Unexpected impact of magnetic disorder on multiband superconductivity

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(Dated: October 30, 2014)

We analyze how the magnetic disorder affects the properties of the two-band $s_\pm$ and $s_{++}$ models, which are subject of hot discussions regarding iron-based superconductors and other multiband systems like MgB$_2$. We show that there are several cases when the transition temperature $T_c$ is not fully suppressed by magnetic impurities in contrast to the Abrikosov-Gor’kov theory, but a saturation of $T_c$ takes place in the regime of strong disorder. These cases are: (1) the purely interband impurity scattering, (2) the unitary scattering limit. We show that in the former case the $s_\pm$ gap is preserved, while the $s_{++}$ state transforms into the $s_\pm$ state with increasing magnetic disorder. For the case (2), the gap structure remains intact.

PACS numbers: 74.70.Xa, 74.20.Rp, 74.62.En, 74.25.F-
I. METHOD

We employ the Eliashberg approach for multiband superconductors and calculate the $\xi$-integrated Green’s functions $g(\omega_n) = \int d\omega \hat{G}(k, \omega_n) = g_{\alpha n} \begin{pmatrix} \delta_{\alpha \beta} & 0 \\ 0 & \delta_{\alpha n} \end{pmatrix}$, where $g_{\alpha n} = g_{\alpha n} \delta_{\alpha \beta} + g_{\alpha n} \tau_2 \delta_{\alpha 2}$, indices $a$ and $b$ correspond to two distinct bands, index $\alpha = a, b$ denote the band space, Pauli matrices define Nambu $(\tau_i)$ and spin $(\sigma_i)$ spaces, $\hat{G}(k, \omega_n) = \big[ \hat{G}_0^{-1}(k, \omega_n) - \Sigma(\omega_n) \big]^{-1}$ is the matrix Green’s function for a quasiparticle with momentum $k$ and the Matsubara frequency $\omega_n = (2n+1)\pi T$ defined in the band space and in the combined Nambu and spin spaces, $\hat{G}_0^{-1}(k, \omega_n) = \big[ i\omega_n \tau_0 \otimes \delta_0 - \xi_{\alpha k} \tau_3 \otimes \sigma_0 \big]^{-1} \delta_{\alpha \beta}$ is the bare Green’s function, $\Sigma(\omega_n) = \sum_{\alpha \beta} \Sigma_{\alpha \beta}^{(i)}(\omega_n) \tau_i$ is the self-energy matrix, $\xi_{\alpha k} (k, \sigma, \epsilon, \mu)$ is the linearized dispersion, $g_{\alpha n}$ and $g_{\alpha n}$ are the normal and anomalous $\xi$-integrated Nambu Green’s functions,

$$g_{\alpha n} = -\frac{i\pi N_{\alpha n}}{\sqrt{\omega_n^2 + \phi_n^2}}, \quad g_{2\alpha n} = -\frac{\pi N_{\alpha n}}{\sqrt{\omega_n^2 + \phi_n^2}}, \quad (1)$$

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

$$\tilde{\omega}_{\alpha n} = \omega_n - \Sigma_{0\alpha}(\omega_n) - \Sigma_{0\alpha}^{\text{imp}}(\omega_n), \quad (2)$$

$$\tilde{\phi}_{\alpha n} = -\Sigma_{2\alpha}(\omega_n) + \Sigma_{2\alpha}^{\text{imp}}(\omega_n). \quad (3)$$

It is also convenient to introduce the renormalization factor $Z_{\alpha n} = \tilde{\omega}_{\alpha n}/\omega_n$ 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

$$\Sigma_{0\alpha}(\omega_n) = \frac{T}{\omega_n^2} \sum_{\omega, n'} \frac{\lambda_{\alpha \beta}^\phi(n - n') g_{0\beta n}}{N_{\beta}}, \quad (4)$$

$$\Sigma_{2\alpha}(\omega_n) = -T \sum_{\omega, n'} \frac{\lambda_{\alpha \beta}^\phi(n - n') g_{2\beta n}}{N_{\beta}}, \quad (5)$$

The coupling functions $\lambda_{\alpha \beta}^\phi(n - n') = 2\lambda_{\alpha \beta}^{\phi,\pi} \int_0^\infty d\Omega \Omega(\Omega)/\big[ (\omega_n - \omega_\mu)^2 + \Omega^2 \big]$ depend on the normalized bosonic spectral function $B(\Omega)$ used in Refs. 7, 8. While the matrix elements $\lambda_{\alpha \beta}^\phi$ can be positive (attractive) as well as negative (repulsive) due to the interplay between spin fluctuations and electron-phonon coupling, the matrix elements $\lambda_{\alpha \beta}^\phi$ are always positive. For simplicity we set $\lambda_{\alpha \beta}^\phi = |\lambda_{\alpha \beta}^\phi| = |\lambda_{\alpha \beta}|$ and neglect possible anisotropy in each order parameter $\tilde{\phi}_{\alpha n}$. Latter effects can lead to changes in the response of the two-band $s_\pm$ system to disorder and have been examined, e.g. in Ref. 29.

