Uniform impurity scattering in two-band $s_\pm$ and $s_{++}$ superconductors

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Abstract The $s_\pm$ and $s_{++}$ models for the superconducting state are subject of intense studies regarding Fe-based superconductors. Depending on the parameters, disorder may leave intact or suppress $T_c$ in these models. Here we study the special case of disorder with equal values of intra- and interband impurity potentials in the two-band $s_\pm$ and $s_{++}$ models. We show that this case can be considered as an isolated point and $T_c$ there has maximal damping for a wide range of parameters.

Keywords Multiband superconductivity · Impurity scattering · Fe-based superconductors

1 Introduction

Fe-based materials - pnictides and chalcogenides - represent a new class of unconventional superconductors with high transition temperatures [2]. While the mechanism of superconductivity is still a mystery, the main candidates are spin or orbital fluctuations. Except for the extreme hole and electron dopings, the Fermi surface consists of two or three hole pockets around the $\Gamma=(0,0)$ point and two electron pockets around the $M=(\pi,\pi)$ point in the 2-Fe Brillouin zone. Scattering between them with the large wave vector results in the enhanced antiferromagnetic fluctuations, which promote the $s_\pm$ type of the superconducting order parameter that change sign between electron and hole pockets [2]. On the other hand, bands near the Fermi level have mixed orbital content and orbital fluctuations enhanced by the electron-phonon interaction may lead to the sign-preserving $s_{++}$ state [3,4]. However, most experimental data including observation of a spin-resonance peak in inelastic neutron scattering, the quasiparticle interference in tunneling experiments, and NMR spin-lattice relaxation rate are in favor of the $s_\pm$ scenario [2].

The $s_\pm$ and $s_{++}$ states are expected to behave differently subject to the disorder [5,6,7,8,9,10,11,12,13]. In general, $s_{++}$ ($s_\pm$) state should be stable (fragile) against a scattering on a nonmagnetic impurities [5,6,7]. Detailed studies revealed that $T_c$ stays finite in the presence of nonmagnetic disorder in the following cases: i) $s_{++}$ state [8,9], ii) $s_\pm \to s_{++}$ transition for the sizeable intraband attraction in the two-band $s_\pm$ model in the strong-coupling $T$-matrix approximation [10] and via the numerical solutions of the Bogoliubov-de Gennes equations [14,15], iii) an unitary limit [16]. Magnetic impurities leave $T_c$ finite [13] in the case of 1) $s_\pm$ superconductor with the purely interband impurity scattering, 2) $s_{++}$ state with the purely interband scattering due to the $s_{++} \to s_\pm$ transition, and 3) the unitary limit for both $s_{++}$ and $s_\pm$ states independent on the exact form of the impurity potential. But even if $T_c$ is suppressed, its behavior may differ from the Abrikosov-Gor'kov (AG) theory for the single-band superconductors [5], which states that $T_c$ is determined by the expression $\ln T_{c0}/T_c = \Psi(1/2 + \Gamma/2\pi T_c) - \Psi(1/2)$, where $\Psi(x)$ is the digamma function, $\Gamma$ is the impurity scattering rate, and $T_{c0}$ is the critical temperature in the absence of impurities [5].
The choice of the “proper” theory for disorder effects in iron-based materials is severely complicated by the fact that the exact form of the impurity potential is not known. In such a situation it is instructive to theoretically explore as many situations as possible. Here we focus on a special case of a uniform impurity potential with equal intra- and interband components. We consider two-band models for the isotropic $s_{\pm}$ and $s_{\mp}$ superconductors with either nonmagnetic or magnetic impurities within the self-consistent $T$-matrix approximation following approach from Refs. [10,13].

