpha_{q,\,\sigma} - \xi_{q,\,\sigma})}{\nu_{q,\,\sigma}(-i\omega_m + \tilde{E}^\alpha_{q,\,\sigma} - \tilde{E}^{\bar{\alpha}}_{q+k,\,\bar{\sigma}})(-i\omega_m + \tilde{E}^\alpha_{q,\,\sigma} - \tilde{E}^\alpha_{q+k,\,\bar{\sigma}})} + f(\tilde{E}^\alpha_{q\bar{\sigma}})\frac{(i\omega_m + \tilde{E}^\alpha_{q\bar{\sigma}} - \xi_{q+k,\,\sigma})(\tilde{E}^\alpha_{q\bar{\sigma}} - \xi_{q\bar{\sigma}})}{\nu_{q\bar{\sigma}}(i\omega_m + \tilde{E}^\alpha_{q\bar{\sigma}} - \tilde{E}^{\bar{\alpha}}_{q+k,\,\sigma})(i\omega_m + \tilde{E}^\alpha_{q\bar{\sigma}} - \tilde{E}^\alpha_{q+k,\,\sigma})}\right\}.$$

The first term in Eq. (54) is written with allowance for smallness of the magnetic field. The resulting static susceptibility is determined in the limit as

$$\chi_0 = \lim_{h\to 0}\frac{3(N_\sigma - N_{\bar{\sigma}})}{4\sigma h}. \quad (55)$$

The generalized dynamic susceptibility

$$\chi(k, i\omega_m) = -\frac{3}{2}D_{\bar{\sigma}\sigma,\,\bar{\sigma}\sigma}(k, i\omega_m) \quad (56)$$

is calculated using formulas (49), (52), and (54), where it is necessary to take into account the difference between

zero value of the Matsubara frequencies ($m = 0$) and nonzero values ($m \neq 0$). For $m = 0$, the functions $R_\sigma(k, i\omega_m)$ and $\Sigma_{\bar\sigma\sigma,\,\bar\sigma\sigma}(k, i\omega_m)$ at small magnetic fields are proportional to $2\sigma h$ and the Green's function (49) can be represented as

$$D_{\bar\sigma\sigma,\,\bar\sigma\sigma}(k, 0) = \left[-\frac{2}{3}\frac{\chi_0 n_f^2}{(2-n_f)^2} + 2\sigma\frac{\partial R_\sigma(k, 0)}{\partial h}\right][1 - 2\sigma\partial\Sigma_{\bar\sigma\sigma,\,\bar\sigma\sigma}(k, 0)/\partial h]^{-1}. \quad (57)$$

For $m \neq 0$, the functions $R_\sigma(k, i\omega_m)$ and $\Sigma_{\bar\sigma\sigma,\,\bar\sigma\sigma}(k, i\omega_m)$ remain finite as $h \longrightarrow 0$ and can be written as products of $i\omega_m$ and the following real functions of ω_m:

$$P_{\bar\sigma\sigma,\,\bar\sigma\sigma}(k, i\omega_m) = i\omega_m P'_{\bar\sigma\sigma,\,\bar\sigma\sigma}(k, \omega_m),$$
$$\Sigma_{\bar\sigma\sigma,\,\bar\sigma\sigma}(k, i\omega_m) = i\omega_m \Sigma'_{\bar\sigma\sigma,\,\bar\sigma\sigma}(k, \omega_m), \quad (58)$$

where

$$P'_{\bar\sigma\sigma,\,\bar\sigma\sigma}(k, \omega_m) = \frac{2}{N}\sum_q\sum_\alpha \frac{\alpha f(\tilde E_q^\alpha)}{\nu_q}(\tilde E_q^\alpha - \xi_q)$$
$$\times[\omega_m^2(\tilde E_q^\alpha - \tilde\varepsilon_f) + (\tilde E_q^\alpha - \xi_{q+k})(\tilde E_q^\alpha - \tilde E_{q+k}^{\bar\alpha})(\tilde E_q^\alpha - \tilde E_{q+k}^{\alpha})][(\tilde E_q^\alpha - \tilde E_{q+k}^{\bar\alpha})^2 + \omega_m^2]^{-1}[(\tilde E_q^\alpha - \tilde E_{q+k}^{\alpha})^2 + \omega_m^2]^{-1}, \quad (59)$$