We use the $T$-matrix approximation to calculate the average impurity self-energy $\Sigma_{\alpha n}$:

$$\Sigma_{\alpha n}^{\text{imp}}(\omega_n) = n_{\text{imp}} \hat{U} + \hat{U} g(\omega_n) \Sigma_{\alpha n}^{\text{imp}}(\omega_n), \quad (6)$$

where $n_{\text{imp}}$ is the impurity concentration. Impurity potential for the non-correlated impurities can be written as $\hat{U} = v_{\text{imp}} \otimes \hat{S}$, where $\hat{S} = \text{diag} \big[ \hat{\sigma} \cdot \hat{S}, -(\hat{\sigma} \cdot \hat{S})^T \big]$ is the 4 x 4 matrix with $(\ldots)^T$ being the matrix transpose and $\hat{S} = (S_x, S_y, S_z)$ being the spin vector. The vector $\hat{\sigma}$ is composed of $\tau$ matrices, $\hat{\sigma} = (\hat{\tau}_1, \hat{\tau}_2, \hat{\tau}_3)$. The potential strength is determined by $(v_{\text{imp}})_{\alpha \beta} = v_{R_{\alpha \beta}}$. For simplicity intraband and interband parts of the potential are set equal to $\mathcal{I}$ and $\mathcal{J}$, respectively, such that $(v_{\text{imp}})_{\alpha \beta} = (\mathcal{I} - \mathcal{J})_{\alpha \beta} + \mathcal{J}$. Components of the impurity potential matrix $U$ is then $U_{\alpha a, \beta b} = \mathcal{I} \mathcal{S}$ and $U_{\alpha b, \beta a} = \mathcal{J} \mathcal{S}$. Coupled $T$-matrix equations for $a a$ and $b b$ components of the self-energy become

$$\Sigma_{\alpha a}^{\text{imp}} = n_{\text{imp}} U_{\alpha a} + U_{\alpha b} g_{\alpha b} \Sigma_{\alpha b}^{\text{imp}} + U_{\alpha b} g_{\alpha b} \Sigma_{\alpha b}^{\text{imp}}, \quad (7)$$

$$\Sigma_{\beta a}^{\text{imp}} = n_{\text{imp}} U_{\beta a} + U_{\beta b} g_{\alpha b} \Sigma_{\beta b}^{\text{imp}} + U_{\beta b} g_{\alpha b} \Sigma_{\beta b}^{\text{imp}}. \quad (8)$$

Renormalizations of frequencies and gaps come from $\Sigma_{0\alpha}^{\text{imp}} = \frac{1}{4} \text{Tr} \left[ \Sigma_{\alpha a}^{\text{imp}} \cdot (\tau_0 \otimes \delta_0) \right]$ and $\Sigma_{2\alpha}^{\text{imp}} = \frac{1}{4} \text{Tr} \left[ \Sigma_{\alpha a}^{\text{imp}} \cdot (\tau_2 \otimes \delta_2) \right]$.

II. RESULTS

Following results were obtained by solving self-consistently frequency and gap equations (2) and (3) with the impurity self-energy from the solution of Eqs. (7), (8) for both finite temperature and at $T_c$. Expressions for $\Sigma_{0\alpha}^{\text{imp}}$ and $\Sigma_{2\alpha}^{\text{imp}}$ are proportional to the effective impurity scattering rate $\Gamma_{\alpha \beta}$ and as in Ref. 7 contain the generalized cross-section parameter $\sigma$ that helps to control the approximation for the impurity strength ranging from Born (weak scattering, $\pi \mathcal{J} N_{\alpha b} \ll 1$) to the unitary (strong scattering, $\pi \mathcal{J} N_{\alpha b} \gg 1$) limits,

$$\Gamma_{\alpha \beta} = \frac{2n_{\text{imp}} \sigma}{\pi N_{\alpha b}} \Bigg\{ \begin{array}{ll} 2\pi J^2 s^2 n_{\text{imp}} N_{b \alpha}, & \text{Born} \\
\left( \frac{2n_{\text{imp}}}{\pi N_{\alpha b}} \right), & \text{unary} \end{array} \Bigg\}. \quad (9)$$

$$\sigma = \frac{\pi J^2 s^2 N_b}{1 + \pi^2 J^2 s^2 N_b N_b} \rightarrow \begin{cases} 0, & \text{Born} \\ 1, & \text{unary} \end{cases}. \quad (10)$$

