

# Magnetic impurity transition in a $d+s$ - wave superconductor

L. S. Borkowski\*

Quantum Physics Division, Faculty of Physics, A. Mickiewicz University, Umultowska 85, 61-614 Poznan, Poland

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\* Corresponding author: e-mail lsb@amu.edu.pl

We consider the superconducting state of  $d + s$  symmetry with finite concentration of Anderson impurities in the limit  $\Delta_s/\Delta_d \ll 1$ . The model consists of a BCS-like term in the Hamiltonian and the Anderson impurity treated in the self-consistent large- $N$  mean field approximation.

Increasing impurity concentration or lowering the ratio  $\Delta_s/\Delta_d$  drives the system through a transition from a state with two sharp peaks at low energies and exponentially small density of states at the Fermi level to one with  $N(0) \simeq (\Delta_s/\Delta_d)^2$ . This transition is discontinuous if the energy of the impurity resonance is the smallest energy scale in the problem.

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**1 Introduction** The order parameter symmetry of high- $T_c$  compounds is believed to be predominantly of  $d$ -wave type. However a subdominant  $s$ -wave component of the order parameter may also occur, especially in materials with orthorhombic distortions. One of such compounds is YBCO, exhibiting strong structural distortion and a substantial anisotropy in the London penetration depth in the  $a$ - $b$  plane.[1] Raman scattering[2] provided evidence for a 5% admixture of  $s$ -wave component while thermal conductivity measurements in rotating magnetic field[3] placed an upper limit of 10%. Angle-resolved photoemission spectroscopy[4] on monocrystalline YBCO gave the ratio of 1.5 for gap amplitudes in the  $a$  and  $b$  directions in the  $CuO_2$ . Measurements of a Josephson current between monocrystalline  $YBa_2Cu_3O_7$  and  $s$ -wave Nb showed that the obtained anisotropy could be explained by a 83%  $d$ -wave with a 17%  $s$ -wave component.[5] In another experiment on YBCO/Nb junction rings the  $s$  to  $d$  gap ratio in optimally doped YBCO was estimated to be 0.1.[6]

Inelastic neutron scattering on monocrystalline and un-twinned samples of YBCO lead to magnetic susceptibilities with intensities and line shapes breaking the tetragonal symmetry.[7–10] It was shown that these data may be interpreted within an anisotropic band model with an order parameter of mixed  $d$  and  $s$  symmetry.[11]

Superconducting states with mixed symmetry are also considered in other classes of compounds, e.g. in the recently discovered ferropnictides.[12]

The effects of dilute concentrations of magnetic and nonmagnetic point defects on a BCS superconductor of pure  $s$  or  $d$ -wave symmetry were intensively studied in the past and are well known. In a  $d$ -wave superconductor with lines of order parameter nodes any amount of disorder induces a nonzero density of states at the Fermi level. In an  $s$ -wave system only magnetic impurities change the response of the superconducting state. For sufficiently strong coupling between the impurity and the conduction band bound states may appear in the energy gap.[13]

In an earlier work on nonmagnetic impurities in a  $d + s$ -wave superconductor it was shown that in the unitary limit a nonzero density of states (DOS) at the Fermi level appears above certain critical impurity concentration, depending on the size of an  $s$ -wave component.[14] However the low-energy DOS is mostly featureless since the  $s$ -wave component prevents a buildup of states due to nonmagnetic scattering. In contrast the presence of magnetic impurities in a superconductor with an  $s$ -wave component may result in sharp peaks in the low-energy DOS for small concentration of defects, provided the energy scale associated with the impurity resonance is small.

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**2 Model and Results** We consider the order parameter of  $d + s$  symmetry on a cylindrical Fermi surface.

$$\Delta_s + e^{i\theta} \Delta_d(\hat{k}), \quad (1)$$

where  $\Delta_s$  and  $\Delta_d$  are amplitudes of  $s$ - and  $d$ -wave component respectively. We assume  $\theta = 0$  and  $\Delta_s \ll \Delta_d$ .

The superconductor is treated in a BCS approximation. The magnetic scatterer is modelled as an Anderson impurity treated within the slave boson mean field approach.[15] The low energy physics is dominated by the presence of strongly scattering impurity resonance. The self-consistent self-energy equations describing the interplay between the superconducting and magnetic degrees of freedom have the following form,

$$\tilde{\omega} = \omega + \frac{nN}{2\pi N_0} \Gamma \frac{\tilde{\omega}}{(-\tilde{\omega}^2 + \epsilon_f^2)}, \quad (2)$$

$$\tilde{\Delta} = \Delta_s + \frac{nN}{2\pi N_0} \Gamma \frac{\tilde{\Delta}}{(-\tilde{\omega}^2 + \epsilon_f^2)}, \quad (3)$$

$$\tilde{\omega} = \omega + \Gamma \left\langle \frac{\tilde{\omega}}{(\tilde{\Delta}^2(k) - \tilde{\omega}^2)^{1/2}} \right\rangle, \quad (4)$$