2 General equations and their analysis

We employ the Eliashberg approach for multiband superconductors [17] and calculate the $\xi$-integrated Green’s functions $\tilde{g}(\omega_n) = \int d\xi \tilde{G}(\k, \omega_n) = \left( \begin{array}{cc} g_{0an} & 0 \\ 0 & 0 \end{array} \right)$, where $\xi_{a,F} = v_{a,F}(k - k_{a,F})$ is the linearized dispersion, $k_{a,F}$ is the Fermi momentum, $g_{0an} = g_{0an} \tau_0 \otimes \sigma_0 + g_{2an} \tau_2 \otimes \sigma_2$, indices $a$ and $b$ correspond to two distinct bands, index $\alpha$ denote the band space, Pauli matrices define Nambu ($\hat{\tau}$) and spin ($\hat{\sigma}$) spaces, $\tilde{G}(\k, \omega_n) = \left[ G_{0}^{-1}(\k, \omega_n) - \tilde{\Sigma}(\omega_n) \right]^{-1}$ is the bare Green’s function, $\tilde{\Sigma}(\omega_n) = \sum_{\iota=1}^{2} \Sigma_{\alpha\beta}^{(\iota)}(\omega_n) \hat{\tau}_\iota$ is the self-energy matrix, $g_{0an}$ and $g_{2an}$ are the normal and anomalous $\xi$-integrated Nambu Green’s functions,

$$g_{0an} = \frac{-i \pi N_{\alpha} \tilde{\omega}_{an}}{\sqrt{\tilde{\omega}_{an}^2 + \tilde{\phi}_{an}^2}}, \quad g_{2an} = -\frac{\pi N_{\alpha} \tilde{\phi}_{an}}{\sqrt{\tilde{\omega}_{an}^2 + \tilde{\phi}_{an}^2}},$$

depending on the density of states per spin of the corresponding band at the Fermi level $N_{a,b}$ and on renormalized (by the self-energy) order parameter $\tilde{\phi}_{an}$ and frequency $\tilde{\omega}_{an}$,

$$\tilde{\omega}_{an} = \omega_n - \Sigma_{0an}(\omega_n) - \Sigma_{2an}(\omega_n), \quad \tilde{\phi}_{an} = \Sigma_{2an}(\omega_n) + \Sigma_{2an}(\omega_n).$$

It is also convenient to introduce the renormalization factor $Z_{\alpha n} = \omega_{\alpha n}/\tilde{\omega}_{\alpha n}$ that enters the gap function $\Delta_{\alpha n} = \tilde{\phi}_{\alpha n}/Z_{\alpha n}$. The self-energy due to the spin fluctuation interaction is then given by

$$\Sigma_{0\alpha}(\omega_n) = T \sum_{\omega_{\beta n}^\prime} \lambda_{\alpha\beta}(n-n\prime) \frac{g_{0\beta n}}{N_{\beta}},$$

$$\Sigma_{2\alpha}(\omega_n) = -T \sum_{\omega_{\beta n}^\prime} \lambda_{\alpha\beta}(n-n\prime) \frac{g_{2\beta n}}{N_{\beta}},$$

The coupling functions $\lambda_{\alpha\beta}(n-n\prime) = 2 \lambda_{\alpha\beta}^{\infty} \frac{\sin^2 \theta_{\alpha\beta}}{\sin^2 \theta_{\alpha\beta} + |\lambda_{\alpha\beta}|^2}$ depend on the normalized bosonic spectral function $B(\Omega)$ used in Refs. [10,11]. While the matrix elements $\lambda_{\alpha\beta}^{\infty}$ can be positive (attractive) as well as negative (repulsive) due to the interplay between spin fluctuations and electron-phonon coupling [18,19], the matrix elements $\lambda_{\alpha\beta}$ are always positive. For simplicity we set $\lambda_{\alpha\beta}^{\infty} = |\lambda_{\alpha\beta}| \equiv |\lambda_{\alpha\beta}|$ and neglect possible k-space anisotropy in each order parameter $\tilde{\phi}_{an}$.

