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On the *s*-Type Superconductivity in Heavy-Fermion Compounds

V. V. Val'kov[a–c] and D. M. Dzebisashvili[a, c]

[a] *Kirenskiĭ Institute of Physics, Siberian Division, Russian Academy of Sciences, Akademgorodok, Krasnoyarsk, 660036 Russia*

[b] *Krasnoyarsk State University, Krasnoyarsk, 660075 Russia*

[c] *Krasnoyarsk State Technical University, Krasnoyarsk, 660074 Russia*

e-mail: vvv@iph.krasn.ru

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The amplitude of scattering of *f* electrons has been calculated for the periodic Anderson model in the strong-correlation limit ($U = \infty$) in the Cooper channel. From the condition of the existence of a pole of this amplitude, an equation is derived for determining the critical temperature (T_c) of the transition to the superconducting phase with the *s* symmetry of the order parameter. The temperature T_c as a function of the electron density and hybridization parameter has been calculated by self-consistently solving the system of equations. The region of the existence of the superconducting phase is found to adjoin the region of the existence of the unsaturated ferromagnetic state and does not overlap it. The results can be used to describe the transition to the superconducting phase with the *s* symmetry of the order parameter in heavy-fermion skutterudite $LaFe_4P_{12}$. In this case, the inclusion of the scattering of fermions by spin fluctuations turns out to be substantial enough to obtain T_c values close to the experimental data.

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It is known that compounds with heavy fermions have superconducting properties differing from the properties predicted by the BCS theory. In particular, superconductivity with an anisotropic order parameter is realized in $CeCu_2Si_2$, UBe_{13}, and UPt_3. To explain these features, it was suggested that the contribution of the spin-fluctuation mechanism of Cooper instability is important. At the same time, recent experiments with heavy-fermion skutterudite $LaFe_4P_{12}$ [1], which is a superconductor for $T < T_C = 4.1$ K, lead to the conclusion that the *s* symmetry of the order parameter is preferable. Such data stimulate works concerning analysis of the electron–phonon mechanism of Cooper pairing that leads to *s*-type superconductivity (see, e.g., [2]). At the same time, it is of current interest to examine such a mechanism of Cooper instability in the Anderson model that takes into account spin-fluctuation scattering and leads to the *s*-type superconductivity. This is the aim of our work.

Heavy-fermion compounds are usually described in the framework of the Anderson periodic model. In this case, the auxiliary-boson method is often used: the Hubbard operators are represented in the form of the product of the Fermi operator and spinless bosom operator. An advantage of such a representation is the possibility of applying the Feynman technique to calculate Green's functions, and a demerit of this representation is the necessity of introducing a constraint. The necessity of eliminating contributions from nonphysical states is a source of difficulties in developing the theory in the framework of the mentioned approach.

In this work, the Cooper instability is analyzed for the Anderson periodic model in the strong electron correlation regime in the atomic representation. To calculate the scattering amplitude, we apply the diagram technique for the Hubbard operators [3, 4]. An exact representation obtained in this work for the Matsubara Green's function of *f* electrons makes it possible to reveal the meaning of renormalization constants appearing when the slave boson representation is used and to demonstrate its limitation.

The Hamiltonian of the Anderson periodic model in the strong electron correlation regime can be represented in the form

$$H = \sum_{\mathbf{k}\sigma}(\varepsilon_{\mathbf{k}} - \mu)c^+_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + \sum_{f\sigma}(E_0 - \mu)X_f^{\sigma\sigma} + \frac{1}{\sqrt{N}}\sum_{\mathbf{k}f\sigma}(V_{\mathbf{k}}e^{-i\mathbf{k}\mathbf{R}_f}c^+_{\mathbf{k}\sigma}X_f^{0\sigma} + \text{H.c.}), \quad (1)$$

where the first term describes the subsystem of itinerant electrons with the dispersion law $\varepsilon_{\mathbf{k}}$, $c^+_{\mathbf{k}\sigma}$ ($c_{\mathbf{k}\sigma}$) is the creation (annihilation) operator of the electron in the state with the quasimomentum $\mathbf{k}$ and the spin moment

projection σ, the second term in Eq. (1) describes the presence of the subsystem of localized electrons with the energy E_0 and chemical potential μ, and the last term of Hamiltonian (1) presents the hybridization of localized and itinerant states with the hybridization interaction parameter $V_{\mathbf{k}}$. The Hubbard operators $X^{mn} = |m\rangle\langle n|$ are constructed on the basis of three single-site states: the electron-free state $\{|m\rangle\}$: $|0\rangle$ and two states $|\sigma\rangle$ with the spin moment projections $\sigma = \pm 1/2$. In the limit of infinitely strong Coulomb repulsion, states with two electrons at one node $|2\rangle$ are forbidden.

