Influence of *f*-levels on the critical temperature of transition metals

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(Submitted March 11, 1975)
Zh. Eksp. Teor. Fiz. **69**, 688–694 (August 1975)

An expression is found for the critical temperature in a regular system of hybridized *sf*-electrons with strong intra-atomic correlation U that is taken into account exactly. It is shown that when there is a localized level ϵ_1 positioned below the Fermi level ϵ_F there is an effective attraction between the *s*-electrons via the *f*-level, which is accompanied, however, by scattering of the effective-exchange type, which hinders the formation of Cooper pairs. The condition for the existence of superconductivity is changed in comparison with that in the molecular-field approximation and is found to be substantially asymmetric with respect to the position of ϵ_1 relative to ϵ_F. The results obtained correspond to the appearance of superconductivity in Ce when it undergoes the α-α' phase transition under pressure.

PACS numbers: 74.10.+v

As is well-known, in the treatment of Cooper pairing in transition metals it is necessary to take into account the interaction of the conduction electrons (s-electrons) with the strongly localized electrons of unfilled shells (f-electrons)[1-5]. Of special interest is the case when a narrow band or a slightly broadened f-electron level is situated near the Fermi surface; this case, apparently, is realized in U and La, and also in Ce under pressure. In this case it is important to take into account the sf-hybridization interaction, which leads to the admixture of a certain proportion of f-states into the s-electrons at the Fermi surface. An important role is also played by the Coulomb repulsion between localized electrons at the same site. This repulsion is usually treated in the molecular-field approximation. In this case, owing to the hydridization, there arises an additional repulsion between the conduction electrons, which hinders the Cooper pairing[4, 5].

In the present paper it is shown that the situation is substantially altered in the case when the Coulomb interaction is strong and the Hartree-Fock approximation is inapplicable inasmuch as the Hubbard splitting of the localized levels cannot be correctly taken into account in it. We shall take the strong correlation of the f-electrons into account exactly, treat the hybridization interaction as a perturbation and analyze the cases of strong and weak hybridization, when the levels of the localized electrons are positioned both above and below the Fermi surface (only the paramagnetic case is considered).

The elementary excitations in the subsystem of localized electrons are the charge (and spin) density fluctuations at the sites. A result of the motion of the s-electrons is the "polarization" of the intrinsic degrees of freedom of the f-states, and the interaction of the conduction electrons via the localized electron states can lead to an additional effective attraction in the framework of the hybridization Hamiltonian, even when the mechanisms associated with the sf Coulomb and exchange interactions are not taken into account[6, 7]. However, as will be shown below, in the case when such attraction arises it is accompanied by scattering of the conduction electrons by the localized f-electrons, this scattering having the character of effective exchange. The latter mechanism decreases the electron-phonon interaction constant, in the same way as paramagnetic impurities hinder Cooper pairing in normal metals[8], and the additional attraction turns out to be insufficient to compensate this decrease.

We shall take the Hamiltonian of the system in the form

$$H=H_s+H_f+H_{sf}+H_{ss},\qquad H_s=\sum_{\mathbf{k}\sigma}\varepsilon_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}{}^+c_{\mathbf{k}\sigma},$$

$$H_f=\sum_{\mathbf{m}\sigma}(\varepsilon_1 n_{\mathbf{m}\sigma}+{}^1/_2 U n_{\mathbf{m}\sigma}n_{\mathbf{m}-\sigma})=\varepsilon_1\sum_{\mathbf{m}\sigma}Z_{\mathbf{m}}{}^{\sigma\sigma}+\varepsilon_2\sum_{\mathbf{m}}Z_{\mathbf{m}}{}^{22}$$

$$H_{sf}=gN^{-1/2}\sum_{\mathbf{k}\sigma\mathbf{m}}(e^{-i\mathbf{k}\mathbf{m}}c_{\mathbf{k}\sigma}{}^+a_{\mathbf{m}\sigma}+\text{h. c.})$$

