

SUPERCONDUCTIVITY AND FERROMAGNETISM IN NONADIABATIC SYSTEM WITH STRONG ELECTRON CORRELATIONS AND MAGNETIC IMPURITY

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The theory of superconductivity in non-adiabatic system with strong electron correlations and paramagnetic impurity was constructed in [1] - [3].

The obtained results allow one to make the following conclusions:

- a. Both the non-adiabatic effects and strong electron correlations, violating Migdal's theorem [4], are enhancing superconductivity.
- b. These effects reduce the influence of the exchange interaction in the paramagnetic phase of the system with magnetic impurities. As a result, the decrease of T_c with impurity concentration is slowed down compared to the conventional superconductors. The critical impurity concentration corresponding to the collapse of superconductivity is increased and the region of ungapped states is substantially enlarged.
- c. The coefficient of the isotope effect α increases with impurity concentration and decreases with increase in Migdal's parameter m . At $m > 0,2$ the coefficient α can be less than 0,5 for both pure and doped superconductors, depending on the value of the impurity concentration.

At low temperatures, the coexistence of superconductivity and ferromagnetic arrangement of impurity spins is possible. This arrangement is due to mediated exchange interaction of ions through the conduction electrons, which gives as a feedback the spatial density of electron spin defined by the paramagnetic susceptibility. This quantity is not zero in superconductor even at $T = 0$ by virtual of the exchange scattering of electrons on paramagnetic impurity. These effects as well as spin-orbital interaction give rise to the spin flip of electrons, and the mixing of electronic states with opposite spin directions, thus weakening the effect of the shift of the Fermi surfaces and gives rise to the possibility of coexistence of superconductivity and ferromagnetism.

The article aims to study the influence of non-adiabatic effects and strong electron correlation on the superconducting transition temperature T_c and the temperature of ferromagnetic arrangement of impurity T_k as functions of concentration of chaotically distributed magnetic impurity and , therefore, on the coexistence of superconductivity and ferromagnetism (see also [5], [6]).

The Hamiltonian of the system is

$$H = H_0 + H_1 + H_2, \quad (1)$$

where H_0 is Hamiltonian of free electrons and phonons, H_1 is electron-phonon interaction, H_2 is interaction of electrons with chaotically distributed magnetic impurity.

In order to study superconducting properties of the system we have to obtain the equations for Greens's functions (normal and anomalous) taking into account the electron-phonon and electron-impurity interactions. For this purpose we will go to the interaction representation and write the perturbation theory for Green functions over interactions H_1+H_2 . After having performed averaging over chaotically distributed impurity and orientations of their spins, we obtain

$$\overline{V_{\alpha_1 \beta_1}(\vec{x}_1) V_{\alpha_2 \beta_2}(\vec{x}_2)} = \frac{c}{V} \sum_{\vec{q}} e^{-i\vec{q}(\vec{x}_1 - \vec{x}_2)} \left\{ V_1(\vec{q}) V_1(-\vec{q}) \delta_{\alpha_1 \beta_1} \delta_{\alpha_2 \beta_2} + \langle S_z \rangle \left[V_1(\vec{q}) V_2(\vec{q}) \delta_{\alpha_1 \beta_1} \sigma_{\alpha_2 \beta_2}^z + V_2(\vec{q}) V_1(-\vec{q}) \delta_{\alpha_2 \beta_2} \sigma_{\alpha_1 \beta_1}^z \right] + V_2(\vec{q}) V_2(-\vec{q}) \left[\langle S_x^2 \rangle \sigma_{\alpha_1 \beta_1}^x \sigma_{\alpha_2 \beta_2}^x + \langle S_y^2 \rangle \sigma_{\alpha_1 \beta_1}^y \sigma_{\alpha_2 \beta_2}^y + \langle S_z^2 \rangle \sigma_{\alpha_1 \beta_1}^z \sigma_{\alpha_2 \beta_2}^z \right] \right\}, \quad (2)$$

where c is the concentration of impurity $\sigma_{\alpha\beta}$ are Pauli matrices. $V_1(\mathbf{q})$, $V_2(\mathbf{q})$ are the Fourier components of the potential of impurity scattering. $\mathbf{S}$ is spin of impurity atom, and $\langle \dots \rangle$ means averaging over orientations of spins of impurity atoms. Hereinafter direct hat line means averaging over chaotically distributed impurity and orientations of their spins. Note that formula (2) can possibly account for ferromagnetic arrangement ($\langle S_z \rangle \neq 0$). Internal field $I = c V_2(0) \langle S_z \rangle$ arises as well. In the derived series of perturbation theory we take in consideration all diagrams, inherit to the doped adiabatic systems with $\langle S_z \rangle \neq 0$, and additional diagrams, containing intersection of two lines of electron-phonon with electron-impurity interactions, in similar way as in the case of paramagnetic phase ($\langle S_z \rangle = 0$) [1, 2]. These additional diagrams determine to first order the effect of nonadiabaticity.