$$\Sigma'_{\bar\sigma\sigma,\,\bar\sigma\sigma}(k, \omega_m) = \frac{2}{N}\sum_q\sum_\alpha \alpha\frac{f(\tilde E_q^\alpha)}{\nu_q}$$
$$\times\{(2\tilde E_q^\alpha - \tilde\varepsilon_f - \xi_{q-k})(\tilde E_q^\alpha - \tilde\varepsilon_f)$$
$$\times[|V_q|^2(\tilde E_q^\alpha - \xi_{q-k}) - |V_{q-k}|^2(\tilde E_q^\alpha - \xi_q)]$$
$$-[|V_q|^2(\tilde E_q^\alpha - \tilde\varepsilon_f) - |V_{q-k}|^2(\tilde E_q^\alpha - \xi_q)] \quad (60)$$
$$\times[-\omega_m^2 + (\tilde E_q^\alpha - \tilde E_{q-k}^{\bar\alpha})(\tilde E_q^\alpha - \tilde E_{q-k}^{\alpha})]\}$$
$$\times[(\tilde E_q^\alpha - \tilde E_{q-k}^{\bar\alpha})^2 + \omega_m^2]^{-1}[(\tilde E_q^\alpha - \tilde E_{q-k}^{\alpha})^2 + \omega_m^2]^{-1}.$$

Thus, for $\omega_m \neq 0$, the spin Green's function (49) takes the following form:

$$D_{\bar\sigma\sigma,\,\bar\sigma\sigma}(k, i\omega_m) = \frac{P'_{\bar\sigma\sigma,\,\bar\sigma\sigma}(k, \omega_m)}{1 - \Sigma'_{\bar\sigma\sigma,\,\bar\sigma\sigma}(k, \omega_m)}. \quad (61)$$

Expressions (57) and (61) determine the spin Green's function as a real function of the Matsubara frequency. These will be used below in self-consistent numerical calculations.

As was mentioned above, HF skutterudite $LaFe_4P_{12}$ features the transition to a superconducting phase with *s*-type symmetry of the order parameter [8]. For this symmetry type, details of variation of the quasi-spin Green's function within the Brillouin zone are insignificant and we can use a widely used approximation [30, 31] in which the generalized susceptibility (56) is replaced by its average value over the Brillouin zone:

$$\chi(k, i\omega_m) \Rightarrow \bar\chi(i\omega_m) = \frac{1}{N}\sum_k \chi(k, i\omega_m). \quad (62)$$

In this case, as can be seen from self-consistency equations (38), the strength operator P depends only on the Matsubara frequency. Taking into account that Σ_{12} and $P(i\omega_n)$ vanish at the point of the superconducting transition, we can introduce the function

$$\rho(i\omega_n) = \frac{P(i\omega_n)}{\Sigma_{12}}, \quad (63)$$

which remains finite at $T = T_c$. Substituting $P(i\omega_n) = \Sigma_{12}\rho(i\omega_n)$ in Eq. (38) and canceling Σ_{12}, we obtain a system of equations for simultaneously determining $\rho(i\omega_n)$ and the critical temperature:

$$\rho(i\omega_n) = -T\sum_{\omega_m}\bar\chi(i\omega_{n-m})\Phi(i\omega_m),$$
$$1 = -2T\sum_{\omega_m}\Phi(i\omega_m), \quad (64)$$

where

$$\Phi(i\omega_m) = \frac{1}{N}$$
$$\times\sum_q \frac{|V_q|^2(i\omega_m + \xi_q) + \rho(i\omega_m)|V_q|^4}{\left|(i\omega_m - \xi_q)(i\omega_m - \tilde\varepsilon_f) - P_{0\sigma,\,0\sigma}(i\omega_m)|V_q|^2\right|^2}. \quad (65)$$

Note that, since system of equations (64) is used to determine the critical temperature, all functions and the Matsubara frequencies are taken for $T = T_c$. The obtained system of self-consistent equations should be supplemented with an equation for the chemical potential,

$$n_e = n_c + n_f, \quad (66)$$

where n_e is the total concentration of electrons per unit cell in both subsystems. The average values of the occupation numbers of itinerant (n_c) and localized (n_f) electrons are calculated using the following formulas:

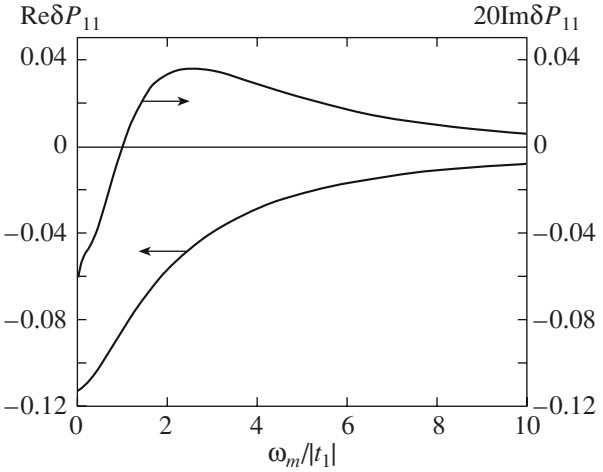


Fig. 1. Typical frequency dependences of the real and imaginary parts of a correction to the normal component of the strength operator.

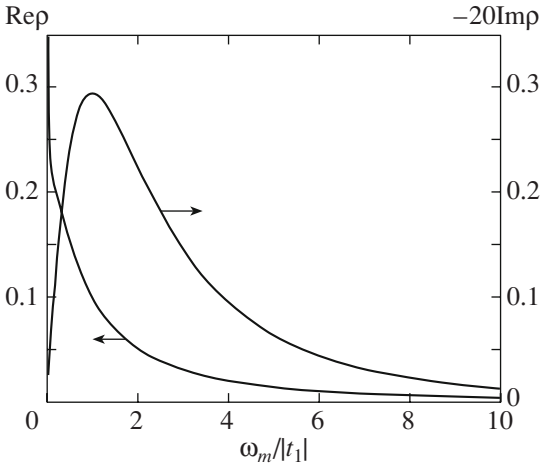


Fig. 2. Typical frequency dependences of the function ρ (63).

$$n_f = 2\frac{T}{N}\sum_{k\omega_n}\exp(i\omega_n\delta)D_{0\sigma,0\sigma}(k, i\omega_n),$$
$$n_c = 2\frac{T}{N}\sum_{k\omega_n}\exp(i\omega_n\delta)G_{k\sigma}(i\omega_n), \quad \delta \longrightarrow +0. \tag{67}$$

For determining the boundaries of the domain of existence of the superconducting phase, the Green's functions $D_{0\sigma,0\sigma}(k, i\omega_n)$ and $G_{k\sigma}(i\omega_n)$ in Eq. (67) are given by expressions (26) and (28) without contributions due to anomalous components of the mass and strength operators.

6. DEPENDENCE OF THE CRITICAL TEMPERATURE ON THE ELECTRON CONCENTRATION

Calculation of the critical temperature using numerical solution of Eqs. (64) involves preliminary determination of the normal component of the strength operator $P_{0\sigma,0\sigma}(k, i\omega_n) = 1 - n/2 + \delta P_{0\sigma,0\sigma}$ (entering into formula (65) for $\Phi(i\omega_m)$) as a function of the Matsubara frequency. This problem was solved using analytical expression (36), in which the spin and irreducible Green's functions averaged over the Brillouin zone were used as described in the preceding section.

Figure 1 shows the typical frequency dependences of the real and imaginary parts of $\delta P_{11} = \delta P_{0\uparrow,0\uparrow}$ obtained using self-consistent calculations for a total electron concentration of $n_e = 1.482$ (the corresponding *f*-electron concentration is $n_f = 0.83$). Since the real components of $\delta P_{11}(i\omega_m)$ are even functions of the frequency, while the imaginary parts are odd, the curves are presented only for the positive Matsubara frequencies. In these calculations, we assumed that the crystalline structure of HF skutterudite $LaFe_4P_{12}$ possesses a cubic symmetry and the bare spectrum of itinerant (band) electrons can be written in the tight binding approximation as

$$\varepsilon_k = 2t_1(\cos k_x + \cos k_y + \cos k_z) \tag{68}$$

with a bandwidth of $W = 12|t_1|$ ($t_1 < 0$) and a hybridization constant equal to one-tenth of the band width, $V/|t_1| = 1.2$. The localized level occurs in the conduction band, at a distance of $W/3$ from the minimum ($E_0/|t_1| = -2$). For other values of the parameters, the qualitative pattern presented in Fig. 1 is retained.

