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Influence of temperature on the impurity-induced $s_{\pm} \to s_{++}$ transition in the two-band model for Fe-based superconductors

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Influence of temperature on the impurity-induced $s_\pm \to s_{++}$ transition in the two-band model for Fe-based superconductors

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Abstract. In Fe-based superconducting materials, the $s_\pm$ state with the sign-changing gap in the clean limit could be changed to the sign-conserving s_{++} state by nonmagnetic impurities. Previous results are obtained for the fixed temperature well below the superconducting critical temperature T_c. We study how the increasing temperature affects the transition between $s_\pm$ and s_{++} states in the two-band model. The calculations show that the $s_\pm \to s_{++}$ transition appears to be dependent on temperature T, i.e. there exists a narrow range of impurity scattering rates, where the s_{++} state in dirty superconductor at low temperature is transformed back to the $s_\pm$ state by increasing T. With the nonmagnetic impurity scattering rate increasing, the temperature of such a reverse transition is shifted to T_c, while the s_{++} state remains solely one for higher degree of disorder.

1. Introduction

Superconducting iron pnictides and chalcogenides constituting a big family of Fe-based high-T_c superconductors (FeBS) are of most interest due to their peculiarities of normal and unconventional superconducting states [1, 2, 3, 4, 5, 6, 7, 8]. Namely, they have the same electronic structure with the Fermi-surface consisting of hole and electron pockets. Moreover, the system possess the multiorbital character which can be described only by multiorbital and, respectively, multiband model. Thus, a minimal model is the two-band model [9, 10, 11]. Another peculiarity is the superconducting state whose origin has not been defined yet. There are two main candidates for the role of superconducting mechanism in FeBS: (i) spin fluctuations leading to the $s_\pm$ superconducting state with a sign-changing gap [8, 12, 13], and (ii) orbital fluctuations enhanced by electron-phonon interaction leading to the sign-conserving s_{++} state [14, 15, 16]. Many experiments (such as the spin resonance peak in inelastic neutron scattering [17, 18, 19, 20], a quasiparticle interference in tunneling experiments [21, 22, 23, 24], the NMR spin-lattice relaxation rate [25, 26], and the temperature dependence of the penetration depth [27, 28, 29]) evidence for mechanism involving the spin fluctuations [27, 28, 29].

Considering the scattering on nonmagnetic impurities in superconductors with different gap structure, one observes different effects. The presence of any nonmagnetic disorder does not affect the superconducting critical temperature T_c in the s_{++} superconductor [30], which is similar to behavior of the conventional s-wave superconductors [31, 32]. On the other hand, T_c for the superconductor with sign-changing $s_\pm$ gap is suppressed by nonmagnetic impurities

[33]. Such a suppression in unconventional superconductors is similar to the suppression of T_c in conventional superconductors by the magnetic impurities according to the Abrikosov-Gor'kov theory [34]. However, a series of experiments show that in the FeBS this suppression is less than it is predicted by the theory [35, 36, 37, 38, 39]. In Refs. [10, 11, 40, 41, 42, 43, 44], it was shown that the possible reason of the inconsistency with the Abrikosov-Gor'kov theory is a transition from the $s_\pm$ to s_{++} state when the impurity scattering rate reaches some critical value $\Gamma^{\rm crit}$.

Here we study the nonmagnetic impurity scattering in the two-band model in a wide temperature range up to T_c. We show that there is a range of $\Gamma^{\rm crit}$ values for different temperatures i.e. while the $s_\pm$ state transforms to the s_{++} state at low temperature, increasing the temperature leads to the transition back to the $s_\pm$ state.

