Unexpected impact of magnetic disorder on multiband superconductivity

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We analyze how the magnetic disorder affects the properties of the two-band $s_\pm$ and s_{++} models, which are the subject of 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 and (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 case (2), the gap structure remains intact.

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I. INTRODUCTION

Since the discovery of Fe-based superconductors (FeBS) in 2008 [1], the main question remains open: What is the driving mechanism for superconductivity in this class of materials? Excluding the cases of extreme hole and electron dopings, the Fermi surface (FS) consisting 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 naturally leads to the enhanced antiferromagnetic fluctuations. They lead to the s-wave-like order parameter that changes sign between electron and hole pockets, the so-called $s_\pm$ state [2]. On the other hand, bands near the Fermi level have mixed orbital content and orbital fluctuations enhanced by the electron-phonon coupling may lead to the sign-preserving s-wave gap, the s_{++} state [3,4]. Most experimental data including observation of the spin-resonance peak in inelastic neutron scattering, quasiparticle interference in tunneling experiments, and NMR spin-lattice relaxation rate are in favor of the $s_\pm$ scenario, although gap anisotropy varies from one material to the other [2]. Therefore, an experimental probe that can uniquely pinpoint the gap structure is of high demand.

It was suggested some time ago that the scattering on impurities may disentangle sign-changing and sign-preserving gaps [5–9]. Usually, nonmagnetic impurity scattering between the bands with different signs of the gaps leads to suppression of the critical temperature T_c similar to magnetic impurity scattering in a single-band BCS superconductor [10]. Then T_c is determined from the Abrikosov-Gor'kov (AG) expression $\ln T_{c0}/T_c = \Psi(1/2 + \Gamma/2\pi T_c) - \Psi(1/2)$, where $\Psi(x)$ is the digamma function, Γ is the impurity scattering rate, and T_{c0} is the critical temperature in the absence of impurities [11]. However, it was recently shown that in the multiband superconductors the behavior may be more complicated [7,10,12]. In particular, T_c is almost constant for varying the amount of nonmagnetic disorder in i) unitary limit of the uniform intra- vs interband scattering potentials [13] and ii) $s_\pm \to s_{++}$ transition for the sizable intraband attraction in the two-band $s_\pm$ model in the strong-coupling T-matrix approximation [7]. Qualitatively these results were confirmed via the numerical solutions of the Bogoliubov-de Gennes equations [14,15]. Several experiments show that the T_c suppression is much weaker than expected in the framework of the AG theory for both nonmagnetic [16–21] and magnetic disorder [16,22–25]. Overall, there is no clear answer to whether the sign-changing order parameter symmetry is prevailing in FeBS. In such a situation, additional information can be gained from studies of the magnetic impurities.

Here we study two-band models for the isotropic $s_\pm$ and s_{++} superconductors with the magnetic impurities in the self-consistent T-matrix approximation [26]. We argue that T_c and order parameter dependencies on the concentration of magnetic impurities have some peculiarities, which may help to identify the order parameter in the clean case. The common wisdom is that the magnetic impurities should suppress superconductivity. We show that while in general there is a suppression of superconducting state with increasing concentration of magnetic disorder, there are several regimes with either the absence of the T_c suppression or the drastic reduction of this effect. But even if T_c is completely suppressed, its behavior may differ from the AG theory for the single-band superconductors. Other prototypical examples of multiband systems where our theory is applicable include MgB_2 and the approximate treatment of the d-wave superconductors like cuprates where the parts of the Fermi surface with the different signs of the gap to some extent can be considered as different bands.