Figure 2 shows characteristic features in the behavior of the function $\rho(i\omega_n)$ (63) introduced in the course of self-consistent calculations of the critical temperature T_c (for the system parameters indicated above). For the same reasons as above, we present only the real and imaginary parts of $\rho(i\omega_n)$ for the positive Matsubara frequencies.

The main result obtained in this part of numerical calculations was that, for frequencies on the order of the width of the conduction band, both $\delta P_{11}(i\omega_m)$ and $\rho(i\omega_m)$ exhibit a strong dependence on ω_m. At low frequencies, the real part of $\delta P_{11}(i\omega_m)$ amounts approximately to –0.1 and the renormalization of the effective hybridization parameter toward a decrease is more pronounced. As a result, the real part of the renormalization factor for the hybridization constant in the region of low frequencies is $1 - n_f/2 - 0.1 = 0.485$. This value is intermediate between those obtained using the Hubbard-I approximation ($1 - n_f/2 = 0.585$) and the slave-boson approach ($1 - n_f = 0.17$). A significant distinctive feature is that, in both latter approximations, the imaginary component of renormalization (which accounts for the scattering) is not taken into account and the frequency dependence is totally ignored.

Figure 3 presents the typical frequency dependences of the Matsubara susceptibility $\chi(i\omega_m) = -3D_{\|}(i\omega_m)$, which was calculated simultaneously with the components of the strength operator. As can be seen, this func-

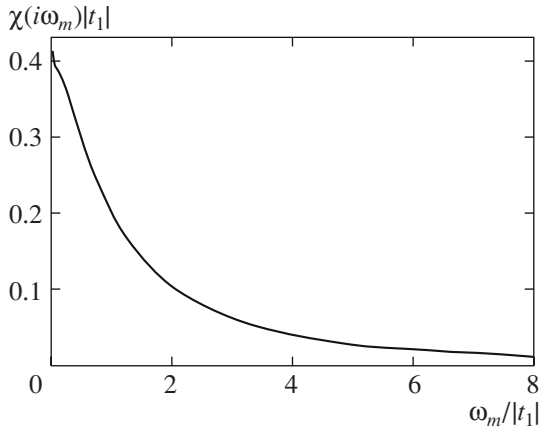


Fig. 3. Typical plot of the dynamic magnetic susceptibility versus Matsubara frequency.

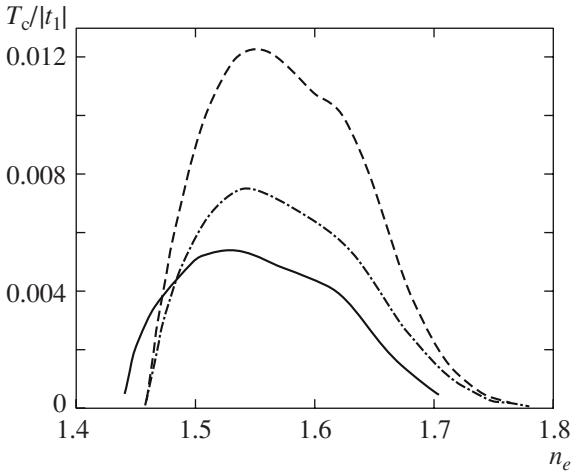


Fig. 4. Plots of the temperature of transition to the superconducting state with *s*-type symmetry of the order parameter versus electron concentration, as calculated using (solid curve) the dynamic spin-fluctuation approximation by Eqs. (64), (dashed curve) static approximation by formula (73), and (dash-dot curve) the mean field approximation by formula (74).

tion at low frequencies is significantly different from zero at low frequencies in the interval $0 < |\omega_m| < W/3$. In addition, the susceptibility exhibits an outburst at $\omega_m = 0$ (see the remark after Eq. (55)).

By jointly solving the equations for $\chi(i\omega_m)$, $\delta P_{11}(i\omega_m)$, $\rho(i\omega_m)$, and chemical potential, it is possible to follow the critical temperature of the transition to a superconducting state with *s*-type symmetry of the order parameter. The results of self-consistent numerical calculations of the critical temperature as a function of the electron concentration, obtained using Eqs. (64) with allowance for the dynamic character of spin fluctuations, are presented in Fig. 4 (solid curve). A characteristic feature of this dependence is that the Cooper instability is observed only in the region of electron concentrations $n_e \geq n_{cr}$, where the upper hybridized subband contains quasi-particles. If the chemical potential occurs in the lower subband, the conditions for *s*-wave superconductivity are not satisfied. As the upper band is occupied, T_c initially exhibits a sharp increase, passes through a maximum at an optimum electron concentration, and then gradually decreases.