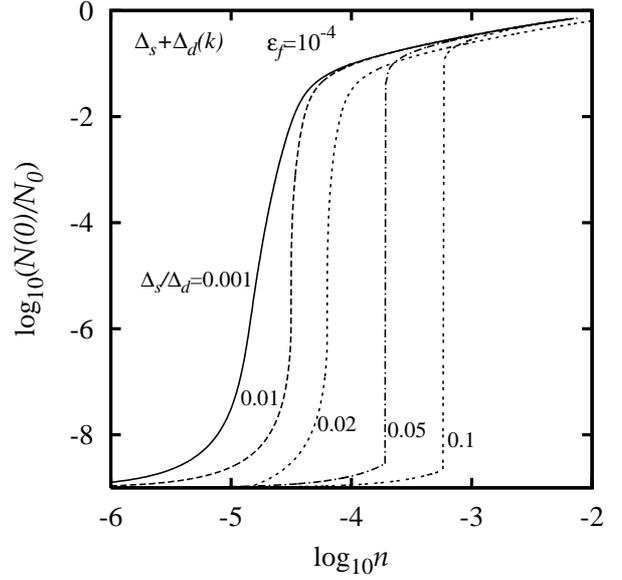
$$\tilde{\Delta} = \Gamma \left\langle \frac{\tilde{\Delta}}{(\tilde{\Delta}^2(k) - \tilde{\omega}^2)^{1/2}} \right\rangle, \quad (5)$$

where  $\tilde{\omega}(\tilde{\omega})$ ,  $\tilde{\Delta}(\tilde{\Delta})$  is the renormalized frequency and order parameter of conduction electrons (impurity) respectively.

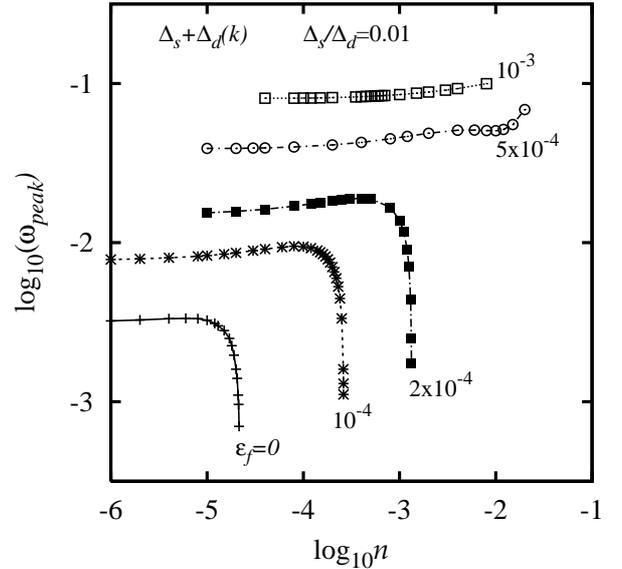
We assume  $\Delta_d/D = 0.01$ , where  $2D$  is the bandwidth of the conduction electron band. In the equations above  $\Gamma$  is the hybridization energy between the impurity and the conduction band and  $\epsilon_f$  is the resonant level energy. Here we assume constant density of states in the normal state  $N_0 = 1/2D$  and do the calculations for a nondegenerate impurity,  $N = 2$ . Brackets denote average over the Fermi surface.

Initial results for the density of states of this system were presented in an earlier paper.[16] For small impurity concentration  $n$ , such that  $\Delta_s$  and  $\Delta_d$  are not significantly affected, there are two peaks located symmetrically near the gap center, provided  $\epsilon_f \ll \Gamma \ll \Delta_s$ . For larger  $n$  the two peaks merge into one peak centrally located at the Fermi energy.

Fig. 1 shows the dependence of the density of states  $N(0)$  at  $E_F$  as a function of impurity concentration. At small  $n$ ,  $N(0)$  is exponentially small,  $N(0)/N_0 \sim (\Delta_s/\Delta_d) \exp(-\alpha(\Delta_s/\Delta_d)^2/n)$ , where  $\alpha$  is a numerical factor. The critical concentration  $n_0$  for the discontinuous transition to  $N(0)/N_0 \simeq \Delta_s/\Delta_d$  is a quadratic function of  $\Delta_s/\Delta_d$ . For  $n > n_0$ ,  $N(0)$  approaches DOS of a  $d$ -wave superconductor in both the magnitude and its functional dependence on  $n$ . These relations are valid when  $\epsilon_f \ll \Gamma, \Delta_s$ .



**Figure 1** Logarithm of the density of states at the Fermi level as a function of impurity concentration for several values of the ratio  $\Delta_s/\Delta_d$ . The resonant impurity level  $\epsilon_f$  is close to the Fermi level.  $\Gamma/D$  is fixed at 0.001.