$$=gN^{-1/2}\sum_{\mathbf{k}\sigma\mathbf{m}}[e^{-i\mathbf{k}\mathbf{m}}c_{\mathbf{k}\sigma}{}^+(Z_{\mathbf{m}}{}^{0\sigma}+2\sigma Z_{\mathbf{m}}{}^{-\sigma2})+\text{h. c}],\tag{1}$$

$$H_{ss}=-{}^1/_2\lambda\sum_{\mathbf{k}\mathbf{k}'\sigma}c_{\mathbf{k}\sigma}{}^+c_{-\mathbf{k}-\sigma}^+c_{-\mathbf{k}'-\sigma}c_{\mathbf{k}'\sigma},$$

$$n_{\mathbf{m}\sigma}=a_{\mathbf{m}\sigma}{}^+a_{\mathbf{m}\sigma},\quad \varepsilon_2=2\varepsilon_1+U,\quad \sigma=\pm{}^1/_2.$$

Here $c_{\mathbf{k}\sigma}$ and $a_{\mathbf{m}\sigma}$ are the second-quantization operators of the s- and f-electrons, **m** is the coordinate of a lattice site, g is the sf-hybridization constant, U is the parameter of the intra-atomic Coulomb interaction of the f-electrons, which is assumed to be the largest energy in the system; H_s is the Hamiltonian of the s-electrons, which we describe by one broad conduction band, H_f is the zeroth-order Hamiltonian of the localized f-electrons, including their strong correlation at the same site. We assume that f-electrons belonging to different sites do not interact, and neglect their degeneracy with respect to the components of the orbital angular momentum. H_{ss} describes, in the framework of the BCS theory, the attraction of the s-electrons that is due to the phonons ($\lambda > 0$), and the summation in this term is restricted to the energy region of width $2\omega_0$ about the Fermi surface.

For convenience in taking the interaction U into account in the zeroth approximation, in H_f and H_{sf} we have changed to the second-quantization operators of the eigenstates of the f-shells[9]:

$$Z_{\mathbf{m}}{}^{\sigma0}=a_{\mathbf{m}\sigma}{}^+(1-n_{\mathbf{m}-\sigma}),\quad Z_{\mathbf{m}}^{2-\sigma}=2\sigma a_{\mathbf{m}\sigma}{}^+n_{\mathbf{m}-\sigma},\quad Z_{\mathbf{m}}{}^{22}=n_{\mathbf{m}\sigma}n_{\mathbf{m}-\sigma},$$
$$Z_{\mathbf{m}}{}^{\sigma\sigma}=n_{\mathbf{m}\sigma}(1-n_{\mathbf{m}-\sigma}),\quad Z_{\mathbf{m}}{}^{00}=(1-n_{\mathbf{m}\sigma})(1-n_{\mathbf{m}-\sigma}),\tag{2}$$
$$Z_{\mathbf{m}}^{\lambda_1\lambda_2}Z_{\mathbf{m}}^{\lambda_3\lambda_4}=Z_{\mathbf{m}}^{\lambda_1\lambda_4}\delta_{\lambda_2\lambda_3},\quad \lambda=0,\sigma,2.$$

Two positions of the Fermi surface relative to the one-electron levels ϵ_1 and $\epsilon_f = \epsilon_1 + U$ (below, all energies are reckoned from the Fermi energy ϵ_F) are of interest: ϵ_F lies near ϵ_1, or near ϵ_f. Then, owing to the large value of U, in H_{sf} we may consider, respectively, only the transitions $|0) \rightarrow |\sigma)$, keeping the terms with

$Z_m^{\sigma 0}$ and $Z_m^{0\sigma}$, or only the transitions $|\sigma) \longleftrightarrow |2)$, keeping the terms $Z_m^{2\sigma}$ and $Z_m^{\sigma 2}$. We shall discuss the first case, and the results for the second case can be obtained in an analogous manner.