We use the $T$-matrix approximation to calculate the average impurity self-energy $\tilde{\Sigma}_{\text{imp}}(\omega_n)$,

$$\tilde{\Sigma}_{\text{imp}}(\omega_n) = n_{\text{imp}} \tilde{U} \mp \tilde{U} \tilde{g}(\omega_n) \tilde{\Sigma}_{\text{imp}}(\omega_n).$$

where $n_{\text{imp}}$ is the impurity concentration.

2.1 Nonmagnetic impurities

First, we consider nonmagnetic disorder. Impurity potential matrix entering equation (6) is defined as $\tilde{U} = \tilde{U} \mp \tilde{\sigma}$, where $\tilde{U} = \tilde{U} \pi \tilde{\sigma}$ for $\tilde{R}_c = 0$ is the impurity site. For simplicity, we set intra- and interband parts of the potential equal to $v$ and $u$, respectively, so that $\tilde{U} = (v-u) n_{\alpha\beta} + u$. Relation between the two will be controlled by the parameter $v: u = uv$.

Apart from the general case, later we are going to examine two important limiting cases: Born limit (weak scattering) with $\pi u N_{a,b} \ll 1$ and the opposite case of a very strong impurity scattering (unitary limit) with $\pi u N_{a,b} \gg 1$.

It is useful to introduce the generalized scattering cross-section

$$\sigma = \frac{\pi^2 N_{a}N_{b}u^2}{1 + \pi^2 N_{a}N_{b}u^2} \rightarrow \begin{cases} 0, & \text{Born}, \\ 1, & \text{unitary} \end{cases}$$

and the impurity scattering rate

$$\Gamma_{a,b} = \frac{2 n_{\text{imp}} \sigma}{\pi N_{a,b}} \rightarrow \begin{cases} 2 n_{\text{imp}}/(\pi N_{a,b}), & \text{Born}, \\ 2 n_{\text{imp}}/(\pi N_{a,b}), & \text{unitary} \end{cases}$$

Then equations on frequency (2) and order parameter (3) become

$$\tilde{\omega}_{an} = \omega_n + i \Sigma_{0an}(\omega_n) + \frac{\Gamma_a}{2D} \left[ \begin{array}{c} \tilde{\omega}_{an} \frac{Q_{an}(1-\eta^2)}{Q_{an}} + \frac{\tilde{\omega}_{bn}}{Q_{bn}} \\ \tilde{\omega}_{bn} \frac{Q_{bn}(1-\eta^2)}{Q_{bn}} + \frac{\tilde{\omega}_{an}}{Q_{an}} \end{array} \right],$$

$$\tilde{\phi}_{an} = \Sigma_{2an}(\omega_n) + \frac{\Gamma_a}{2D} \left[ \begin{array}{c} \tilde{\phi}_{an} \frac{Q_{an}(1-\eta^2)}{Q_{an}} + \frac{\tilde{\phi}_{bn}}{Q_{bn}} \\ \tilde{\phi}_{bn} \frac{Q_{bn}(1-\eta^2)}{Q_{bn}} + \frac{\tilde{\phi}_{an}}{Q_{an}} \end{array} \right].$$

where $Q_{an} = \sqrt{\tilde{\omega}_{an}^2 + \tilde{\phi}_{an}^2}, D = (1-\sigma^2) + \sigma(1-\sigma) \frac{2 Q_{an} \tilde{\omega}_{an} + \tilde{\omega}_{bn}}{Q_{an} Q_{bn}} + \frac{N_{a}^2 + N_{b}^2 \eta^2}{N_{a} N_{b} \eta^2} + \sigma^2(1-\eta^2)^2$. 
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Let’s consider the main limits. Since in the Born approximation $\sigma \to 0$, then $D = 1$, $\Gamma_a = 2n_{\text{imp}}\pi N_b u^2$ and

$$\tilde{\omega}_{an} = \omega_n + i\Sigma_0(\omega_n) + \frac{\gamma_{aa}\tilde{\omega}_{an} + \gamma_{ab}\tilde{\omega}_{bn}}{Q_a + Q_b}, \quad (11)$$