To examine the Cooper instability in the Anderson periodic model, we introduce the Matsubara Green's function for the itinerant and localized electrons

$$G_{\mathbf{k}\sigma}(\tau - \tau') = -\langle T_\tau \tilde{c}_{\mathbf{k}\sigma}(\tau)\tilde{c}^+_{\mathbf{k}\sigma}(\tau')\rangle,$$
$$D_{\alpha\beta}(f\tau; g\tau') = -\langle T_\tau \tilde{X}^\alpha_f(\tau)\tilde{X}^{-\beta}_g(\tau')\rangle. \quad (2)$$

In these expressions, the standard notation is used [3–5].

Analysis of the diagram series for the Green's function of f electrons shows that, after the pairing of all c operators in each order of perturbation theory, a diagram representation appears which is formally similar to the representation for the Hubbard model in terms of the effective Matsubara-frequency-dependent Fourier transform of the hopping integral:

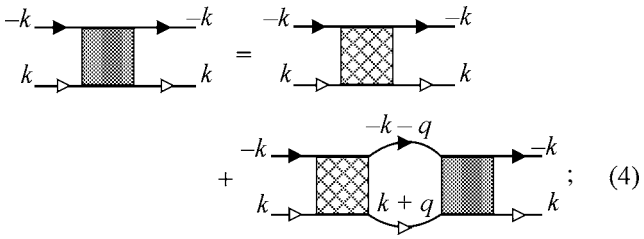
$$\tilde{t}_{\mathbf{k}}(\omega_n) = |V_{\mathbf{k}}|^2 G^{(0)}_{\mathbf{k}}(\omega_n) = |V_{\mathbf{k}}|^2 (i\omega_n - \xi_{\mathbf{k}})^{-1}, \quad (3)$$

where $\xi_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - \mu$. Such exact rearrangement is possible because the hybridization interaction operator is linear in the Fermi operators $c_{\mathbf{k}\sigma}$ and $c^+_{\mathbf{k}\sigma}$.

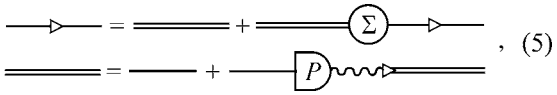
A qualitatively similar reduction of the diagram series for the electron Green's function is possible for the case of electron–phonon interaction [5]. In this case, the diagram series corresponding to the effective frequency-dependent fermion–fermion interaction appears. A feature of the case under consideration is that the introduction of the effective interaction is possible, because the interaction operator is linear with respect to the Fermi operators rather than to the Bose operator, as for the electron–phonon interaction.

The extension of the above analogy leads to the conclusion that the effective interaction (through the additional Fermi subsystem) appears in the subsystem of the f electrons such as the indirect interaction through the phonon subsystem appears. In this case, this effective interaction under certain conditions can be expected to be a source of Cooper instability. To analyze this problem, we consider the collision of the f electrons with the opposite projections of spin moments in the paraphase.

The solution of the problem of the Cooper instability is reduced to the determination of the conditions under which a pole appears in the scattering amplitude of the f electrons with the opposite projections of the spin moments. The equation for this amplitude can be represented in the diagram form



here, the dark squares correspond to the desired amplitude $\Gamma(k; -k|k; -k)$ [$\Gamma(k + q; -k - q|k; -k)$ in the right-hand side of the equation], and k and q are the 4-vectors $k = (\mathbf{k}, i\omega_n)$ and $q = (\mathbf{q}, i\omega_m)$, and respectively, with $\omega_n = (2n + 1)\pi T$ and $\omega_m = 2m\pi T$, where n and $m = 0, \pm 1, \pm 2, \ldots$. The bare amplitude $\Gamma^{(0)}(k; -k|k + q; -k - q)$ [the first term of Eq. (4) for $q = 0$] is shown by the light square. The line with a light (dark) arrow denotes the Green's function $G(k)$ of f electrons with the spin-moment projection $\sigma = +1/2$ ($\sigma = -1/2$). The equation for the function $G(k)$ with the inclusion of the above rearrangement of the diagram series has the form