II. METHOD

We employ the Eliashberg approach for multiband superconductors [26] and calculate the ξ-integrated Green's

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functions

$$\hat{\mathbf{g}}(\omega_n) = \int d\xi \hat{\mathbf{G}}(\mathbf{k},\omega_n) = \begin{pmatrix} \hat{g}_{an} & 0 \\ 0 & \hat{g}_{bn} \end{pmatrix},$$

where $\hat{g}_{\alpha n} = g_{0\alpha n}\hat{\tau}_0 \otimes \hat{\sigma}_0 + g_{2\alpha n}\hat{\tau}_2 \otimes \hat{\sigma}_2$, indices a and b correspond to two distinct bands, index $\alpha = a,b$ denote the band space, Pauli matrices define Nambu ($\hat{\tau}_i$) and spin ($\hat{\sigma}_i$) spaces, $\hat{\mathbf{G}}(\mathbf{k},\omega_n) = [\hat{\mathbf{G}}_0^{-1}(\mathbf{k},\omega_n) - \hat{\Sigma}(\omega_n)]^{-1}$ is the matrix Green's function for a quasiparticle with momentum $\mathbf{k}$ and the Matsubara frequency $\omega_n = (2n+1)\pi T$ defined in the band space and in the combined Nambu and spin spaces, $\hat{G}_0^{\alpha\beta}(\mathbf{k},\omega_n) = [\mathrm{i}\omega_n \hat{\tau}_0 \otimes \hat{\sigma}_0 - \xi_{\alpha\mathbf{k}}\hat{\tau}_3 \otimes \hat{\sigma}_0]^{-1}\delta_{\alpha\beta}$ is the bare Green's function, $\hat{\Sigma}(\omega_n) = \sum_{i=0}^{3} \Sigma_{\alpha\beta}^{(i)}(\omega_n)\hat{\tau}_i$ is the self-energy matrix, $\xi_{\alpha,\mathbf{k}} = v_{\alpha,F}(k - k_{\alpha,F})$ is the linearized dispersion, $g_{0\alpha n}$ and $g_{2\alpha n}$ are the normal and anomalous ξ-integrated Nambu Green's functions,

$$g_{0\alpha n} = -\frac{\mathrm{i}\pi N_\alpha \tilde{\omega}_{\alpha n}}{\sqrt{\tilde{\omega}_{\alpha n}^2 + \tilde{\phi}_{\alpha n}^2}}, \quad g_{2\alpha n} = -\frac{\pi N_\alpha \tilde{\phi}_{\alpha n}}{\sqrt{\tilde{\omega}_{\alpha n}^2 + \tilde{\phi}_{\alpha n}^2}}, \tag{1}$$

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 $\tilde{\phi}_{\alpha n}$ and frequency $\tilde{\omega}_{\alpha n}$,

$$\mathrm{i}\tilde{\omega}_{an} = \mathrm{i}\omega_n - \Sigma_{0a}(\omega_n) - \Sigma_{0a}^{\mathrm{imp}}(\omega_n), \tag{2}$$

$$\tilde{\phi}_{an} = \Sigma_{2a}(\omega_n) + \Sigma_{2a}^{\mathrm{imp}}(\omega_n). \tag{3}$$

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

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

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

The coupling functions $\lambda_{\alpha\beta}^{\phi,z}(n-n') = 2\lambda_{\alpha\beta}^{\phi,z}\int_0^\infty d\Omega\Omega B(\Omega)/[(\omega_n - \omega_{n'})^2 + \Omega^2]$ depend on the normalized bosonic spectral function $B(\Omega)$ used in Refs. [7] and [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 [27,28], the matrix elements $\lambda_{\alpha\beta}^{z}$ are always positive. For simplicity we set $\lambda_{\alpha\beta}^{z} = |\lambda_{\alpha\beta}^{\phi}| \equiv |\lambda_{\alpha\beta}|$ 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 $\hat{\Sigma}^{\mathrm{imp}}$:

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

where n_{imp} is the impurity concentration. Impurity potential for the noncorrelated impurities can be written as $\hat{\mathbf{U}} = \mathbf{V} \otimes \hat{S}$, where $\hat{S} = \mathrm{diag}[\vec{\hat{\sigma}} \cdot \vec{S}, -(\vec{\hat{\sigma}} \cdot \vec{S})^T]$ is the 4×4 matrix with $(\ldots)^T$ being the matrix transpose and $\vec{S} = (S_x,S_y,S_z)$ being the spin vector [30]. The vector $\vec{\hat{\sigma}}$ is composed of τ matrices, $\vec{\hat{\sigma}} = (\hat{\tau}_1,\hat{\tau}_2,\hat{\tau}_3)$. The potential strength is determined by $(\mathbf{V})_{\alpha\beta} = V_{\mathbf{R}_i=0}^{\alpha\beta}$. For simplicity intraband and interband parts of the potential are set equal to $\mathcal{I}$ and $\mathcal{J}$, respectively, such that $(\mathbf{V})_{\alpha\beta} = (\mathcal{I} - \mathcal{J})\delta_{\alpha\beta} + \mathcal{J}$. Components of the impurity potential matrix $\hat{\mathbf{U}}$ is then $\hat{U}_{aa,bb} = \mathcal{I}\hat{S}$ and $\hat{U}_{ab,ba} = \mathcal{J}\hat{S}$. Coupled T-matrix equations for aa and ba components of the self-energy become

$$\hat{\Sigma}_{aa}^{\mathrm{imp}} = n_{\mathrm{imp}}\hat{U}_{aa} + \hat{U}_{aa}\hat{g}_a\hat{\Sigma}_{aa}^{\mathrm{imp}} + \hat{U}_{ab}\hat{g}_b\hat{\Sigma}_{ba}^{\mathrm{imp}}, \tag{7}$$

$$\hat{\Sigma}_{ba}^{\mathrm{imp}} = n_{\mathrm{imp}}\hat{U}_{ba} + \hat{U}_{ba}\hat{g}_a\hat{\Sigma}_{aa}^{\mathrm{imp}} + \hat{U}_{bb}\hat{g}_b\hat{\Sigma}_{ba}^{\mathrm{imp}}. \tag{8}$$

Renormalizations of frequencies and gaps come from $\Sigma_{0a}^{\mathrm{imp}} = \frac{1}{4}\mathrm{Tr}[\hat{\Sigma}_{aa}^{\mathrm{imp}} \cdot (\hat{\tau}_0 \otimes \hat{\sigma}_0)]$ and $\Sigma_{2a}^{\mathrm{imp}} = \frac{1}{4}\mathrm{Tr}[\hat{\Sigma}_{aa}^{\mathrm{imp}} \cdot (\hat{\tau}_2 \otimes \hat{\sigma}_2)]$.

III. 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) and (8) for both finite temperature and at T_c. Expressions for $\Sigma_{0\alpha}^{\mathrm{imp}}$ and $\Sigma_{2\alpha}^{\mathrm{imp}}$ are proportional to the effective impurity scattering rate $\Gamma_{a,b}$ and as in Ref. [7] contain the generalized cross-section parameter σ 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,

$$\Gamma_{a,b} = \frac{2n_{\mathrm{imp}}\sigma}{\pi N_{a,b}} \to \begin{cases} 2\pi\mathcal{J}^2 s^2 n_{\mathrm{imp}} N_{b,a}, \text{Born} \\ \frac{2n_{\mathrm{imp}}}{\pi N_{a,b}}, \text{unitary} \end{cases} \tag{9}$$

$$\sigma = \frac{\pi^2\mathcal{J}^2 s^2 N_a N_b}{1 + \pi^2\mathcal{J}^2 s^2 N_a N_b} \to \begin{cases} 0, \text{Born} \\ 1, \text{unitary} \end{cases} \tag{10}$$