$$\tilde{\phi}_{an} = \Sigma_{2a}(\omega_n) + \frac{\gamma_{aa}\tilde{\phi}_{an} + \gamma_{ab}\tilde{\phi}_{bn}}{Q_a + Q_b}, \quad (12)$$

where $\gamma_{aa} = 2\pi n_{\text{imp}} N_a u^2$ and $\gamma_{ab} = 2\pi n_{\text{imp}} N_b u^2$. Obviously, for the finite interband scattering $\gamma_{ab}$ (i.e. finite $\eta$) different bands are mixed in equations. This leads to the AG-like suppression of $T_c$.

In the unitary limit $\sigma \to 1$, $\Gamma_a = 2n_{\text{imp}}/(\pi N_a)$, and we have to consider two cases.

I). Uniform impurity potential with $\eta = 1$:

$$\tilde{\omega}_{an} = \omega_n + i\Sigma_0(\omega_n) + \frac{n_{\text{imp}}}{\pi N_a N_b D_{ab}} \left[ N_a \tilde{\omega}_{an} + N_b \tilde{\omega}_{bn} \right],$$

$$\tilde{\phi}_{an} = \Sigma_{2a}(\omega_n) + \frac{n_{\text{imp}}}{\pi N_a N_b} N_a \tilde{\phi}_{an} + N_b \tilde{\phi}_{bn},$$

where $D_{ab} = 2\tilde{\omega}_{an}\tilde{\phi}_{an} + \tilde{\omega}_{bn}\tilde{\phi}_{bn} + N_a^2 + N_b^2$. Again, different bands are mixed so we have a suppression of $T_c$.

II). All other cases with $\eta \neq 1$:

$$\tilde{\omega}_{an} = \omega_n + i\Sigma_0(\omega_n) + \frac{n_{\text{imp}}}{\pi N_a N_b} \left[ N_a \tilde{\omega}_{an} + N_b \tilde{\omega}_{bn} \right], \quad (13)$$

$$\tilde{\phi}_{an} = \Sigma_{2a}(\omega_n) + \frac{n_{\text{imp}}}{\pi N_a N_b} N_a \tilde{\phi}_{an} + N_b \tilde{\phi}_{bn}. \quad (14)$$

We get the same result, as for the intraband impurities since the other band (b) does not contribute to the equations. Surprisingly, but here the Anderson theorem works independent of the gap signs in different bands. Thus, $T_c$ should be finite for arbitrary impurity concentration.

Here we conclude, that there is a special case of $T_c$ suppression in the unitary limit for the uniform impurity potential $\eta = 1$. Such situation arise due to the structure of the denominator $D$ in equations (9)-(10). It vanishes for $\eta = \sigma = 1$ and one has to accurately take the limit $\eta \to 1$ first and only then put $\sigma \to 1$. It is the $\eta = 1$ case, that was considered in Ref. [4]. For all other values of $\eta$ (even for a slight difference between intraband and interband potentials) impurities are not going to affect the critical temperature.

2.2 Magnetic impurities

Now we switch to the magnetic disorder. Impurity potential for the non-correlated impurities can be written as $\tilde{U} = U \otimes \tilde{S}$, where $\tilde{S} = \text{diag} (\tilde{\sigma}_1 \cdot \mathbf{S}, -\tilde{\sigma}_1 \cdot \mathbf{S})$ is the $4 \times 4$ matrix with $(\cdot) T$ being the matrix transpose and $\mathbf{S} = (S_x, S_y, S_z)$ being the spin vector [20]. The vector $\tilde{\sigma}_1$ is composed of $\tau$ matrices, $\tilde{\sigma}_1 = (\tilde{\tau}_1, \tilde{\tau}_2, \tilde{\tau}_3)$. The potential strength is determined by $(V)_{\alpha\beta} = V_{\alpha\beta}^m a_{\alpha\beta}^m$.