, (5)

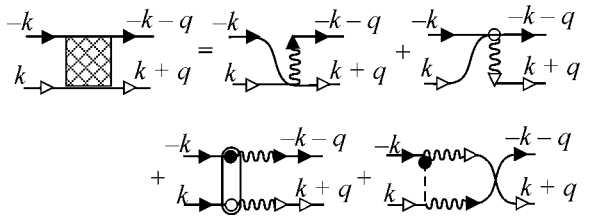
where the double solid line corresponds to the collective Green's function $G^{(0)}(k)$ and the thin solid line stands for the bare propagator $G_0(\omega_n) = (i\omega_n - E_0 + \mu)^{-1}$. The light circle with Σ inside corresponds to the operator $\Sigma(k)$ and the semicircle means the force operator $P(k)$. The wavy line stands for the effective interaction $\tilde{t}_{\mathbf{k}}(\omega_n)$ defined in Eq. (3).

Solving system of Eqs. (5), we obtain the following representation for the function $G(k)$:

$$G(k) = \frac{i\omega_n - \xi_{\mathbf{k}}}{(i\omega_n - E_0 + \mu - \Sigma(k))(i\omega_n - \xi_{\mathbf{k}}) - P(k)|V_{\mathbf{k}}|^2},$$

which contains the force operator $P(k)$ in addition to the mass operator. This operator affects the spectral characteristics and renormalization of the hybridized constant. It follows from the representation obtained for $G(k)$ that the salve-boson approximation appears if the frequency dependence of the renormalization factor, as well as its imaginary component, is disregarded. Since the last factors are significant according to the analysis, the use of the simplest approximations in the slave-boson approach significantly distorts the real physics.

Taking into account scattering by spin fluctuations, we conclude that the bare amplitude is determined by the diagrams



(6)

and can be analytically written in the form

$$\Gamma^{(0)}(k;\ -k|k+q;\ -k-q) = \frac{|V_{\mathbf{k}+\mathbf{q}}|^2}{(\omega_n+\omega_m)^2+\xi^2_{\mathbf{k}+\mathbf{q}}} \quad (7)$$

$$\times\{2\xi_{\mathbf{k}+\mathbf{q}}+|V_{\mathbf{k}+\mathbf{q}}|^2[\tilde{\chi}\delta(\omega_m)+2\chi\delta(2\omega_n+\omega_m)]\}.$$

Here, χ is the magnetic susceptibility of the system, $\tilde{\chi} = \chi - C_n/4T$, and $C_n = \langle\Delta\hat{n}_f\Delta\hat{n}_f\rangle$ is the density–density correlation function. The appearance of χ and C_n is caused by the inclusion of the relaxation on spin and charge fluctuations [6].

Taking into account Eq. (7) for the bare amplitude, it is easy to check that the total scattering amplitude $\Gamma(k+q;\ -k-q|k;\ -k)$ is independent of the quasi-momentum $\mathbf{q}$ but depends on ω_m. This property allows one to reduce the determination of the desired amplitude $\Gamma_\omega(\mathbf{k}) \equiv \Gamma(k; -k|k; -k)$ to the solution of the system of equations

$$\begin{aligned}
&[1-T\tilde{\chi}\Phi_2(\omega)]\Gamma_\omega(\mathbf{k}) - 2T\chi\Phi_2(\omega)\tilde{\Gamma}_\omega(\mathbf{k})\\
&\quad - T\sum_\omega \Phi_1(\omega)\Gamma_\omega(\mathbf{k}) = \Gamma^{(0)}_\omega(\mathbf{k}),\\
&[1-T\tilde{\chi}\Phi_2(\omega)]\tilde{\Gamma}_\omega(\mathbf{k}) - 2T\chi\Phi_2(\omega)\Gamma_\omega(\mathbf{k})\\
&\quad - T\sum_\omega \Phi_1(\omega)\Gamma_\omega(\mathbf{k}) = \tilde{\Gamma}^{(0)}_\omega(\mathbf{k}),
\end{aligned} \quad (8)$$