We shall seek, as usual[10], an expression for the s-electron vertex part $\Gamma_{\alpha\beta,\nu\delta}(p_1, p_{1'}; p_2, p_{2'})$ $(p = \mathbf{k},\omega)$ of the two-particle Matsubara Green function G^{II} for $p_1 + p_{1'} = 0$. The first nonzero term $\Gamma^{(1)}(p_1, p_2)$ of the perturbation-theory series in g, λ is equal to

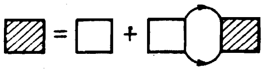
$$\begin{gathered}\Gamma^{(1)}(p_1, p_2)=\gamma^s+\gamma^f,\ \gamma^s=-\lambda,\ \gamma^f=\gamma_1+\gamma_2,\\ \gamma_1(p_1, p_2)=2\varepsilon_1 Kg^4\varphi_1\varphi_2,\ \gamma_2(p_1, p_2)=\beta Ag^4\varphi_1\Delta_{12},\\ K=P_\sigma+P_0,\ A=P_\sigma-P_0+K^2,\ \varphi_i=(\omega_i^2+\varepsilon_1^2)^{-1},\ \Delta_{12}=\delta(\omega_1-\omega_2),\ \beta=T^{-1}\end{gathered} \tag{3}$$

Here we have omitted the spin indices corresponding to the singlet interaction, and also the conservation laws for the quasi-momenta and frequencies. The term γ^s corresponds to the H_{ss}-interaction and γ^f to the H_{sf}-interaction. This term appears only in fourth order in g. The calculation of γ^f contains certain specific features arising from the non-Fermi commutation relations for the Z-operators (2). The details of this calculation are given in the Appendix. The quantity P_σ is the probability that there is an f-electron with spin σ at the site, and P_0 is the probability that there is no f-electron:

$$\begin{gathered}P_\sigma=\langle Z_m^{\sigma\sigma}\rangle_f=(2+e^{\beta\varepsilon_1})^{-1},\ P_0=\langle Z_m^{00}\rangle_f=(1+2e^{-\beta\varepsilon_1})^{-1},\\ \langle\ldots\rangle_f=\mathrm{Sp}\, e^{-\beta H_f}(\ldots).\end{gathered} \tag{4}$$

First of all we note that the vertex γ_2 is nonzero only for $\omega_1 = \omega_2$, while the vertex γ_1 changes sign on change of the sign of ϵ_1 and, for $\epsilon_1 < 0$, the interaction described by it corresponds to the effective attraction of the s-electrons via an f-level that was discussed above.

The problem of calculating Γ reduces formally to the BCS case, where the leading approximation is the ladder approximation[10]:



(5)

Here the shaded and unshaded squares correspond to Γ and $\Gamma^{(1)}$ respectively, and the thin lines to the zeroth-order s-electron Green function $G_{\mathbf{k}\sigma}^{(0)}(\omega)$. In our case, however, because γ_2 is diagonal in ω_1 and ω_2, the graph (5) corresponds to a system of two equations for the diagonal and nondiagonal parts of Γ. Because of the factorization of $\Gamma^{(1)}$ in ω_1 and ω_2, the system (5) can be solved exactly. The condition for the existence of a pole of Γ corresponds to the vanishing of the determinant

$$\begin{vmatrix} 1-a_{ss} & a_{sf} \\ a_{fs} & 1-a_{ff} \end{vmatrix}=0, \tag{6}$$