For simplicity, intraband and interband parts of the potential are set equal to $I$ and $\mathcal{J}$, respectively, such that $(V)_{\alpha\beta} = (I - J)\delta_{\alpha\beta} + J$. Components of the impurity potential matrix $\tilde{U}$ is then $\tilde{U}_{aa,bb} = \tilde{I} S$ and $\tilde{U}_{ab,ba} = J \tilde{S}$. We introduce the parameter $\eta$ to control the ratio of intra- and interband scattering potentials, so that $\mathcal{J} = \eta \mathcal{J}$. Coupled $T$-matrix equations for $aa$ and $ba$ components of the self-energy become

$$\Sigma_{2a}^{\text{imp}} = n_{\text{imp}} \tilde{U}_{aa} + \tilde{U}_{aa} \tilde{\phi}_{aa} + \tilde{U}_{ab} \tilde{\phi}_{ba}$$

$$\Sigma_{2b}^{\text{imp}} = n_{\text{imp}} \tilde{U}_{ba} + \tilde{U}_{ba} \tilde{\phi}_{aa} + \tilde{U}_{bb} \tilde{\phi}_{ba}.$$  

Renormalizations of frequencies and gaps come from

$$\tilde{\omega}_{aa}^{\text{imp}} = \frac{1}{4} \text{Tr} \left[ \Sigma_{2a}^{\text{imp}} \cdot (\tilde{\phi}_0 \otimes \tilde{\phi}_0) \right]$$

and

$$\tilde{\omega}_{ba}^{\text{imp}} = \frac{1}{4} \text{Tr} \left[ \Sigma_{2a}^{\text{imp}} \cdot (\tilde{\phi}_2 \otimes \tilde{\phi}_2) \right].$$

Expressions for $\Sigma_{2a}^{\text{imp}}$ and $\Sigma_{2b}^{\text{imp}}$ are proportional to the effective impurity scattering rate $\Gamma_{a,b}$ and as in the case of nonmagnetic impurities contain the generalized cross-section parameter $\sigma$ that helps to control the approximation for the impurity strength ranging from Born (weak scattering, $\pi \mathcal{J} N_{a,b} \ll 1$) to the unitary (strong scattering, $\pi \mathcal{J} N_{a,b} \gg 1$) limits,

$$\Gamma_{a,b} = \frac{2n_{\text{imp}}}{\pi N_{a,b} \mathcal{J}}$$

$$\sigma = \frac{\mathcal{J}^2 S^2 N_{a,b}}{1 + \mathcal{J}^2 S^2 N_{a,b}^2} \rightarrow \begin{cases} 0, & \text{Born}, \\ 1, & \text{unitary}. \end{cases} \quad (18)$$

We assume that spins are not polarized and $s^2 = (S^2) = S(S+1)$. Since $s$ enters all equations only in conjunction with $I$ or $\mathcal{J}$, without losing generality we set $s = 1$ assuming that $I$ and $\mathcal{J}$ are both renormalized by $s$.

For the uniform impurity potential $\eta = 1$ in the Born limit $\sigma = 0$ we find

$$\tilde{\omega}_{an} = \omega_n + i\Sigma_0(\omega_n) + \frac{n_{\text{imp}}}{\pi N_a N_b} \left[ N_a \tilde{\omega}_{an} + N_b \tilde{\omega}_{bn} \right],$$

$$\tilde{\phi}_{an} = \Sigma_{2a}(\omega_n) - \mathcal{J}^2 n_{\text{imp}} \left[ N_a \tilde{\phi}_{an} + N_b \tilde{\phi}_{bn} \right].$$

Here contribution from both $a$ and $b$ bands are mixed so we expect a suppression of $T_c$ by disorder.