**Figure 2** Position of the peak in the conduction electron DOS as a function of impurity concentration for  $d + s$  superconductor for several values of the resonant level energy. Energy is scaled by half of the conduction electron bandwidth  $D$  and  $\Gamma/D = 0.001$ . The suppression of  $\Delta_s$  and  $\Delta_d$  was not taken into account.

Qualitatively similar scaling of  $N(0)$  as a function of  $\Delta_s/\Delta_d$  in presence of nonmagnetic impurities in the unitary limit was obtained in ref. [14]. The difference between magnetic and nonmagnetic defects in a superconductor with  $\Delta_s/\Delta_d \ll 1$  is the character of the transition from

the exponentially small  $N(0)$  to finite  $N(0)$  in the strong scattering limit. In contrast to nonmagnetic impurities, the transition caused by resonantly scattering magnetic impurities is discontinuous, and there are two sharp peaks of  $N(\omega)$  on both sides of the transition.[16] The position of peaks as a function of impurity concentration for different values of  $\epsilon_f$  is shown in Fig 2. These peaks strongly alter the low-energy and low-frequency response and may be detected in thermodynamic or transport measurements. The increase of  $\Delta_s$  shifts the resonances towards  $E_F$  and makes them more narrow.

The  $d$ -wave component of the superconducting order parameter is more sensitive to pair breaking by magnetic impurities in the limit  $T \ll T_K$ , where  $T_K = \sqrt{\Gamma^2 + \epsilon_f^2}$ , than the  $s$ -wave part. Depending on the relative size of  $\Delta_d$  and  $\Delta_s$  there may be another impurity transition for larger  $n$ , when the order parameter nodes disappear due to vanishing of the  $d$ -wave component and a full gap opens up. The impurity peak is then split and  $N(0)$  falls to zero again. However a detailed description of this possibility requires a careful analysis involving four energy scales:  $\Delta_d$ ,  $\Delta_s$ ,  $\Gamma$ , and  $\epsilon_f$ .

Can such transition be observed experimentally? The transition may be tuned either by varying impurity concentration or the ratio  $\Delta_s/\Delta_d$ . The density of states of the normal state at  $E_F$ ,  $N_0$ , also has an effect. It appears in equations 2 and 3. One should bear in mind, however, that both the superconducting transition temperature and the impurity resonance energy scale  $T_K$  are exponentially sensitive to changes of  $N_0$ . Experiments conducted at very low temperatures may give different signatures of low-energy behavior depending on the location of the system on the phase diagram relative to the impurity critical point.

In a  $d+s$ -superconductor in the limit of high concentration of point defects the  $d$ -wave component vanishes while the  $s$ -wave part of the order parameter remains unaffected. The situation is different in presence of magnetic scatterers. If the  $s$ -wave component is small and the energy scale of the resonance due to impurity scattering is at most of the order  $\Delta_s$ , increasing impurity concentration may drive  $\Delta_s \rightarrow 0$  while  $\Delta_d$  will be reduced and finite. This follows from the fact that the largest pair breaking occurs when the energy scales of the impurity resonance and the order parameter are comparable. If  $\Delta_d \gg T_K$ , the rate of suppression of  $\Delta_d$  with increasing  $n$  is small.

The  $d+s$  superconductor with a subdominant  $s$ -wave component doped with magnetic impurities has a different phase diagram in the  $T$ - $n$  plane compared to the same superconductor with nonmagnetic defects. If the impurity resonance scale  $T_K$  is comparable to  $\Delta_s$  and  $\Delta_s \ll \Delta_d$ , the  $s$ -wave component may vanish at  $T \simeq T_K$ .

**3 Conclusions** The  $T = 0$  impurity transition discussed in this work may be detected in the low temperature limit. While the slave boson mean field formalism used in this paper cannot be applied at temperatures exceeding  $T_K$ ,

we may also qualitatively describe the expected behavior of the system as a function of temperature. At finite but small impurity concentration there may be even four phase transitions as a function of temperature: normal to  $d$ -wave,  $d$ -wave to  $d+s$ -wave,  $d+s$  to  $d$ -wave, and  $d$ -wave to  $d+s$ -wave. Due to the difference of magnitudes the small  $\Delta_s$  may be driven to zero faster with increasing  $n$  than  $\Delta_d$ . Nonmonotonic behavior around  $T \sim T_K$  is a consequence of strong scattering by the resonance state forming on the impurity site. As  $T \rightarrow 0$ , the impurity scattering becomes weaker and the  $s$ -wave component may appear again. Whether this particular scenario is realized, depends on the relative size of energy scales:  $\Delta_s/\Delta_d$ ,  $\Delta_s/T_K$ , and  $\epsilon_f/\Gamma$ .

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