In order to elucidate the role of dynamic spin fluctuations in the formation of an *s*-wave superconducting state, let us compare the obtained dependence of T_c on the electron concentration to the analogous dependences calculated within simpler models, in particular, using (a) the approximation ignoring the dynamics of spin fluctuations (static approximation) and (b) the mean-field approximation.

In the static approximation, the quasi-spin Green's functions are nonvanishing only for zero Matsubara frequency. In real experiments, this corresponds to high temperatures and, accordingly, this approximation may be called the high-temperature limit. Indeed, according to formula (61), the Green's function $D_{\bar{\sigma}\sigma,\bar{\sigma}\sigma}(k, i\omega_m)$ is inversely proportional to T^2. This allows all harmonics of the magnetic susceptibility except for $\omega_m = 0$ to be ignored at high temperatures. In this case, Eq. (64) yields the following solution for $\rho(i\omega_m)$:

$$\rho(i\omega_n) = -\frac{T\bar{\chi}(0)\Phi_1(i\omega_n)}{1 + T\bar{\chi}(0)\Phi_2(i\omega_n)}, \tag{69}$$

where

$$\Phi_1(i\omega_m) = \frac{1}{N} \times \sum_q \frac{|V_q|^2(i\omega_m + \xi_q)}{\left|(i\omega_m - \xi_q)(i\omega_m - \tilde{\varepsilon}_f) - P_{0\sigma,0\sigma}(i\omega_m)|V_q|^2\right|^2}, \tag{70}$$

$$\Phi_2(i\omega_m) = \frac{1}{N} \times \sum_q \frac{|V_q|^4}{\left|(i\omega_m - \xi_q)(i\omega_m - \tilde{\xi}_f) - P_{0\sigma,0\sigma}(i\omega_m)|V_q|^2\right|^2}.$$

On the other hand, we have $\rho(i\omega_n) = -T\bar{\chi}(0)\Phi(i\omega_n)$. Then, summing $\rho(i\omega_n)$ over the Matsubara frequencies and taking into account the second equation (64), we obtain the following sum rule:

$$2\sum_{\omega_n} \rho(i\omega_n) = \bar{\chi}(0), \tag{71}$$

which allows the equation for the critical temperature T_c to be written in an explicit form as

$$1 + 2T\sum_{\omega_n} \frac{\Phi_1(i\omega_n)}{1 + T\bar{\chi}(0)\Phi_2(i\omega_n)} = 0. \tag{72}$$

It should be noted that the same equation was previously derived [32] under the condition that the Cooper channel has a pole in the scattering amplitude calculated for the normal phase with allowance for the static spin-fluctuation contributions. This coincidence shows that inclusion of the anomalous components of the strength operator into the theory of a superconducting phase corresponds to allowance for the spin and charge fluctuations. In this context, it should be noted that Zaitsev [33] solved the problem of Cooper instability and demonstrated importance of taking into account the scattering on spin fluctuations for the Hubbard model in the regime of strong correlations. Figure 4 (dashed curve) shows the dependence of the critical temperature on the concentration of electrons as calculated using formula (72). The static approximation used in this study can be justified not only at high temperatures. Since only the smallness of all nonzero components of the dynamic susceptibility as compared to that for $\omega_m = 0$ is important, it should be noted that this condition can be also satisfied, for example, in the vicinity of the point of ferromagnetic instability at temperatures on the order of the Curie point, which may be relatively low.