where

$$\begin{aligned}
\tilde{\Gamma}_\omega(\mathbf{k}) &= \Gamma(\tilde{k};\ -\tilde{k}|k;\ -k), \quad \tilde{k} = (\mathbf{k}, -i\omega_n),\\
\Gamma^{(0)}_\omega(\mathbf{k}) &= \Gamma^{(0)}(k;\ -k|k;\ -k),\\
\tilde{\Gamma}^{(0)}_\omega(\mathbf{k}) &= \Gamma^{(0)}(\tilde{k};\ -\tilde{k}|k;\ -k),
\end{aligned} \quad (9)$$

$$\Phi_1(\omega) = \frac{1}{N}\sum_{\mathbf{q}} 2\xi_{\mathbf{q}} l(q), \quad \Phi_2(\omega) = \frac{1}{N}\sum_{\mathbf{q}} |V_{\mathbf{q}}|^2 l(q),$$

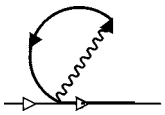
$$l(q) = \frac{|V_{\mathbf{q}}|^2}{\left|(i\omega-\xi_{\mathbf{q}})(i\omega-E_0-\Sigma+\mu)-P(\omega)|V_{\mathbf{q}}|^2\right|^2}.$$

Calculating the scattering amplitude $\Gamma_\omega(\mathbf{k})$ from the system of Eqs. (8) and determining its pole, we arrive at the following equation for the transition temperature to the superconducting phase with the *s* symmetry of the order parameter ($\alpha = 3\chi T - C_n/4$):

$$1 + T\sum_\omega \Phi_1(\omega)/[1+\alpha\Phi_2(\omega)] = 0. \quad (10)$$

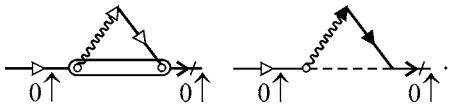
The analytical summation over the Matsubara frequencies in this equation can be performed only for $\alpha = 0$. For finite α values, the summation was performed numerically. Since α depends on the magnetic susceptibility, this quantity is used in the theory to include scattering on the spin degrees of freedom of the system under consideration. This procedure of the inclusion of relaxation processes was considered in [6], where high-temperature superconductors were described.

In numerical calculations, $G(k)$ is found self-consistently. In the one-loop approximation, the mass operator $\Sigma_{0\sigma,\,0\sigma}$ is described by one diagram



(11)

and the correction to the force operator $\delta P_{0\sigma,\,0\sigma}$ is described by two diagrams



(12)

Using the diagram technique, we arrive at the analytical expressions

$$\Sigma_{0\sigma,\,0\sigma} = -\frac{T}{N}\sum_{\mathbf{q},\,\omega_m} |V_{\mathbf{q}}|^2 G^{(0)}_{\mathbf{q}}(\omega_m) G(\mathbf{q},\omega_m) \quad (13)$$

for $\Sigma_{0\sigma,\,0\sigma}$ and

$$\delta P_{0\sigma,\,0\sigma}(\omega_n) = \beta\frac{1}{N}\sum_{\mathbf{q}} |V_{\mathbf{q}}|^2 G^{(0)}_{\mathbf{q}}(\omega_n) G(\mathbf{q},\omega_n) \quad (14)$$

for $\delta P_{0\sigma,\,0\sigma}(\omega_n)$, where $\beta = 3\chi T + C_n/4$. We note that the force operator is a function of the Matsubara frequency, whereas the mass operator is an uncertain constant leading to the shift of the localized level. These features are used to write expression (9) for $l(q)$.

Taking into account Eqs. (13) and (14), the infinite self-consistency system of equations for determining the chemical potential, mass operator, number of localized electrons, and force-operator correction $\delta P_{0\sigma,\,0\sigma}(\omega_n)$ is written. The numerical solution of this system makes it possible to calculate the dependence of the transition temperature on the superconducting phase with the *s*-type symmetry of the order parameter. The calculated T_c values are shown in two figures as functions of the concentration for various values of the hybridization parameter.