where

$$\begin{gathered}a_{ss}=\lambda\beta^{-1}\sum_{\omega,|\omega|<\omega_0} B^{(0)}(\omega)R^{-1}(\omega),\quad a_{ff}=-2\varepsilon_1 Kg^4\beta^{-1}\sum_{\omega}\varphi^2(\omega)B^{(0)}(\omega)R^{-1}(\omega),\\ a_{sf}a_{fs}=-2\varepsilon_1 Kg^4\lambda\left(\beta^{-1}\sum_{\omega,|\omega|<\omega_0}\varphi(\omega)B^{(0)}(\omega)R^{-1}(\omega)\right)^2, \qquad (7)\\ B^{(0)}(\omega)=\sum_{\mathbf{k}}G_{\mathbf{k}}^{(0)}(\omega)G_{-\mathbf{k}}^{(0)}(-\omega)=\rho\pi|\omega|^{-1},\quad R(\omega)=1+Ag^4\varphi(\omega)B^{(0)}(\omega).\end{gathered}$$

We emphasize that the appearance of the denominator $R(\omega)$ in the expressions (7) is due entirely to taking processes that are diagonal in ω_1 and ω_2, i.e., the vertex γ_2, into account.

Before analyzing (6) and (7), we shall discuss what is altered by complicating the vertex part γ^f and the s-lines. Complicating γ^f can lead only to a renormalization of the atomic level ϵ_1, and we shall assume that this has been performed at the outset. It is more important to consider the influence of hybridization effects. To take this influence into account it is sufficient to replace the zeroth-order s-electron Green function in (5) by[11]

$$G_{\mathbf{k}}=\frac{i\omega-\varepsilon_1}{(i\omega-\varepsilon_k)(i\omega-\varepsilon_1)-Kg^2}. \tag{8}$$

This leads to a change in the density of states of the s-electrons near the Fermi surface and to the replacement of $B^{(0)}(\omega)$ in (7) by $B(\omega)$:

$$\rho(E)=\rho\frac{\varepsilon_1^2-E^2}{\varepsilon_1^2-E^2+Kg^2}\qquad B(\omega)=\frac{\pi\rho(\omega^2+\varepsilon_1^2)}{|\omega|(\omega^2+\varepsilon_1^2+Kg^2)}. \tag{9}$$

In obtaining (9) we have assumed that $\rho g^2 < |\epsilon_1|$, and we shall assume that this condition is fulfilled everywhere below.

With (9) taken into account, the expressions (7) finally have the form

$$\begin{gathered}a_{ss}=\rho\lambda\pi\beta^{-1}\sum_{\omega,|\omega|<\omega_0}\frac{\omega^2+\varepsilon_1^2}{(\omega^2+\varepsilon_1^2+Kg^2)(|\omega|+2\pi T_s)},\\ a_{ff}=-2\rho g^4\varepsilon_1 K\pi\beta^{-1}\sum_{\omega}[(\omega^2+\varepsilon_1^2+Kg^2)(\varepsilon_1^2+\omega^2)(|\omega|+2\pi T_s)]^{-1},\\ a_{sf}a_{fs}=(-2\rho g^4\varepsilon_1 K)\rho\lambda\left\{\pi\beta^{-1}\sum_{\omega,|\omega|<\omega_0}[(\omega^2+\varepsilon_1^2+Kg^2)(|\omega|+2\pi T_s)]^{-1}\right\}^2,\\ T_s=A\rho g^4/2(\varepsilon_1^2+Kg^2).\end{gathered} \tag{10}$$

In the expression for T_s we have omitted the $|\omega|^2$ appearing with $\epsilon_1^2 + Kg^2$, bearing in mind that the principal contribution to the sums is given by the region of small $|\omega|$.

We shall consider the case of weak hybridization ($|\epsilon_1| > g$). It is easy to see that in this case we can neglect the off-diagonal elements of the determinant (6). Then the critical temperature T_c is determined by the equation

$$a_{ss}=\rho\lambda\frac{\varepsilon_1^2}{\varepsilon_1^2+Kg^2}\ln\frac{\omega_0+T_s}{T_c+T_s}=1. \tag{11}$$

If the localized level ϵ_1 lies above the Fermi surface ($\epsilon_1 > 0$, $P_\sigma = 0$, $P_0 = 1$, $T_s = 0$), the role of the sf-interaction reduces to an effective decrease of the electron-phonon interaction constant: $\lambda_{eff} = \lambda\epsilon_1^2/(\epsilon_1^2 + g^2)$. The constant λ_{eff} is distinguished by the absence of the additional repulsion that arises in the molecular-field approximation (cf. formula (14) of the paper by Kocharyan and Khomskiĭ[5])[1)], so that exact allowance for the Coulomb interaction appreciably alters the expression for T_c.