Note that $\Gamma_{\alpha}$ here is twice as large as defined in Ref. 7. We assume that spins are not polarized and $s^2 = (S^2) = S(S + 1)$. Also, we introduce the parameter $\eta$ to control the ratio of intra- and interband scattering potentials, $\mathcal{I} = \mathcal{J} \eta$.

In Fig. 1(a,b) and 2 we plot $T_c$ and the gap function $\Delta_{\alpha n}$ for the first Matsubara frequency $\omega_n = 3\pi T$ vs. $\Gamma_{\alpha \beta}$ for a set of $\sigma$’s for both $s_\pm$ and $s_{++}$ superconductors. Real part of the analytical continuation of $\Delta_{\alpha n}$ to real frequencies, the gap function $\text{Re} \Delta_{\alpha}(\omega)$, is shown in Fig. 1(c,d). First, we discuss the $s_\pm$ state. $T_c$ becomes insensitive to impurities for the pure interband scattering, $\mathcal{I} = 0$. This partially confirms qualitative arguments that $s_\pm$ state with magnetic disorder behave like the $s_{++}$ state with non-magnetic impurities and...
agrees with the quantitative theoretical calculations in the Born limit. For the finite $I$, intraband scattering on magnetic disorder average gaps to zero thus suppressing $T_c$. On the other hand, in the unitary limit ($\sigma = 1$) at $T \rightarrow T_c$ we have $\omega_{an} = \omega_n + i\Sigma_{\text{imp}}(\omega_n) + \frac{\Gamma_a}{2} \text{sgn}(\omega_n)$ and $\phi_{an} = \Sigma_{2a}(\omega_n) + \frac{\Gamma_a}{2} \frac{\phi_{\text{imp}}}{|\omega_n|}$ for any value of $\eta$ including the case of intraband-only impurities, $1/\eta = 0$. This form is the same as for non-magnetic impurities and thus analogously to the Anderson theorem there is no impurity contribution to the $T_c$ equation. The only exception here is the special case of uniform impurities, $\eta = 1$, when $\omega_{an} = \omega_n + i\Sigma_{\text{imp}}(\omega_n) + \frac{\text{imp}}{\pi(N_a+N_b)} \text{sgn}(\omega_n)$ and $\phi_{an} = \Sigma_{2a}(\omega_n) + \frac{\text{imp}}{\pi(N_a+N_b)} \left(N_a \frac{\phi_{\text{imp}}}{|\omega_n|} + N_b \frac{\phi_{\text{imp}}}{|\omega_n|} \right)$. Both gaps are mixed in equation for $\phi_{an}$, 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. For the initially unequal gaps, $|\Delta_a| \neq |\Delta_b|$, there is an initial decrease of $T_c$ for small $\Gamma_a$ until the renormalized gaps become equal and then $T_c$ saturates since the analog of Anderson theorem achieved.

In general, multiband $s_{++}$ state should always be fragile against paramagnetic disorder since magnetic scattering between bands of the same sign effectively equivalent to the pairbreaking scattering within the single (quasi)isotropic band. Surprisingly, we find a regime with the saturation of $T_c$ for the finite amount of disorder right after the initial AG downfall, see Fig. 1(b). The saturation of $T_c$ is observed for the interband-only impurities; presence of the intraband magnetic disorder finally suppress $T_c$ to zero. But depending on the “strength” of scattering $\sigma$, decrease of $T_c$ may be quite slow compared to the AG law.

To understand the origin of the $T_c$ saturation we analyzed the gap function dependence on the scattering rate $\Gamma_a$, see Fig. 2. For the $s_{++}$ state after the certain value of the scattering rate the smaller gap, $\Delta_b$, becomes negative. What we see is the $s_{++} \rightarrow s_\pm$ transition. As soon as system becomes effectively $s_\pm$, the scattering on magnetic impurities cancels out in the $T_c$ equation similar to the Anderson theorem and $T_c$ saturates. Before saturation, the initial AG downfall takes place. The transition is also seen in the gap function on real frequencies, Fig. 1(d).