The calculations are performed under the assumption that the bare electron band is characterized by the

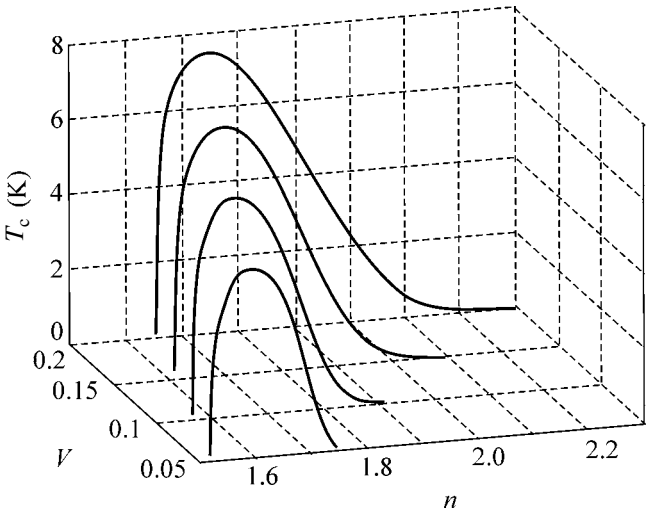


Fig. 1. Superconducting transition temperature in the Anderson periodic model with the inclusion of the spin-fluctuation scattering processes.

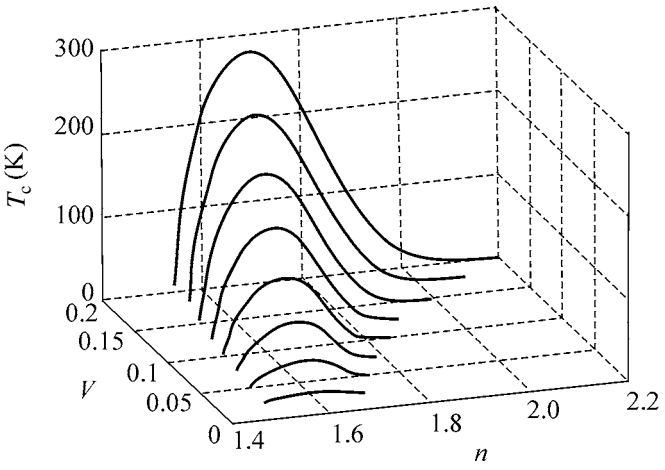


Fig. 2. Superconducting transition temperature in the Anderson periodic model disregarding the spin-fluctuation scattering processes.

semi-elliptic density of states $g(\varepsilon) = (8/\pi W^2)\sqrt{(W/2)^2 - \varepsilon^2}$. All the energy parameters of the system are measured in the bare band width W. The position of the localized level corresponds to the middle of the band. The magnetic susceptibility in the calculations is taken to be equal to the susceptibility of heavy-fermion compounds, i.e., is more than two orders of magnitude larger than the characteristic values of the Pauli susceptibility for usual metals. As seen in Fig. 1, when the spin-fluctuation scattering processes are taken into account, a change in the hybridization parameter in the range of 0.05–0.2 does not lead to a significant increase in the critical temperature.

The situation is different if relaxation processes are disregarded. The calculations show that the critical temperature in this case increases significantly in the mentioned region of the parameter V. The corresponding behavior is shown in Fig. 2.

The results presented for the Cooper instability raise the question of the mutual location of the regions of various phases. The conditions of the existence of the far-range magnetic order in the one-impurity model were revealed by Anderson. For the Anderson periodic model, the region of the existance of the ferromagnetic order that was recently determined by Izyumov et al. [7] is shown in Fig. 3. The abbreviations FM, SF, and P are used for the ferromagnetic phase, saturated ferromagnetic state, and paramagnetic phase, respectively. Small numerical differences in the shape of the boundaries of the SF and FM regions exist only because the ratio of the energy parameters V and E_0 to the bandwidth in our analysis is taken to be one fourth of that taken in [7]. To calculate the boundary of the superconducting-phase boundary, we use Eq. (10). In the low-temperature limit, the contributions from scattering by spin fluctuations can be disregarded. In this case, the summation over the Matsubara frequencies can be performed in the explicit form. As a result, we obtain