For the sake of simplicity we are choosing Einstein spectrum and write the phonon Green's function in the form

$$D(\vec{p} - \vec{p}_1, \Omega - \Omega_1) = -|g_{\vec{p}\vec{p}_1}|^2 \frac{\omega_0^2}{(\Omega - \Omega_1)^2 + \omega_0^2} = |g_{\vec{p}\vec{p}_1}|^2 D(\Omega, \Omega_1). \quad (3)$$

Investigations of the influence of strong electron correlations on electron - phonon or electron- impurity interaction [7, 8] show that as the exchange momentum q increases, these quantities increase weakly with the next dramatic drop. These results allow one to get an approximate form of the above - mentioned quantities

$$|g_{\vec{p}\vec{p}_1}|^2 = \left(\frac{2k_F}{q_c} \right)^2 g^2 \theta(q_c - |\vec{p} - \vec{p}_1|),$$

$$V_i(\vec{p} - \vec{p}_1) V_j(\vec{p}_1 - \vec{p}) = V_i V_j \left(\frac{2k_F}{q_{cl}} \right)^2 \theta(q_{cl} - |\vec{p} - \vec{p}_1|). \quad (4)$$

In order to derive analytical expression for vertex functions we consider the weak coupling approximation $T_c / \omega_0 \ll 1$ and I / E , $I / \omega_0 \ll 1$ and use the method of direct calculation [4], [9].

Generalizing the method of Grin functions and mass operators determinations [2], [3] for a case $\langle S_z \rangle \neq 0$ and also the method of calculation of superconducting transition temperature in adiabatic systems [10], we obtain the equation:

$$\ln \frac{T_c}{T_{C0}} = \Psi\left(\frac{1}{2}\right) - \frac{1}{2} \left[1 - \frac{\bar{b}}{\sqrt{\bar{b}^2 - I^2}} \right] \Psi\left(\frac{1}{2} + \rho_+\right) - \frac{1}{2} \left[1 + \frac{\bar{b}}{\sqrt{\bar{b}^2 - I^2}} \right] \Psi\left(\frac{1}{2} + \rho_-\right), \quad (5)$$

where T_{C0} is the temperature of superconducting transition for the pure nonadiabatic system:

$$T_{C0} = \frac{2\omega_0 \gamma}{\sqrt{e}(1+m)\pi} \exp \frac{1}{2} \left(\frac{m}{m+1} \right) \exp \left(-\frac{Z}{\lambda_\Delta} \right), \quad (6)$$

$$\lambda_\Delta = \lambda \left[1 + 2\lambda P_V^0(Q_c, 0, \omega_0) + \lambda P_c^0(Q_c, 0, \omega_0) \right],$$

$$\lambda_z = \lambda \left[1 + \lambda P_V^0(Q_c, 0, \omega_0) \right], \quad (7)$$

$$Z = 1 + \lambda \frac{1}{1+m}, \quad m = \frac{2\omega_0}{E}, \quad Q_c = \frac{q_c}{2K_F}.$$

Here P_V^0 and P_c^0 are vertex and crossing functions for pure system. Ψ is Euler's psi-function, m is Migdal's parameter, $\rho_{\pm}$ are parameters of impurity scattering, determined by relationships

$$\rho_{\pm} = \frac{1}{Z} \frac{\left[\bar{a} + \sqrt{\bar{b} - I^2} \right]}{2\pi T_C}, \quad \bar{a} = \frac{2}{3} \bar{\Gamma}_{S_0} + \bar{\Gamma}_{ex} S(S+1) + \bar{\Gamma}_{ex} \langle S_z^2 \rangle;$$

$$\bar{b} = \frac{2}{3} \bar{\Gamma}_{S_0} - \bar{\Gamma}_{ex} (\langle S_x^2 \rangle + \langle S_y^2 \rangle), \quad \bar{\Gamma} = \Gamma [1 + 2\lambda P_V(Q_c 00)], \quad (8)$$