When the level ϵ_1 lies below the Fermi surface ($\epsilon_1 < 0$, $P_\sigma = 1/2$, $P_0 = 0$, $T_s = 3/4\rho g^4/(2\epsilon_1^2 + g^2)$), Eq. (11) is soluble only under the condition $\epsilon_1^2 > \rho g^4/T_{c0}$, $T_{c0} \approx \omega_0 e^{-1/\rho\lambda}$. For low values of $|\epsilon_1|$ Cooper pairing is impossible at any temperature. The appearance, for $\epsilon_1 < 0$, of a mechanism hindering Cooper pairing ($T_s \neq 0$) resembles, in its physical meaning, the situation with paramagnetic impurities in a normal metal, considered by Abrikosov and Gor'kov[8]: in second order of perturbation theory in g there are terms corresponding to effective sf-exchange, which hinder the appearance of singlet Cooper pairs. For $\epsilon_1 > 0$ and $P_\sigma = 0$ this scattering channel, associated with the vertex γ_2, disappears. In our case T_s plays the same role as the inverse relaxation time τ_s^{-1} of conduction electrons interacting with an impurity subsystem[8].

It is possible to see this by representing H_{sf} from (1) in the form of an effective Hamiltonian of second order in g[12]:

$$\tilde{H}=-N^{-1}\sum_{\substack{\mathbf{kk}'\\ \sigma\sigma'}}\sum_{\mathbf{m}} J_{\mathbf{kk}'}e^{-i(\mathbf{k}-\mathbf{k}')\mathbf{m}}Z_{\mathbf{m}}^{\sigma'\sigma}c_{\mathbf{k}\sigma}^{+}c_{\mathbf{k}'\sigma'}$$

$$+N^{-1}\sum_{\mathbf{mm}'}\sum_{\mathbf{k}\sigma} J_{\mathbf{kk}}e^{ik(\mathbf{m}-\mathbf{m}')}Z_{\mathbf{m}}^{\sigma 0}Z_{\mathbf{m}'}^{0\sigma}, \tag{12}$$

$$J_{\mathbf{kk}'}=-\frac{g^2}{2}\left(\frac{1}{\varepsilon_k-\varepsilon_1}+\frac{1}{\varepsilon_{k'}-\varepsilon_1}\right).$$

We separate out from this Hamiltonian the part $\tilde{H}_{sf}$ corresponding to the effective sf-exchange interaction. For $\epsilon_1 < 0$, $P_0 = 0$,

$$Z_{\mathbf{m}}^{+-}=S_{\mathbf{m}}^{+},\quad Z_{\mathbf{m}}^{-+}=S_{\mathbf{m}}^{-},\quad Z_{\mathbf{m}}^{\sigma\sigma}=1/2+2\sigma S_{\mathbf{m}}^{z},$$

$$\tilde{H}_{sf}=-2N^{-1}\sum_{\substack{\mathbf{kk}'\\ \sigma\sigma'}}\sum_{\mathbf{m}} J_{\mathbf{kk}'}e^{-i(\mathbf{k}-\mathbf{k}')\mathbf{m}}\mathbf{S}_{\mathbf{m}}(\mathbf{s})_{\sigma\sigma'}c_{\mathbf{k}\sigma}^{+}c_{\mathbf{k}'\sigma'}.$$

We now find the contribution to the vertex part Γ from $\tilde{H}_{sf}$, to second order in J. By direct calculation we convince ourselves that, in the case of weak hybridization ($|\omega|$, $\epsilon_k < |\epsilon_1|$), the corresponding vertex coincides with γ_2 from (3) (which determines T_S), including the factor A, which, for $P_0 = 0$, is equal to $S(S + 1)$. We note, however, that full correspondence between T_S and τ_S^{-1} from[8] does not exist, inasmuch as we are considering a periodic system.