$$1 = \frac{1}{N}\sum_{q} \frac{|V_{\mathbf{q}}|^2 \xi_{\mathbf{q}} \left\{ \frac{\tanh(\tilde{E}_{\mathbf{q}}^{+}/2T_c)}{\tilde{E}_{\mathbf{q}}^{+}} - \frac{\tanh(\tilde{E}_{\mathbf{q}}^{-}/2T_c)}{\tilde{E}_{\mathbf{q}}^{-}} \right\}}{(\tilde{E}_{\mathbf{q}}^{+})^2 - (\tilde{E}_{\mathbf{q}}^{-})^2}, \quad (15)$$

where $\tilde{E}_{\mathbf{q}}^{\pm} = (\varepsilon_{\mathbf{q}} + E_0 + \Sigma)/2 \pm \nu_{\mathbf{q}}/2 - \mu$, $\nu_{\mathbf{q}} = \{(\varepsilon_{\mathbf{q}} - E_0 - \Sigma)^2 + 4(1 - n_d/2)|V_{\mathbf{q}}|^2\}^{1/2}$, and n_d is the number of the localized electrons per one site. The boundary of the superconducting-phase region that is obtained by analyzing this equation adjoins the ferromagnetic-phase

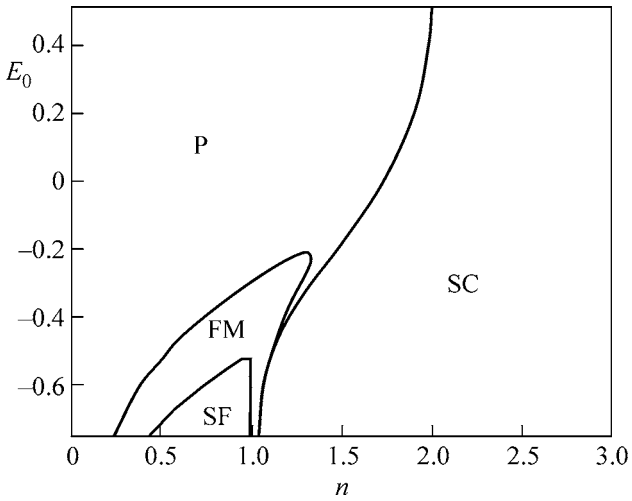


Fig. 3. Phase diagram of the Anderson periodic model for $V = 0.125$.

boundary and does not intersect it (Fig. 3). Nonintersection is important in view of the competition between the magnetic and superconducting phases and is consistent with the general conception of antagonism between the superconductivity and magnetism.

We note that the superconducting phase exists only when the upper hybridized band is filled. This result easily follows from Eq. (15). Indeed, if the chemical potential is in the lower band, the main contribution to the integral comes from the region where $\tilde{E}_{\mathbf{q}}^{-} = 0$. In this case, the integral is negative and Eq. (15) has no solution. If the chemical potential μ is in the upper band, the principal positive integral value is collected near the point $\tilde{E}_{\mathbf{q}}^{+} = 0$. In this case, a solution always exists according to numerical calculations.

According to the above results, the analysis of the Anderson periodic model by the diagram technique for the Hubbard operators can be reduced to the analysis of the properties of the Hubbard model for strongly correlated f electrons with the effective interaction $\tilde{t}_{\mathbf{k}}(\omega_n)$ depending on the Matsubara frequency. A similar conclusion was drawn previously in [7], where the normal phase of the Anderson periodic model is analyzed by the generating functional method. In view of these facts, it is easy to understand that the mechanism of the Cooper instability in the Anderson periodic model is similar to the kinematic mechanism leading to s pairing in the Hubbard model in the strong electron correlation regime [8].

In summary, we note that the spin-fluctuation scattering processes are important for describing the superconducting phase of heavy-fermion compounds in the Anderson periodic model. In this work, we examined the effect of these processes only on the superconductivity with the s symmetry of the order parameter, because, according to [1], this order parameter of the superconducting phase is realized in the heavy-fermion skutterudite $CeFe_4P_{12}$.

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