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Magnetic impurity-induced states in the gap of an s± superconductor

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We consider a two-band superconductor (SC) whose order parameter (OP) components in each band are constants of opposite sign. Conduction electrons interact with impurities described by the Anderson model. We calculate the density of states (DOS) of this system within a mean-field slave-boson approximation. The position of impurity-induced states in the energy gap depends strongly on the relative size of the energy of the impurity resonant level ε_f, its width Γ and the size of OP components Δ_1, Δ_2. In the Kondo limit the bound states are at the gap center or in its vicinity. In the mixed valence regime these bound states can be located far from the gap center. However they never reach the edge of the smaller of the two superconducting gaps. We also briefly discuss the consequences of varying the relative strengths of pairing and impurity coupling on low-energy properties of the system.

1 Introduction Experimental evidence suggests that in many of the recently discovered Fe-based superconductors (SCs) [1] Cooper pairs are formed in more than one band. The order parameter (OP) may have an overall s-wave symmetry with a different magnitude and possibly different sign in each band. The simplest model of this kind is a two-band SC with an OP constant over each of the Fermi surface sheets (see *e.g.* reviews [2–6]). This state is often referred to as s±.

Properties of such SC in presence of disorder has been a subject of a great interest recently [7–18]. Strongly scattering impurities cause resonant states to appear in the SC gap, significantly altering low-temperature properties. The resonant states induced by magnetic impurities in SCs with an s-wave OP component are much sharper than in the case of nonmagnetic scattering. In an earlier work on magnetic impurities in a d + s-wave SC we showed that there may even be a discontinuous transition in the impurity and conduction electron spectrum [19].

2 Model and results We calculate density of states (DOS) of an s± state doped with finite concentration of magnetic impurities, using the large-N, mean field slave boson formalism developed for a single Anderson impurity in a normal state [20–22], and extended to include superconducting interaction and finite concentration of impurities [23, 24] in a one-band SC. The SU(N) Hamiltonian takes the form

$$H = \sum_{k,i,m} \varepsilon_{ki} c^{\dagger}_{kim} c_{kim} + E_0 \sum_m f^{\dagger}_m f_m + V \sum_{k,i,m} [c^{\dagger}_{kim} f_m b + h.c.] + \sum_{k,i,m} [\Delta_i c^{\dagger}_{ki} c^{\dagger}_{-ki-m} + h.c.] + \lambda \left(\sum_m f^{\dagger}_m f_m + b^{\dagger} b - 1 \right), \tag{1}$$

where E_0 is the energy of a localized orbital, V is the hybridization matrix element between localized states and conduction states with dispersion ε_{ki}, where $i = 1,2$ is the band index, λ is a Lagrange multiplier preventing double occupancy of the impurity site, $\sum_m f^{\dagger}_m f_m + b^{\dagger} b = 1$. The OP has two different components in each of the bands, Δ_1, Δ_2, differing in magnitude and sign. We assume $\Delta_2/\Delta_1 = -0.4$ for most of the calculations, which is close to experimental data [25–27]. The conduction bands are assumed to have a flat normal-state DOS, $N_0 = N_1(\omega) + N_2(\omega) = 1/2D$. Following the argument of Bang [10], the DOS ratio of the two bands is assumed to be, $N_2(\omega)/N_1(\omega) = 2.6$.

In general the mean-field approach requires solving equations determining the resonant level energy ε_f and width Γ and the gap equations for Δ_1 and Δ_2, given V, E_0, and the impurity concentration [23, 24]. However, since we are not interested in the temperature dependence of physical quantities, we avoid deriving Γ and ε_f from V and E_0, and work with assumed values of Γ and ε_f. They can always be related to V and E_0 in a full calculation.

$$G_i(\omega) = G_{0i}(\omega)^{-1} - \Sigma(\omega) = \tilde{\omega}\tau_0 - \varepsilon_{ki}\tau_3 - \tilde{\Delta}_i(k)\tau_1, \tag{2}$$

$$G_f(\omega)^{-1} = G_f(\omega)^{-1} - \Sigma_f(\omega) = \overline{\omega} - \varepsilon_f\tau_3 - \overline{\Delta}\tau_1, \tag{3}$$

where renormalized quantities are calculated self-consistently from the Dyson equations. We simplify the calculations assuming small impurity concentration in order to avoid the renormalization of Δ_i.