$\bar{\Gamma}_{S_0}$ is damping caused by the spin - orbital interaction :

$$\bar{\Gamma}_{S_0} = \Gamma_{S_0} [1 + 2\lambda P_V(Q_c 00)]; \quad \Gamma_{S_0} = \pi N_0 c_{S_0} V_{S_0}^2, \quad I = c V_2(0) \langle S_z \rangle, \quad (9)$$

c_{S_0} is the concentration of nonmagnetic impurity, V_{S_0} is the potential of impurity scattering.

Equation (5) describes the superconducting transition temperature in the phase of ferromagnetic arrangement of impurity's atoms and attributes the paramagnetic effect of internal field to the influence of electron scattering on the impurity atoms. By the form this equation coincides with the corresponding equation of the adiabatic theory. But for all that the remarkable redetermination of the quantities T_{C0} and $\rho_{\pm}$ have taken place. The quantity T_{C0} increases owing to the effects of non-adiabaticity and can achieve the values inherent to high- T_C materials at intermediate values of coupling constant but the parameters of impurity scattering $\bar{a}$ and $\bar{b}$ decrease in comparison with the case of the adiabatic systems.

In the limit $T_C \rightarrow 0$ on the basis of (25) expression for the critical concentration of impurity can be easily derived (Γ_{cr})

$$\ln \frac{\Gamma_{cr}}{\Gamma_{cr}^p} = \ln \frac{2\bar{\Gamma}}{\sqrt{\bar{a}^2 - \bar{b}^2 + I^2}} + \frac{\bar{b}}{2\sqrt{\bar{b}^2 - I^2}} \ln \frac{\bar{a} + \sqrt{\bar{b}^2 - I^2}}{\bar{a} - \sqrt{\bar{b}^2 - I^2}}, \quad (10)$$

where $\bar{\Gamma} = \bar{\Gamma}_{ex} S(S+1)$, Γ_{cr}^p is the critical concentration of impurity in the paramagnetic phase, determined by the relationship:

$$\Gamma_{cr}^p = \frac{\pi T_{C0}}{2\gamma f_c}; \quad f_c = f_c(m) = \frac{1}{Z} \left[1 - 2\lambda \frac{m}{1+m} \right]. \quad (11)$$

The last formula shows a significant increase of the critical concentration of impurity in non-adiabatic systems at $I = 0$ than in usual superconductors due to large values of T_{C0} and $f_c(m) < 1$. The temperature of superconducting transition T_C in the ferromagnetic phase is determined by equation (5) and the critical concentration of impurity by relationships (10).

Besides that, to obtain explicit dependence of T_C on the concentration of impurity is too difficult a task because we have to know temperature dependence of the quantities $\langle S_z \rangle$ and $\langle S_z^2 \rangle$. In order to obtain qualitative picture how the quantity T_C behaves in the ferromagnetic phase we are studying the behavior of this quantity near the temperature of magnetic arrangement T_k , determining the slope of curve $T_C(I)$ and values of the critical concentrations of impurity in two limit cases: $\Gamma_{S_0}/\Gamma \gg 1$ and $\Gamma_{S_0}/\Gamma \ll 1$. In order to perform these calculations we approach used at study of the adiabatic systems. We proceed from the statement that the quantity T_C decreases and the temperature T_k increases as the concentration of impurity increases. From this point of view the curves T_C and T_k as functions of impurity

concentration intersects on the phase diagram (T, Γ) or (temperature, concentration of impurity) at the point (T^*, Γ^*) . Near this point equation (5) can lead to

$$\frac{T_c - T^*}{T^*} = \frac{Y}{Y-1} \frac{\bar{\Gamma} - \bar{\Gamma}^*}{\bar{\Gamma}^*} = \frac{Y}{Y-1} \frac{\Gamma - \Gamma^*}{\Gamma^*}, \quad (12)$$

where

$$Y = \frac{3f_c}{2} \Psi' \left(\frac{1+3f_c}{2} \right) - \frac{15}{2f_c} \frac{1}{(S+1)^2 + S^2} \left(\frac{1}{2\pi N_0 V_2} \right)^2 \left(1 - \frac{\bar{\Gamma}_{s0}}{\bar{\Gamma}^*} \right)^{-1} \times \\ \times \left\{ \Psi' \left(\frac{1+3f_c}{2} \right) + \frac{1}{f_c} \left(1 - \frac{\bar{\Gamma}_{s0}}{\bar{\Gamma}^*} \right)^{-1} \right. \\ \left. \times \left[\Psi \left(\frac{1}{2} + \frac{f_c}{2} \left(1 + \frac{2\bar{\Gamma}_{s0}}{\bar{\Gamma}^*} \right) \right) - \Psi \left(\frac{1+3f_c}{2} \right) \right] \right\}. \quad (13)$$