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

In Figs. 1(a), 1(b), and 2 we plot T_c and the gap function $\Delta_{\alpha n}$ for the first Matsubara frequency $\omega_{n=1} = 3\pi T$ vs Γ_a for a set of σ's for both $s_\pm$ and s_{++} superconductors. Real part of the analytical continuation of $\Delta_{\alpha n}$ to real frequencies, the gap function $\mathrm{Re}\Delta_\alpha(\omega)$, is shown in Figs. 1(c) and 1(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 the $s_\pm$ state with magnetic disorder behaves like the s_{++} state with nonmagnetic impurities [10] and agrees with the quantitative theoretical calculations in the Born limit [31]. For the finite $\mathcal{I}$, intraband scattering on magnetic disorder average gaps to zero thus suppressing T_c. On the other hand, in the unitary limit ($\sigma = 1$) at $T \to T_c$ we have $\tilde{\omega}_{an} = \omega_n + \mathrm{i}\Sigma_{0a}(\omega_n) + \frac{\Gamma_a}{2}\mathrm{sgn}(\omega_n)$ and $\tilde{\phi}_{an} = \Sigma_{2a}(\omega_n) + \frac{\Gamma_a}{2}\frac{\tilde{\phi}_{an}}{|\tilde{\omega}_{an}|}$ for any value of η including the case of intraband-only impurities, $1/\eta = 0$. This form is the same as for nonmagnetic 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 $\tilde{\omega}_{an} = \omega_n + \mathrm{i}\Sigma_{0a}(\omega_n) + \frac{n_{\mathrm{imp}}}{\pi(N_a+N_b)}\mathrm{sgn}(\omega_n)$ and $\tilde{\phi}_{an} = \Sigma_{2a}(\omega_n) + \frac{n_{\mathrm{imp}}}{\pi(N_a+N_b)^2}(N_a\frac{\tilde{\phi}_{an}}{|\tilde{\omega}_{an}|} + N_b\frac{\tilde{\phi}_{bn}}{|\tilde{\omega}_{bn}|})$. Both gaps are

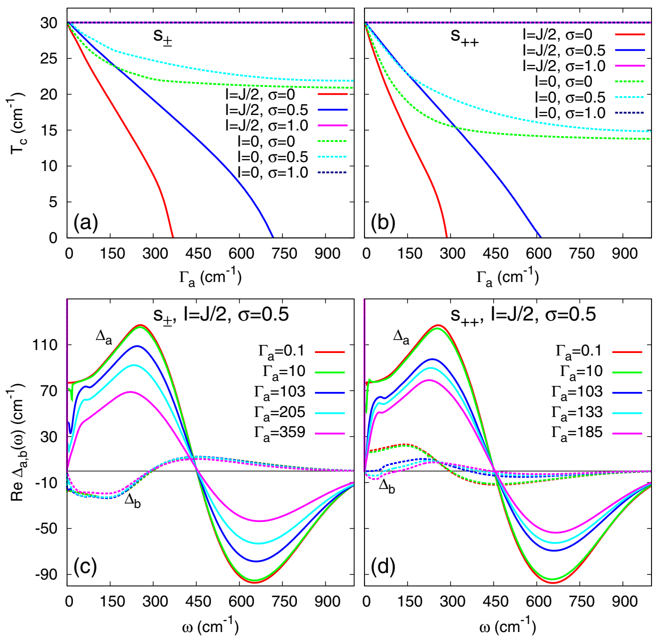

FIG. 1. (Color online) T_c dependence on the scattering rate Γ_a (a),(b) and frequency dependence of gaps $\mathrm{Re}\Delta_\alpha(\omega)$ (c),(d) for various values of Γ_a for the $s_\pm$ (a),(c) and the s_{++} (b),(d) superconductors. $N_b/N_a = 2$ and coupling constants are $(\lambda_{aa},\lambda_{ab},\lambda_{ba},\lambda_{bb}) = (3,-0.2,-0.1,0.5)$ so that $\langle\lambda\rangle < 0$ for the $s_\pm$ state and $(3,0.2,0.1,0.5)$ for the s_{++} state.