2. Model and Method

We use the same two-band model as in Refs. [10, 11, 43] with the following Hamiltonian,

$$H = \sum_{\mathbf{k},\alpha,\sigma} \xi_{\mathbf{k},\alpha} c^\dagger_{\mathbf{k}\alpha\sigma} c_{\mathbf{k}\alpha\sigma} + \sum_{\mathbf{R}_i,\sigma,\alpha,\beta} \mathcal{U}^{\alpha\beta}_{\mathbf{R}_i} c^\dagger_{\mathbf{R}_i\alpha\sigma} c_{\mathbf{R}_i\beta\sigma} + H_{SC}, \quad (1)$$

where the operator $c^\dagger_{\mathbf{k}\alpha\sigma}(c_{\mathbf{k}\alpha\sigma})$ creates (annihilates) a quasiparticle with the band index $\alpha = (a,b)$, momentum $\mathbf{k}$, and spin σ, $\xi_{\mathbf{k},\alpha}$ is a dispersion of quaziparticles linearized near the Fermi level, with $\mathbf{v}_{F\alpha}$ and $\mathbf{k}_{F\alpha}$ being the Fermi velocity and the Fermi momentum of the band α, respectively. The second term in the Hamiltonian contains the impurity potential $\mathcal{U}_{\mathbf{R}_i}$ at site $\mathbf{R}_i$, while the last term, whose the exact form is not important for the current discussion, is responsible for the superconductivity. We assume that the superconducting pairing is provided by the exchange of spin fluctuations (repulsive interaction) and may include some attractive interaction (for example, electron-phonon coupling).

The presence of nonmagnetic disorder is considered using the Eliashberg approach for the multiband superconductors [45]. To simplify the calculations, we use the quasiclassical ξ-integrated Green's functions,

$$\hat{\mathbf{g}}(\omega_n) = \begin{pmatrix} \hat{\mathrm{g}}_{an} & 0 \\ 0 & \hat{\mathrm{g}}_{bn} \end{pmatrix}, \quad (2)$$

where $\omega_n = (2n+1)\pi T$ is the Matsubara frequency, and

$$\hat{\mathrm{g}}_{\alpha n} = g_{0\alpha n} \hat{\tau}_0 \otimes \hat{\sigma}_0 + g_{2\alpha n} \hat{\tau}_2 \otimes \hat{\sigma}_2, \quad (3)$$

Here $\hat{\tau}_i$ and $\hat{\sigma}_i$ are the Pauli matrices corresponding to Nambu and spin spaces, respectively; $g_{0\alpha n}$ and $g_{2\alpha n}$ are the normal and anomalous (Gor'kov) ξ-integrated Green's functions in the Nambu representation,

$$g_{0\alpha n} = -\frac{\mathrm{i}\pi N_\alpha \tilde{\omega}_{\alpha n}}{\sqrt{\tilde{\omega}^2_{\alpha n} + \tilde{\phi}^2_{\alpha n}}}, \qquad g_{2\alpha n} = -\frac{\pi N_\alpha \tilde{\phi}_{\alpha n}}{\sqrt{\tilde{\omega}^2_{\alpha n} + \tilde{\phi}^2_{\alpha n}}}, \quad (4)$$

which depend on density of states per spin at the Fermi level of the corresponding band $(N_{a,b})$, and on the renormalized by the self-energy order parameter $\tilde{\phi}_{\alpha n}$ and frequency $\tilde{\omega}_{\alpha n}$. The order parameter $\tilde{\phi}_{\alpha n}$ is connected to the gap function $\Delta_{\alpha n}$ via the renormalization factor $Z_{\alpha n} = \tilde{\omega}_{\alpha n}/\omega_n$, i.e.

$$\Delta_{\alpha n} = \tilde{\phi}_{\alpha n}/Z_{\alpha n}. \quad (5)$$

The impurity part of self-energy $\hat{\mathbf{\Sigma}}^{\rm imp}$ is calculated in a noncrossing diagrammatic approximation described by the $\mathcal{T}$-matrix approximation with the following equation,

$$\hat{\mathbf{\Sigma}}^{\rm imp}(\omega_n) = n_{\rm imp}\hat{\mathbf{U}} + \hat{\mathbf{U}}\hat{\mathbf{g}}(\omega_n)\hat{\mathbf{\Sigma}}^{\rm imp}(\omega_n), \quad (6)$$