The value of the quantity T_c in the ferromagnetic phase near Γ^* depends on the parameters Γ_{s0}/Γ , V_2 , N_0 and f_c (m). Effects of non-adiabaticity in this formula are revealed in $f_c(m) < 1$ at nonzero Migdal's parameter ($m \neq 0$). At $m = 0$ $f_c(m) = 1$ we obtain results of adiabatic theory for the case of isotropic scattering of impurity. We consider the most interesting case: strong spin-orbital interaction ($\Gamma_{s0}/\Gamma \gg 1$). In this limit we derive

$$Y = \left\{ \frac{3f_c}{2} + \frac{15S(S+1)}{2f_c[(S+1)^2 + S^2]} \left(\frac{1}{2\pi N_0 V_2} \right)^2 \frac{\Gamma}{\Gamma_{s0}} \right\} \Psi' \left(\frac{1+3f_c}{2} \right). \quad (14)$$

On the basis of (10) we obtain also expressions for the critical concentration of impurity in the ferromagnetic phase for the $\Gamma_{s0}/\Gamma \gg 1$. This expression has the following form

$$\ln \frac{\Gamma_{cr}}{\Gamma_{cr}^p} \approx - \frac{3\bar{\Gamma}_{cr}}{2\bar{\Gamma}_{s0} k^2 (S+1)^2} \left[1 + \frac{\bar{\Gamma}_{cr}}{2\bar{\Gamma}_{s0}} \ln \frac{\bar{\Gamma}_{cr}}{2\bar{\Gamma}_{s0}} \right], \quad (15)$$

where $k = 2\pi N_0 V_2 f_c Z$.

We obtain $\Gamma_{cr} < \Gamma_{cr}^p$ and with increase of Γ_{s0} the critical concentration coincides with the critical concentration Γ_{cr}^p in the paramagnetic phase. The same procedure like in the case of the adiabatic systems can be performed for the case of low values of the spin orbital ($\Gamma_{s0}/\Gamma \ll 1$). In this case in non-adiabatic system $\Gamma_{cr} \ll \Gamma_{cr}^p$ but is greater than the same value in usual superconductors.

To determine Curie's T_k temperature we calculate spin density of electron $\langle \sigma_z \rangle$ determined by the relationship:

$$\langle \sigma_z \rangle = \frac{1}{\beta V} \sum_{\vec{p}\Omega} [\bar{G}_{\uparrow\uparrow}(\vec{p}\Omega) - \bar{G}_{\downarrow\downarrow}(\vec{p}\Omega)] \quad (16)$$

where $\bar{G}$ is the complete Green function averaged over chaotically distributed positions of impurity atoms and orientation of their spins.

In result of calculations we obtain:

$$\langle \sigma_z \rangle - \langle \sigma_z \rangle_n = -N_0 i\pi \sum_{\Omega} \left[\frac{1}{\sqrt{1+U_{1+}^{-2}+U_{2+}^{-2}}} - \frac{1}{\sqrt{1+U_{1-}^{-2}+U_{2-}^{-2}}} \right] \varphi(\Omega) , \quad (17)$$

where

$$\langle \sigma_z \rangle_n = -\frac{2 N_0 I}{Z}$$

$U_{1\pm}$ and $U_{2\pm}$ are determined by complex system of equations [5], [6].