The superconducting properties of a periodic sf-exchange Hamiltonian have been considered in detail in papers by Izyumov and Skryabin[13] (in the ferromagnetic case). As we have seen, the hybridization model reduces partially to an effective sf-exchange Hamiltonian only in the case of weak hydridization ($|\epsilon_1|/g > 1$) and for $\epsilon_1 < 0$. Both the possibility of the appearance of an effective attraction as a result of polarization of the intrinsic degrees of freedom of the f-shells (the vertex part γ_1) and the hybridization effects are then lost. Also lost is the possibility of treating the disappearance of localized moments on change of the sign of ϵ_1. The fact that, unlike Izyumov and Skryabin[13], we have chosen the paramagnetic state of the system to analyze the superconducting properties is also connected with the incomplete reducibility of the Hamiltonian (1) to $\tilde{H}_{sf}$. The magnetic properties of the system (1) in the simplest approximation were analyzed in a paper by Smith[14], who showed that, in second order in g, the system is paramagnetic when $\epsilon_1 < 0$. The fact that the paramagnetic state is energetically favored is mainly connected with the hybridization effects (with the last term in $\tilde{H}$ (12), which describes jumps of f-electrons from site to site across the s-band). The effective exchange gives a contribution to the magnetic energy only in fourth order in g, and, evidently, cannot change the magnetic properties of the system.

In the case of strong hybridization ($|\epsilon_1|/g < 1$) the determinant (6) is always nonzero, whence it follows that in these conditions the normal state is stable against Cooper pairing at all temperatures.

Thus, the region in which the sf-interaction completely eliminates the possibility of Cooper pairing is essentially asymmetric about the Fermi surface:

$$-(\rho g^2/T_{c0})^{1/2}<\varepsilon_1/g<1. \tag{13}$$

Thus, if we want to take a non-superconducting transition metal over into a superconducting state, we must try to increase ϵ_1. Such a situation is apparently realized in Ce, which becomes superconducting in the $\alpha-\alpha'$ transition under pressure[15].

In conclusion we note that the results obtained above are carried over automatically to the case when the level ϵ_f of the second f-electron lies near ϵ_F (see the Appendix). For this it is sufficient to change to a hole representation, which reduces to replacing ϵ_1 by $-\epsilon_f$ in (13).

The authors thank E. G. Maksimov and D. I. Khomskiĭ for useful discussions.

APPENDIX

The vertex part $\gamma^{f}_{\alpha\beta,\gamma\delta}(p_1p_2, p_3p_4)$ obtained by expanding the S-matrix to order g^4 in the expression for G^{II} contains four Z-operators: $\langle TZ_{\mathbf{m}_1\alpha}(\tau_1)Z^{+}_{\mathbf{m}_3\gamma}(\tau_3)Z_{\mathbf{m}_2\beta}(\tau_2)Z^{+}_{\mathbf{m}_4\delta}(\tau_4)\rangle_f$, where $Z^{+}_{\mathbf{m}\sigma} \equiv Z^{\sigma 0}_{\mathbf{m}}$ and $Z_{\mathbf{m}\sigma} \equiv Z^{0\sigma}_{\mathbf{m}}$. The averaging is performed independently at each site, and therefore there are two possibilities: either all four operators refer to the same site, or they refer in pairs to two distinct sites.