where $n_{\rm imp}$ is the concentration of impurities, $\hat{\mathbf{U}} = \mathbf{U} \otimes \hat{\tau}_3$, is the matrix of impurity potential $(\mathbf{U})_{\alpha\beta} = \mathcal{U}^{\alpha\beta}_{\mathbf{R}_i}$, consisting of intra- and interband parts $(\mathbf{U})_{\alpha\beta} = (v-u)\,\delta_{\alpha\beta} + u$. The relation between intra- and interband impurity scattering is set by a parameter $\eta = v/u$. Without loss of generality we set $\mathbf{R}_i = 0$.

It is convenient to introduce the generalized cross-section parameter

$$\sigma = \frac{\pi^2 N_a N_b u^2}{1+\pi^2 N_a N_b u^2} \to \begin{cases} 0, & \text{Born limit,} \\ 1, & \text{unitary limit} \end{cases} \tag{7}$$

and the impurity scattering rate

$$\Gamma_{a(b)} = 2n_{\rm imp}\pi N_{b(a)} u^2 (1-\sigma) \tag{8}$$
$$= \frac{2n_{\rm imp}\sigma}{\pi N_{a(b)}} \to \begin{cases} 2n_{\rm imp}\pi N_{b(a)}u^2, \text{Born limit,} \\ \dfrac{2n_{\rm imp}}{\pi N_{a(b)}}, \text{unitary limit,} \end{cases}$$

For σ an Γ_α, there are two limiting cases: (i) the Born limit corresponding to the weak impurity potential ($\pi u N_{a(b)} \ll 1$), and (ii) the unitary limit corresponding to the strong impurity scattering ($\pi u N_{a(b)} \gg 1$).

3. Results and Discussions

For the calculations, we use the following parameters: the ratio between densities of states is chosen as $N_b/N_a = 2$, and matrix of coupling constants $\hat{\lambda}$ is set to be $(\lambda_{aa};\lambda_{ab};\lambda_{ba};\lambda_{bb}) = (3;-0.2;-0.1;0.5)$. That gives a positive averaged coupling constant, $\langle\lambda\rangle = (\lambda_{aa}+\lambda_{ab})\,N_a/N + (\lambda_{ba}+\lambda_{bb})\,N_b/N > 0$, where $N = N_a + N_b$. This set of parameters leads to the $s_\pm$ superconducting state with the critical temperature $T_{c0} = 40$ K in the clean limit and unequal gaps. The larger gap is positive (band a) while the smaller one is negative (band b). The $s_\pm \to s_{++}$ transition takes place when the sign of the small gap is changed while the sign of the large gap remains positive [10].

Here we present the smaller gap $\Delta_{b,n}$ for the lowest Matsubara frequency ($n=0$) depending both on the impurity scattering rate and the temperature for two different cases: (i) the Born limit with $\sigma = 0$; and (ii) the intermediate scattering with $\sigma = 0.5$. Qualitatively, the results for both limiting cases appears to be similar. Thus, we present the results only for $\sigma = 0.5$, see figure 1.

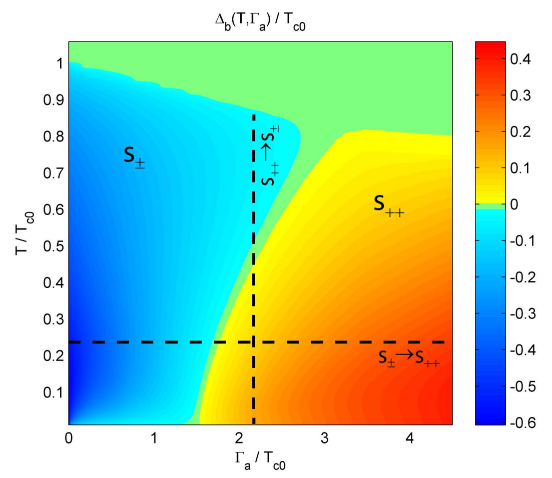

Figure 1. Dependence of the lowest-frequency Matsubara gap function $\Delta_{b,n=0}$, indicated by the color code, for the band b on Γ_a and T in the intermediate scattering limit, $\sigma = 0.5$. All quantities are normalized by T_{c0}. Green color marks the state with the vanishingly small gap, $\Delta_{b,n} < 10^{-3}T_{c0}$.