Depending on the relative size of Γ/ε_f, there may be either two impurity-induced bands or one, see Fig. 1. For $\Gamma \gtrsim \varepsilon_f$, the gap between the impurity bands vanishes, see Fig. 2. Large ratios of Γ/ε_f, characteristic of the Kondo limit, favor a single resonance located at the gap center.

An increase of impurity concentration n may lead to merging of the resonant states, as shown in Fig. 3. In this case DOS at the Fermi level scales as $N_{\mathrm{tot}}(0) \sim (n - n_c)^{1/2}$, where n_c is the critical value, at which N_{tot} (0) becomes greater than zero.

For $T_K \gg \Delta_1$, where $T_K = \sqrt{\Gamma^2 + \varepsilon_f^2}$, the location of impurity induced-states ω_b depends on the ratio Γ/ε_f. For $\Gamma/\varepsilon_f \gg 1$, ω_b is close to 0. For $\Gamma \sim \varepsilon_f$, ω_b approaches Δ_1, but does not reach the gap edge, see Fig. 4. This is in contrast to a conventional s-wave SC, where in the limit $T_K/T_c \to \infty$ the impurity states disappear into the gap edge.

Dependence of ω_b on the size of the smaller gap Δ_2 in the Kondo limit is shown in Fig. 5. As $|\Delta_2|$ decreases, $|\omega_b|$ moves to the center of the gap. The ratio N_2/N_1 has no influence on

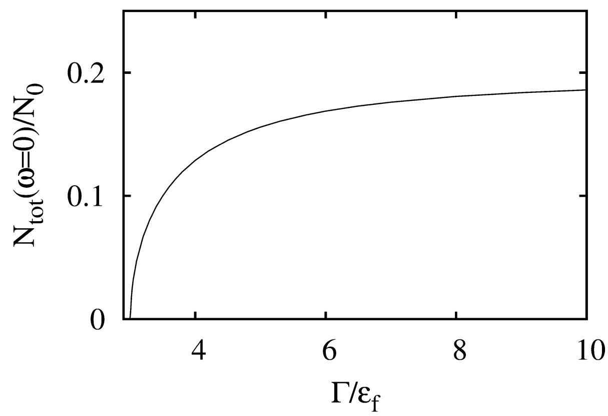

Figure 2 DOS at $\omega = 0$ as a function of Γ/ε_f. Impurity concentration is $n = 10^{-4}$ and $\Delta_2 = -0.4\ \Delta_1$.

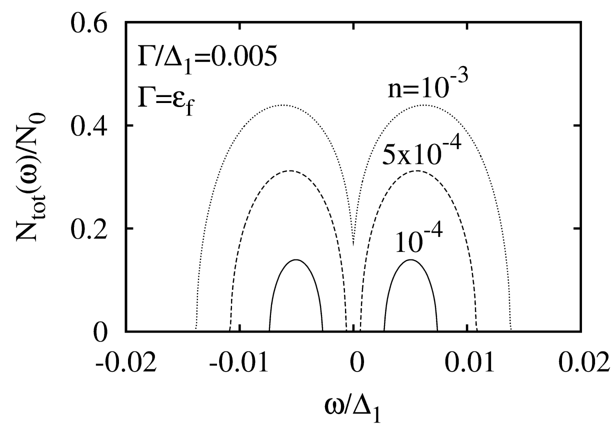

Figure 3 DOS near the gap center for different impurity concentrations n. For larger n there is a single maximum of $N_{\mathrm{tot}}(\omega)$ at $\omega = 0$. Here $\Delta_2 = -0.4\ \Delta_1$.

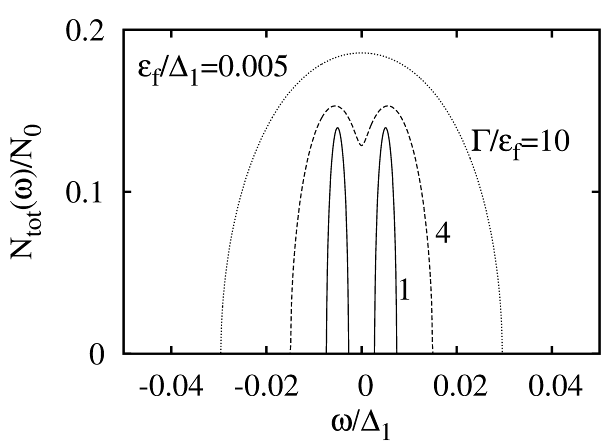

Figure 1 DOS near the gap center as a function of the ratio Γ/ε_f. Impurity concentration is fixed at $n = 10^{-4}$. The smaller gap is $\Delta_2/\Delta_1 = -0.4$.