Similar to the $s_\pm \rightarrow s_{++}$ transition for the non-magnetic disorder, there is a simple physical argument behind the $s_{++} \rightarrow s_\pm$ transition here. Namely, with increasing interband magnetic disorder, the gap functions on the different Fermi surfaces tend to the same value and if one of the gaps is smaller than another, it cross zero and change sign. A similar effect has been mentioned in Refs.10,32 for a two-band systems with $s_{++}$ symmetry in the Born limit. Note that here we do not consider possible time-reversal symmetry broken $s_\pm + is_{++}$ state that may be energetically favorable below $T_c$ in cases when
translational symmetry is broken\textsuperscript{33}.

Since one of the gaps changes sign it necessary goes through zero. That corresponds to the gapless superconductivity. Therefore, the transition should manifest itself in the density of states measurable by tunneling and ARPES $N(\omega) = -\sum\alpha \text{Im} g_{\alpha\alpha}(\omega)/\pi$, where $g_{\alpha\alpha}(\omega)$ is the retarded Green’s function, and in the temperature dependence of the London penetration depth $\lambda_L$,

$$\frac{1}{\lambda_L^2} = \sum_{\alpha} \frac{\omega_p^2}{\omega_{\alpha n}} T \frac{\pi N^2 \sqrt{\omega_{\alpha n}^2 + \phi_{\alpha n}^2}}{g_{\alpha n}} ,$$

where $\omega_p/c$ is the ratio of the plasma frequency to the sound velocity that we set to unity for simplicity. In Fig. 3 and 4 we show $N(\omega)$ and $1/(\omega_p \lambda_L)^2$ for the case of $\mathcal{I} = \mathcal{J}/2$ and $\sigma = 0.5$ for $s_\pm$ and $s_{++}$ superconductors. In the former case, Fig. 3 reflects the expected situation of the gradually decreasing gaps. The gapless superconductivity with a finite residual $N(\omega = 0)$ appears for $\Gamma_a > 300$ cm\textsuperscript{-1} when $\text{Re}\Delta_n(\omega = 0)$ vanishes, see 1(c). As for the $s_{++}$ case in Fig. 4, with increasing impurity scattering rate $\Gamma_a$, the smaller gap vanishes leading to a finite residual $N(\omega = 0)$. Then the gap reopens and $\Delta_{bn} \neq 0$ until $T_c$ reaches zero for $\Gamma_a \sim 600$ cm\textsuperscript{-1}, but the superconductivity remains gapless with finite $N(0)$ due to the $\text{Re}\Delta_n(\omega = 0) \rightarrow 0$, see Fig. 1(d). Penetration depth in the clean limit shows the activated behavior controlled by the smaller gap. For the $s_{++}$ superconductor it goes to the $T^2$ behavior in the gapless regime showing a pronounced dip in Fig. 4 around $\Gamma_a = 100$ cm\textsuperscript{-1} and crosses over to a new activated behavior in the $s_{+-}$ state after the transition.

III. CONCLUSIONS

We have shown that contrary to the common wisdom in two-band models few exceptional cases exist with the saturation of $T_c$ for the finite amount of magnetic disorder. The particular case is the $s_{\pm}$ state in the unitary limit or with the purely interband impurity scattering potential. The latter satisfies qualitative assessment of direct relation between magnetic impurities in $s_{\pm}$ state...
and non-magnetic impurities in isotropic s-wave state. We demonstrate that $s_{++}$ superconductivity may be robust against magnetic impurities with the purely interband scattering due to the transition to the $s_{\pm}$ state. Therefore, it may manifest itself in optical and tunneling experiments, as well as in a photoemission and thermal conductivity on FeBS and other multiband systems.

The authors are grateful to S.-L. Drechsler, P.J. Hirschfeld, K. Kikoin, and S.G. Ovchinnikov for useful discussions. We acknowledge partial support by the Dynasty Foundation and ICFPM (MMK), the Ministry of Education and Science of the Russian Federation (Grant No. 14Y26.31.0007), RFBR (Grants 12-02-31534 and 13-02-01395), President Grant for Government Support of the Leading Scientific Schools of the Russian Federation (NSh-2886.2014.2), DFG Priority Program 1458, and FP7 EU-Japan program IRON SEA.

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