The transition goes through the gapless state with the finite larger gap and the vanishing smaller gap [10]. As the line of transition is not vertical in figure 1, the critical scattering rate is a temperature-dependent $\Gamma_a^{\rm crit}(T)$. Moreover, if we stay at a fixed Γ_a in the range $1.1T_{c0} < \Gamma_a < 1.6T_{c0}$ for $\sigma = 0$ or $1.5T_{c0} < \Gamma_a < 3.2T_{c0}$ for $\sigma = 0.5$ and increase the temperature, we observe that while at low temperatures the transition to the s_{++} state already took place ($\Delta_{b,n} > 0$), at higher temperatures the system goes back to the $s_\pm$ state ($\Delta_{b,n} < 0$). Thus, there is a temperature-dependent $s_{++} \to s_\pm$ transition. With the increasing Γ_a, the temperature of this transition is shifted to T_c and the system becomes s_{++} for the whole temperature range.

In figure 2 we present temperature dependencies of the gap function $\Delta_{\alpha,n=0}$ for several fixed values of Γ_a with $\sigma = 0.5$. Gap in the band a has the same positive sign for all values of Γ_a and vanishes at T_c. In the clean limit and for the small Γ_a, the sign of the smaller gap $\Delta_{b,n}$ is negative at all temperatures, see figure 2(b). With the impurity scattering rate increased, the gap at low temperatures changes sign while at higher temperatures the sign is either reversed again (small Γ_a) or the gap vanishes ($\Gamma_a \gtrsim 2T_{c0}$). Therefore, the transition from the $s_\pm$ state to the s_{++} state is characterized by two parameters, namely, the critical scattering rate $\Gamma_a^{\rm crit}$ and the critical temperature $T^{\rm crit}$. The latter changes from zero to T_c. Thus the s_{++} state becomes dominant in the initially clean $s_\pm$ system for $\Gamma_a > \Gamma_a^{\rm crit}$ and $T < T^{\rm crit}$. This is true in both the Born limit and the intermediate scattering limit.

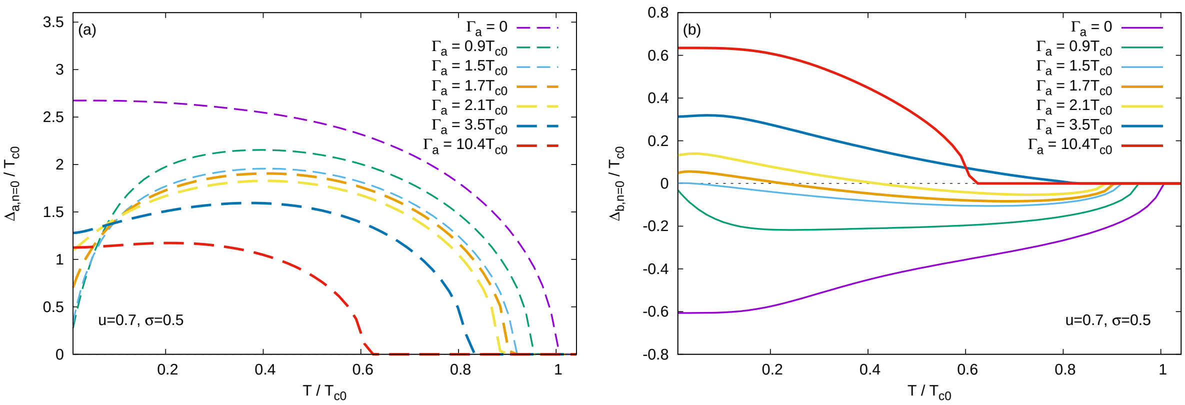

Figure 2. Temperature dependence of the lowest-frequency Matsubara gap $\Delta_{\alpha,n=0}$ normalized by T_{c0} for fixed values of Γ_a in the intermediate scattering limit ($\sigma = 0.5$) with the band index $\alpha = a$ (**a**) and $\alpha = b$ (**b**).