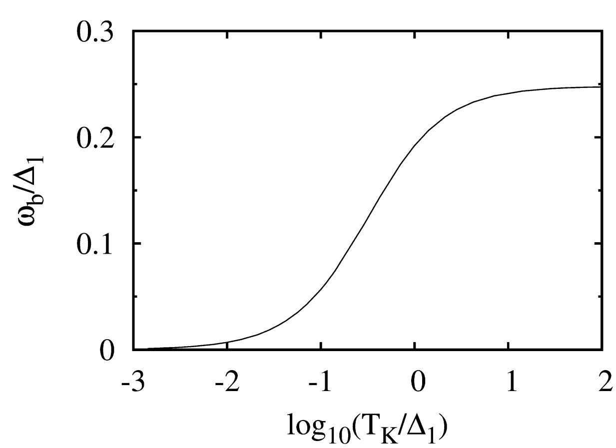

Figure 4 Position of bound states in the gap as a function of the ratio T_K/Δ_1, where $T_K = \sqrt{\Gamma^2 + \varepsilon_f^2}$. Here $\Delta_2 = -0.4\Delta_1$.

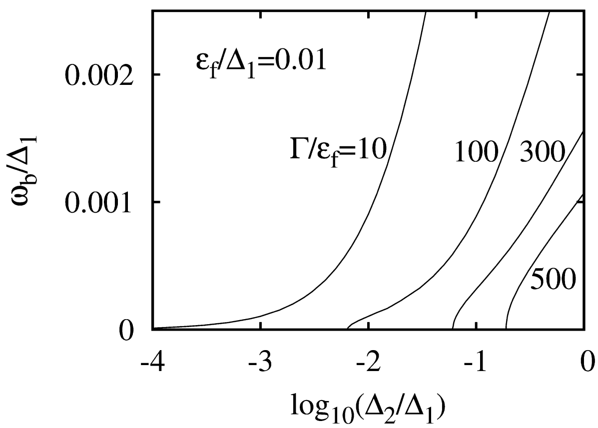

Figure 5 Position of bound states in the gap in the limit $\Gamma/\varepsilon_f \gg 1$. Here we assumed $\varepsilon_f/\Delta_1 = 0.01$. Δ_1 is kept constant. In the limit $\Gamma/\varepsilon_f \to \infty$ the impurity-induced state is located in the center of the gap.

ω_b and therefore both Figs. 4 and 5 are not sensitive to the change of DOS.

3 Conclusions Distinguishing among different OP symmetries in multiband SCs is more challenging than in the one-band case. The opposite sign of the OP components imply that the position of bound states in the energy gap is closer to the gap center in comparison to analogous problem in a one-band s-wave SC. In a conventional s-wave SC the impurity-induced states merge with the edges of the gap in the limit $T_K/T_c \to \infty$. However, in the same limit in an s± state these states are located in the center of the gap.

Impurity resonances are located further away from the Fermi level in the mixed-valence regime, when $\Gamma \sim \varepsilon_f$, and both Γ and ε_f are comparable to Δ_1 and $|\Delta_2|$. When both Γ and ε_f are much greater than Δ_1 and Δ_2, impurities may cause a relatively broad band and experimental measurements of thermodynamic and some transport properties may mimic those od d-wave SC.

Whether low-energy DOS is gapless or gapful, depends on n, as well as on the relative magnitude of the energy scales Γ, ε_f, Δ_i. When $\omega_b \ll \Delta_1$, very small change of impurity concentration or hybridization may significantly change the low-energy behavior of the system. When Γ exceeds Γ_c, at which N_{tot} (0) becomes nonzero, N_{tot} (0) rises quickly and saturates in a relatively narrow range of Γ values. Sample inhomogeneities may lead to $N_{tot}(\omega) > 0$ in some regions and N_{tot} $(\omega) = 0$ in others, further complicating interpretation of measurements. The transition between N_{tot} $(0) = 0$ and N_{tot} $(0) > 0$ is a consequence of the OP sign change. This transition is continuous in the problem studied here but in general it may also be a discontinuous one [19]. Finally, it should be pointed out that the bound states due to magnetic impurities are generally much sharper than in the case of nonmagnetic scatterers.

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