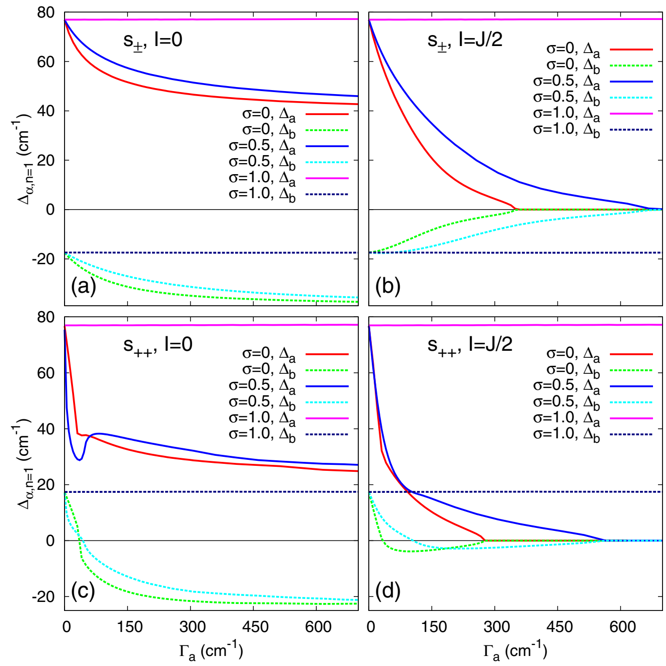

FIG. 2. (Color online) Matsubara gap $\Delta_{\alpha n=1}$ dependence on the scattering rate Γ_a for the $s_\pm$ (a),(b) and the s_{++} (c),(d) superconductors with only interband scattering, $\mathcal{I} = 0$ (a),(c), and with $\mathcal{I} = \mathcal{J}/2$ (b),(d). Parameters are the same as in Fig. 1.

mixed in the equation for $\tilde{\phi}_{an}$, thus they tend to zero with an 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, $\mathcal{I} = \mathcal{J}$, 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 Γ_a until the renormalized gaps become equal and then T_c saturate 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; the presence of the intraband magnetic disorder finally suppresses T_c to zero. But depending on the "strength" of scattering σ, 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 Γ_a, see Fig. 2. For the s_{++} state after the certain value of the scattering rate, the smaller gap Δ_b becomes negative. What we see is the $s_{++} \to s_\pm$ transition. As soon as the 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 $s_\pm \to s_{++}$ transition for the nonmagnetic disorder, there is a simple physical argument behind the $s_{++} \to s_\pm$ 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 crosses zero and change sign. A similar effect has been mentioned in Refs. [10] and [32] for a two-band systems with s_{++} symmetry in the Born limit. Note that here we do not consider a possible time-reversal symmetry broken $s_\pm + is_{++}$ state that may be energetically favorable below T_c in cases when translational symmetry is broken [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 $N(\omega) = -\sum_\alpha \mathrm{Im} g_{0\alpha}(\omega)/\pi$, where $g_{0\alpha}(\omega)$ is the retarded Green's function, and in the temperature dependence of the London penetration depth λ_L, $\frac{1}{\lambda_L^2} = \sum_\alpha \frac{\omega_{P\alpha}^2}{c^2} T \sum_n \frac{g_{2\alpha n}^2}{\pi N_\alpha^2 \sqrt{\tilde{\omega}_{\alpha n}^2 + \tilde{\phi}_{\alpha n}^2}}$, where $\omega_{P\alpha}/c$ is the ratio of the plasma frequency to the sound velocity that we set to unity for simplicity. In Figs. 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 $\Gamma_a > 300\ \mathrm{cm}^{-1}$ when $\mathrm{Re}\Delta_\alpha(\omega = 0)$ vanishes, see Fig. 1(c). As for the s_{++} case in Fig. 4, with increasing impurity scattering rate Γ_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 $\Gamma_a \sim 600\ \mathrm{cm}^{-1}$, but the superconductivity remains gapless with finite $N(0)$ due to the $\mathrm{Re}\Delta_\alpha(\omega = 0) \to 0$, see Fig. 1(d). Penetration depth in the clean limit shows the