Also, we have checked that the similar behavior holds for the higher Matsubara frequencies, see figure 3 for the illustration of the gaps behavior for $n = 3$ and $n = 10$ in the Born limit.

4. Conclusions

In the two-band model for FeBS with the $s_\pm$ superconducting ground state in the clean limit, we studied dependence of the superconducting gaps $\Delta_{\alpha,n}$ on both temperature and the nonmagnetic impurity scattering rate. We show that the disorder-induced transition from the $s_\pm$ to the s_{++} state appears to be dependent on temperature. That is, in the narrow region of scattering rates, while the ground state is s_{++}, it transforms back to the $s_\pm$ state at higher temperatures up to T_c. With the increasing impurity scattering rate, temperature of such a $s_{++} \to s_\pm$ transition shifts to the critical temperature T_c. The $s_\pm \to s_{++}$ transition is characterized by the two parameters: (i) the critical scattering rate $\Gamma_a^{\rm crit}$ and (ii) the critical temperature $T^{\rm crit} \leq T_c$. The s_{++} state becomes dominant in the initially clean $s_\pm$ system for $\Gamma_a > \Gamma_a^{\rm crit}$ and $T < T^{\rm crit}$.

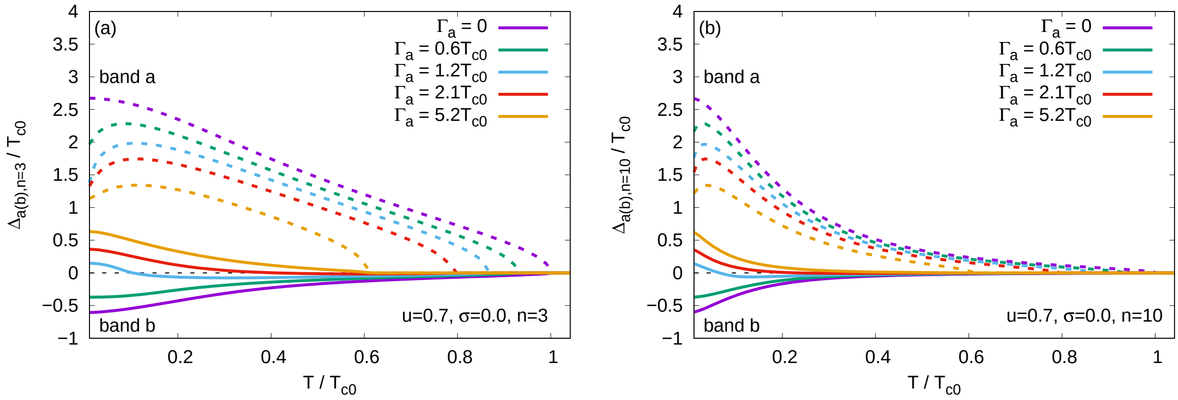

Figure 3. Temperature dependence of the gap for higher Matsubara frequencies, $\Delta_{\alpha,n=3}$ (**a**) and $\Delta_{\alpha,n=10}$ (**b**), normalized by T_{c0} for fixed values of Γ_a in the Born limit ($\sigma = 0$). Gaps corresponding to the band index a (band index b) are shown by dashed (solid) curves.

Experimentally, one can observe the reentrant $s_\pm$ state by increasing the temperature for the fixed amount of disorder that results in the low-temperature s_{++} state. For example, the spin resonance peak in the inelastic neutron scattering should be absent in the low-temperature s_{++} state, but have to appear in the $s_\pm$ state at higher temperatures [8, 13, 17, 18]. Temperature dependence of the penetration depth should also bear specific signatures of the gapless behavior accompanying the $s_{++} \to s_\pm$ transition [11].

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