In the first case the contribution to γ^f is proportional to the Fourier component with respect τ_1, τ_2, τ_3, τ_4 of

$$N^{-1}\sum_{\mathbf{m}}\langle TZ_{\mathbf{m}\alpha}(\tau_1)Z_{\mathbf{m}\gamma}^{+}(\tau_3)Z_{\mathbf{m}\beta}(\tau_2)Z_{\mathbf{m}\delta}^{+}(\tau_4)\rangle_f\exp\{i(\mathbf{k}_1-\mathbf{k}_2+\mathbf{k}_3-\mathbf{k}_4)\mathbf{m}\},$$

a method for calculating which is given in [16] using the example of the Anderson model. Carrying out the Fourier transformation, we obtain an expression in the form of two terms:

$$\gamma_1+\gamma_2'=(\delta_{\alpha\gamma}\delta_{\beta\delta}-\delta_{\alpha\delta}\delta_{\beta\gamma})\frac{(-1)g^4[i(\omega_1+\omega_2)-2\varepsilon_1](P_0+P_\sigma)}{(i\omega_1-\varepsilon_1)(i\omega_2-\varepsilon_1)(i\omega_3-\varepsilon_1)(i\omega_4-\varepsilon_1)}$$

$$+\frac{\beta g^4}{(i\omega_1-\varepsilon_1)(i\omega_2-\varepsilon_1)}[\delta_{\alpha\gamma}\delta_{\beta\delta}(P_\sigma\Delta_{14}\Delta_{23}-P_0\Delta_{13}\Delta_{24})$$

$$-\delta_{\alpha\delta}\delta_{\beta\gamma}(P_\sigma\Delta_{13}\Delta_{24}-P_0\Delta_{14}\Delta_{23})]\delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4}.$$

In the second case the contribution to γ^f is proportional to the Fourier component of an expression of the form

$$N^{-1}\sum_{\substack{\mathbf{m}_1\mathbf{m}_2\\ (\mathbf{m}_1\neq\mathbf{m}_2)}}\langle TZ_{\mathbf{m}_1\alpha}(\tau_1)Z^{+}_{\mathbf{m}_1\gamma}(\tau_3)\rangle_f\langle TZ_{\mathbf{m}_2\beta}(\tau_2)Z^{+}_{\mathbf{m}_2\delta}(\tau_4)\rangle_f$$

$$\times\exp\{i(\mathbf{k}_1-\mathbf{k}_3)\mathbf{m}_1+i(\mathbf{k}_2-\mathbf{k}_4)\mathbf{m}_2\}.$$

We represent the sum over $\mathbf{m}_1$ and $\mathbf{m}_2$ for $\mathbf{m}_1 \neq \mathbf{m}_2$ in the form of a sum over all $\mathbf{m}_1$ and $\mathbf{m}_2$ of $(1 - \delta_{\mathbf{m}_1\mathbf{m}_2})$. Here only the second term is related to the vertex part $\Gamma^{(1)}$ and leads to

$$\gamma_2''=\delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4}\frac{(P_\sigma+P_0)^2}{(i\omega_1-\varepsilon_1)(i\omega_2-\varepsilon_1)}(\delta_{\alpha\gamma}\delta_{\beta\delta}\Delta_{13}\Delta_{24}-\delta_{\alpha\delta}\delta_{\beta\gamma}\Delta_{14}\Delta_{23}).$$

The sum of γ_2' and γ_2'' gives γ_2 in (3).

We note that if we had considered the case in which the level ϵ_f lies near the Fermi surface, the expressions for $\gamma_{1,2}$ would have differed from those given above only by the replacement of ϵ_1 by $-\epsilon_f$ and of P_0 by $P_2 = \langle Z^{22}_{\mathbf{m}}\rangle = \{1 + 2\exp(\beta\epsilon_f)\}^{-1}$.

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[1] This formula can also be formally obtained in our case, if Eq. (6) is replaced by $1 - a_{ss} - a_{ff} = 0$.

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Translated by P. J. Shepherd
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