In the unitary limit ($\sigma = 0$) at $T \to T_c$ we have

$$\tilde{\omega}_{an} = \omega_n + i\Sigma_0(\omega_n) + \frac{n_{\text{imp}}}{\pi \left( N_a + N_b \right)} \text{sgn}(\omega_n),$$

$$\tilde{\phi}_{an} = \Sigma_{2a}(\omega_n) + \frac{n_{\text{imp}}}{\pi \left( N_a + N_b \right)} \left[ N_a \tilde{\phi}_{an} + N_b \tilde{\phi}_{bn} \right].$$
Both gaps are mixed in equation for $\tilde{\omega}_{n}$, thus they tend to zero with increasing amount of disorder. That’s also true away from the unitary limit and that’s why there is a special case of uniform potential of the impurity scattering, $I = J$, when the strongest $T_{c}$ suppression occurs.

3 Numerical results

Following results were obtained by solving self-consistently frequency and gap equations (2)-(3) for both finite temperature and at $T_{c}$ with the impurity self-energy as in Eqs. (9)-(10) for the nonmagnetic disorder or from the solution of Eqs. (15)-(16) for the magnetic impurities. For definiteness we choose $N_{b}/N_{a} = 2$ and coupling constants to be $(\lambda_{aa}, \lambda_{ab}, \lambda_{ba}, \lambda_{bb}) = (3, 0.2, 0.1, 0.5)$ for the $s_{++}$ state and $(3, -0.2, -0.1, 0.5)$ for the $s_{\pm}$ state with $\langle \lambda \rangle < 0$.

Typical results [10,13] of the dependence on the impurity scattering rate $I_{a}$ for the critical temperature $T_{c}$ and gaps $\Delta_{a,\pm}$ for the first Matsubara frequency $\omega_{n=1} = 3\pi T$ are shown in Fig. 1 (nonmagnetic) and in Fig. 2 (magnetic disorder). Scattering on magnetic impurities suppress both $s_{\pm}$ and $s_{++}$ states due to the finite interband scattering component. The $s_{++}$ state initially transforms to the $s_{\pm}$ state, but then follows its fate with increasing $I_{a}$. The only exception is the unitary limit. On the other hand, both states survive the nonmagnetic disorder but for different reasons: the $s_{++}$

due to the Anderson theorem, while the $s_{\pm}$ state transforms to the $s_{++}$. Unitary limit, again, gives constant result.

For the uniform impurity potentials the situation, however, becomes different. Results for $T_{c}$ and $\Delta_{an=1}$
Fig. 4 Uniform magnetic impurity potential $\eta = 1$: $T_c$ (a,c) and Matsubara gap $\Delta_{\alpha=1}$ (b,d) dependence on the scattering rate $I_n$ for the $s_\pm$ (a,b) and the $s_{++}$ (c,d) superconductors.

is shown in Fig. 3 for the nonmagnetic disorder and in Fig. 4 for the magnetic one. While behavior in the Born and intermediate scattering ($\sigma = 0.5$) limits are in general similar to those for $\eta \neq 1$, critical temperature and gaps in the unitary limit are not independent on disorder any more. Following the analytical results in the previous section, $T_c$ gradually decrease with increasing $I_n$. There is even a $s_\pm \to s_{++}$ transition for the magnetic impurities in the unitary limit, which is not seen for $\eta \neq 1$. On the other hand, there is no transition to the $s_\pm$ state for $\sigma = 0.5$, which appeared for $s_{++}$ state with unequal intra- and interband impurity potentials.

4 Conclusions

We have studied the case of uniform impurity potential, that is, the equal strength of intra- and interband scattering, $u = v$ and $I = J$ ($\eta = 1$). It appears to be qualitatively different from the other cases. This is particularly demonstrated in the unitary limit where for $\eta \neq 1$ there is an independence of gaps and $T_c$ on the values of both nonmagnetic and magnetic scattering. On the contrary, for the uniform impurity potential, there is a suppression of gaps and critical temperature due to the disorder.

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