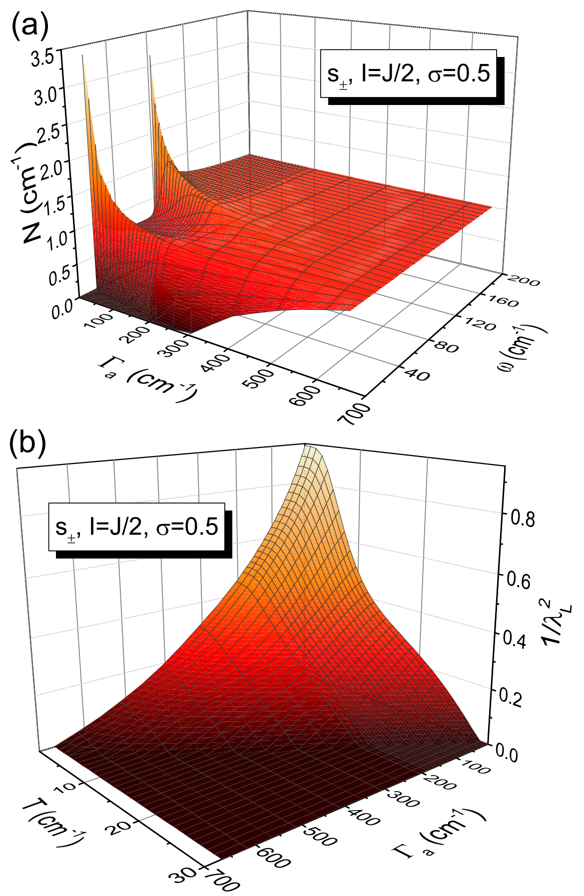

FIG. 3. (Color online) Density of states N as a function of frequency ω and interband magnetic impurities scattering rate Γ_a (a) and inverse squared penetration depth $1/\lambda_L^2$ vs. Γ_a and T (b) for the $s_\pm$ superconductor with $\mathcal{I} = \mathcal{J}/2$, $\sigma = 0.5$, and parameters as in Fig. 1.

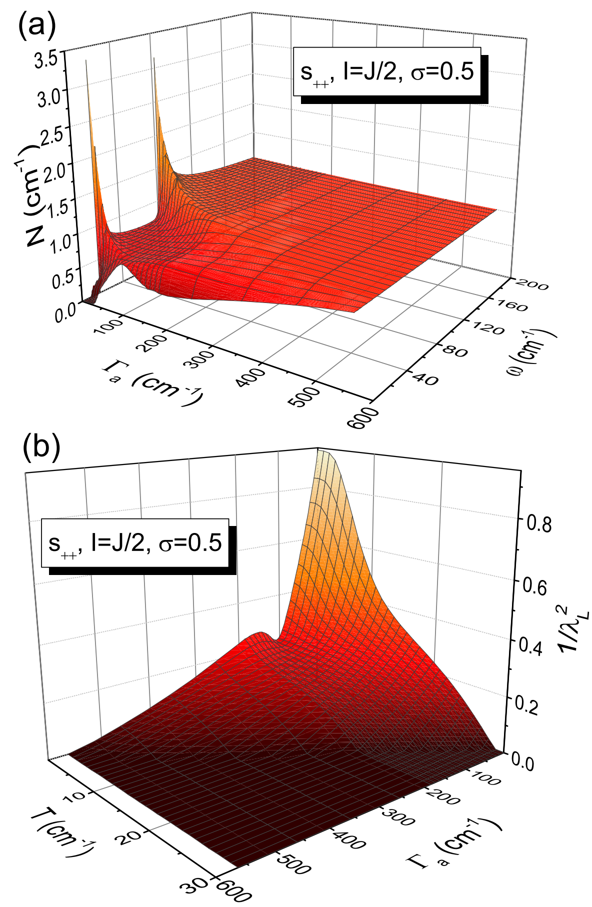

FIG. 4. (Color online) Density of states N as a function of frequency ω and Γ_a (a) and inverse squared penetration depth $1/\lambda_L^2$ vs Γ_a and T (b) for the s_{++} superconductor with $\mathcal{I} = \mathcal{J}/2$, $\sigma = 0.5$, and parameters as in Fig. 1. Note the s_{++} to $s_\pm$ transition at $\Gamma_a \sim 100$ cm^{-1} and the gapless region right after that.

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^{-1} and crosses over to a new activated behavior in the s_{+-} state after the transition.

IV. 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 the $s_\pm$ state and nonmagnetic impurities in the 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. Since this transition goes through the gapless regime, there should be clear signatures in the thermodynamics of the system. 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.

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