We consider behavior of the quantities T_k near the temperature of superconducting transition T_C . In the weak coupling approximation ($\Delta / E \ll 1$) and for concentrations of impurity ($\Gamma / E \ll 1$), which is not too large, using the same approach as in the case of adiabatic systems [10] with insignificant improvement in the case of electron-phonon interaction for Curie temperature T_k , we derive near the intersection point (T^* , Γ^*) the following expression

$$\frac{T_K - T^*}{T^*} = \frac{1 - \alpha \frac{3f_c}{2} \Psi' \left(\frac{1}{2} + \frac{3f_c}{2} \right)}{1 + \alpha \left[1 - \frac{3f_c}{2} \Psi' \left(\frac{1}{2} + \frac{3f_c}{2} \right) \right]} \frac{\Gamma - \Gamma^*}{\Gamma^*} , \quad (18)$$

where

$$\begin{aligned} \alpha = & \frac{2}{f_c b_1 \left(\frac{3f_c}{2} \right)} \left[1 - \frac{\Gamma_{s0}}{\Gamma^*} \right]^{-1} \left\{ \Psi' \left(\frac{1}{2} + \frac{3f_c}{2} \right) + \frac{1}{f_c} \left[1 - \frac{\Gamma_{s0}}{\Gamma^*} \right]^{-1} \times \right. \\ & \times \left[-\Psi \left(\frac{1}{2} + \frac{3f_c}{2} \right) + \Psi \left(\frac{1}{2} + \frac{f_c}{2} + \frac{\Gamma_{s0}}{\Gamma^*} f_c \right) \right] \Bigg\} , \\ & b_1 \left(\frac{3f_c}{2} \right) = -\frac{1}{2} \Psi'' \left(\frac{1}{2} + \frac{3f_c}{2} \right) - \frac{3f_c}{2} \frac{1}{6} \Psi''' \left(\frac{1}{2} + \frac{3f_c}{2} \right) . \end{aligned} \quad (19)$$

Formula (18) can possibly allow one to determine T_k near the superconducting transition temperature T_C and the slope of the curve $\left(\frac{dT_K}{d\Gamma} \right)$. So, we can present the qualitative

behavior of T_k as a function of concentration of impurity in the superconducting phase. The common examination of (12) and (18) allows by an uneasy way to obtain the phase diagram (T_C , Γ).

The dependence of the temperature of superconducting transition T_C is given in fig. 1 at the ferromagnetic arrangement as well as of Curie temperature T_k in superconducting state at different values of Migdal's parameter $m = 2\omega_0 / E$ for systems large values of spin-orbital interaction ($\Gamma / \Gamma_{s0} \ll 1$). Curves 1 - 3 correspond to T_C and the curves 1' - 3' correspond to T_k . We obtain favorable conditions for coexistence of superconductivity and ferromagnetism. We have derived that both the exchange interaction and the spin-orbital interaction lower the «splitting» of Fermi surface by conservation of the spin of electron. The quantities T_C as a function of concentrations of impurity at given m ($m = 0, 1; 1, 0; 0$) go to the corresponding curves of paramagnetic phase with the critical concentrations $\Gamma_{cr} = \Gamma_{cr}^p$.