The mean-field approximation is obtained under the condition of vanishing of the one-loop corrections to the strength operator, which formally corresponds to the case where the susceptibility of localized electrons is zero. Setting $\bar{\chi}(0) = 0$ in Eq. (72), considering Hubbard-I approximation for the normal component of the strength operator ($P_{0\sigma,0\sigma}(i\omega_n) = 1 - n_f/2$), and summing over Matsubara frequencies, we can rewrite the equation for T_c as follows:

$$1 = \frac{1}{N}\sum_q \frac{|V_q|^2\xi_q}{(\tilde{E}_q^+)^2 - (\tilde{E}_q^-)^2} \times \left[\frac{\tanh(\tilde{E}_q^+/2T_c)}{\tilde{E}_q^+} - \frac{\tanh(\tilde{E}_q^-/2T_c)}{\tilde{E}_q^-}\right]. \quad (73)$$

This relation, with a correction for the two-band structure, corresponds to the equation for T_c in the t-model in the mean-field approximation, where the scattering on spin fluctuations is ignored. This can be readily checked by taking into account the aforementioned equivalence of the diagram series for the Green's functions in the Anderson model and the series for Green's functions in the Hubbard model for $U = \infty$. The plot of $T_c(n_e)$ calculated in the mean-field approximation using formula (73) is depicted in Fig. 4 by the dash-dot curve.

A comparison of the curves in Fig. 4 shows to what extent allowance for the scattering on spin fluctuations influences the domain of existence of a superconducting phase. In particular, comparison of the dashed and dash-dot curves shows that taking this scattering into consideration even in the static approximation leads to a significant decrease in the critical temperature as compared to that in the mean-field approximation, while the values of critical concentrations for these curves nearly coincide. This behavior is related to the fact that the contributions of the strength operator components in the static approximation vanish as $T \longrightarrow 0$.

A different situation is observed in the case of allowance for the dynamic spin-fluctuation processes of scattering, where the sums over the Matsubara frequencies are calculated explicitly. As is known, this summation in the region of lowest temperatures can be replaced by integration ($T\sum_m \longrightarrow \int d\omega/2\pi$). Calculations show that contributions to the strength operator components remain finite even as $T \longrightarrow 0$. It is this difference that accounts for a significant shift of the boundary of the domain of superconductivity due to allowance for the dynamics of scattering on spin fluctuations. Figure 4 shows that, besides producing this shift, the dynamic spin fluctuations induce an additional decrease in the critical temperature. The magnitude of this decrease depends on the particular system parameters, but the indicated trends are retained in all cases.

7. CONCLUSIONS

The results presented above show that the superconducting phase with s-type symmetry of the order parameter observed in HF skutterudite $LaFe_4P_{12}$ [8] can be described using the periodic Anderson model with recourse to the electron mechanism of the Cooper instability. This scenario of electron pairing is qualitatively analogous to that of the formation of high-temperature superconductivity proposed [25] for the Hubbard model in the regime of strong electron correlations. At the same time, features of the Anderson model led to some modifications. For example, the mixing of band and localized states results in the fact that all kernels of the integral equations of self-consistency can be expressed via characteristics of a two-band mixon spectrum of Fermi excitations. It is established that the superconducting phase is achieved only for the electron concentrations at which occupied quasi-particle states appear in the upper mixon band.

Going beyond the mean-field approximation leads to an infinite system of integral equations for the superconducting phase. Solutions of these equations describe the behavior of the normal and anomalous components of the mass and strength operators. It should be emphasized that the influence of the strength operator components is not restricted to renormalization of the spectrum of elementary excitations. As can be seen from our results for the representations of Green's functions, this operator also significantly influences the values of the spectral intensity and the mean normal and anomalous components. It is also important that the strength operator mediates in the influence of the processes of scattering on spin fluctuations. The inclusion of these processes leads to a decrease in the critical temperature of the transition into a supercon-

ducting phase, which comes close to the experimental T_c values.

We have studied the conditions of transition to the superconducting state with *s*-type symmetry of the order parameter in the regime of strong electron correlations and developed spin fluctuations. As was mentioned above, this situation is met in HF skutterudites $LaFe_4P_{12}$ [8] and $PrRu_4As_{12}$ [9]. At the same time, the traditional HF superconductors are characterized by the anisotropic order parameter. The approach developed in this study is also applicable to the description of *d*-wave superconductivity, with the process of scattering on spin fluctuations realized via the strength operator components. However, in order to obtain the mechanism of Cooper instability leading to the *d*-wave pairing state, it is necessary to construct preliminarily an effective low-energy Hamiltonian for the periodic Anderson model in the limit of large but yet finite Coulomb repulsion *U*. Recently, we obtained [34] such a Hamiltonian in the regime of mixed valence.

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