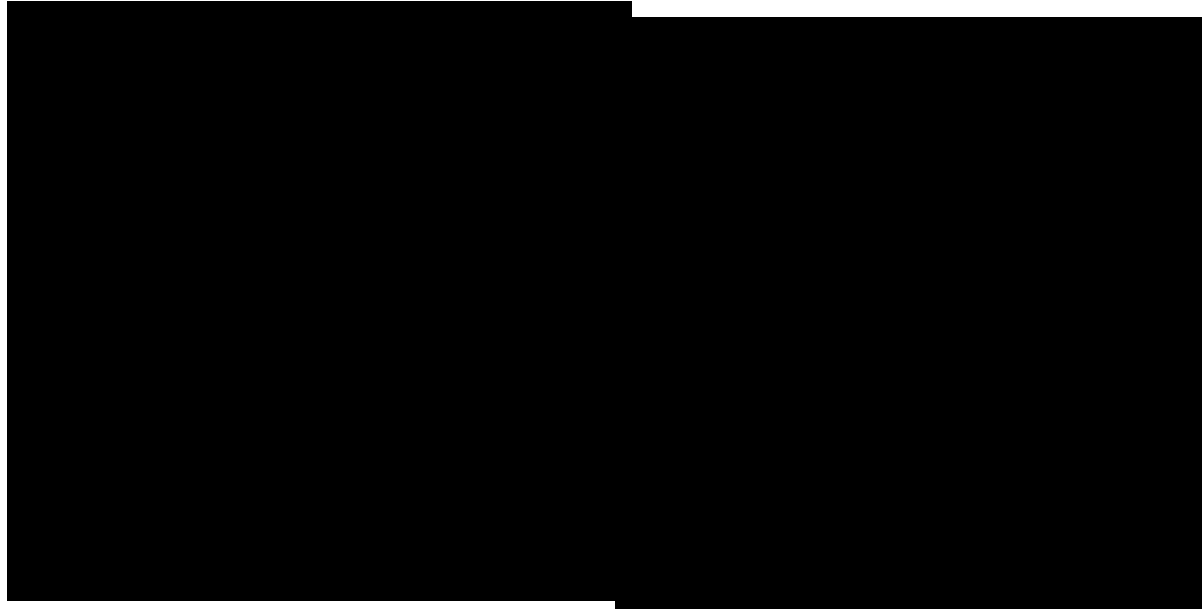


Fig.1. The critical temperature T_C and the temperature of ferromagnetic arrangement T_k plotted as functions of inverse relaxation time Γ at $\Gamma_{s0} / \Gamma \gg 1$.

Fig.2. The critical temperature T_C and T_k plotted as function of inverse relaxation time Γ at $\Gamma_{s0}/\Gamma \ll 1$.

The value T_k as function of concentration of impurity increases and has the form of curve with convexity down. But from all of that the field with coexistence of superconductivity and ferromagnetism is arisen between the curves of T_C and T_k . In this figure $m = 0,1$ the field with coexistence is bounded by curves 1 and 1', at $m = 1$ by curves 2 and 2', at $m = 0$ and by curves 3 and 3'. Therefore, maximum field of coexistence corresponds to the value $m = 0.1$ and is lessened with increase of m . For arbitrary m ($0.1 < m < 1$) this field is greater than in the case of adiabatic systems ($m = 0$). The quantities T^* and Γ^* in the non-adiabatic system are greater than in adiabatic systems at different values of m .

Figure 2 corresponds to the case of low values of the spin-orbital interaction ($\Gamma_{s0}/\Gamma \ll 1$). As can be seen from the figure in this case the coexistence of superconductivity and ferromagnetism is possible at low temperatures and small concentrations of impurity. Extent of this field depends greatly on the parameter m . It has minimum value at $m = 0$ (adiabatic systems), maximum one at $m = 0.1$, then it decreases with increase of m remaining greater than the field inherent to adiabatic systems.

Such picture is determining by the maximum in T_C dependence on m at the point $m \approx 0.1$.

In fig.1 and fig.2 we show crosshatched region corresponding to the coexistence of superconductivity and ferromagnetism: we have first field between curves 3 and 3' with $m = 0$ (adiabatic systems), second field between curves 2 and 2' with $m = 1$ (non-adiabatic systems) and third between curves 1 and 1' with $m = 0.1$. Due to the nonadiabaticity this field of coexistence expands with increase of concentration of impurity. We observe also increase of the temperature T^* and the concentration of impurity Γ^* , at which the ferromagnetic arrangement arises in non-adiabatic systems in comparison to adiabatic ones.

We make the following conclusions:

1. Upon doping a non-adiabatic system with magnetic impurities, a ferromagnetic spin ordering of impurity ions can set in at low temperatures. In such regions superconductivity

and ferromagnetism coexist. The decisive role is then played by the competition of the following mechanisms: on one hand the splitting of the Fermi surfaces by the internal magnetic field destroying superconductivity and on the other hand the exchange and spin-orbital interactions which produce spin-flips and favor the formation of Cooper pairs.

2. The extent of the coexistence region of superconductivity and magnetism on (T, c) phase diagram is determined by the ratio of exchange (Γ_{ex}) and spin-orbital (Γ_{SO}) interactions.

For $\Gamma_{\text{SO}} / \Gamma_{\text{ex}} \ll 1$ the phase coexistence exists only at very low temperature and impurity concentrations. For $\Gamma_{\text{SO}} / \Gamma_{\text{ex}} \gg 1$ the coexistence region is substantially enlarged and the critical concentration coincides with that of a paramagnetic phase.

3. Non-adiabatic effects lead to the increase of the coexistence region of superconductivity and ferromagnetism for the above-mentioned values of the ratio $\Gamma_{\text{SO}} / \Gamma_{\text{ex}}$. In this region the behavior is determined by the Migdal's parameter m : the region is maximal for $m \sim 0.1$ and for the rest of the interval $0.1 < m < 1$ it still remains larger than for adiabatic systems.

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