Multiband superconductivity of doped cuprates

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Abstract. Numerous indications point to the multiband nature of the superconductivity in doped cuprates. The electronic structure of these compounds evolves with doping. Based on experimental findings, a simple model for the description of cuprate superconductor characteristics on the doping is developed. The leading interband pairing channel between an itinerant band and defect states created by doping is postulated. Bare gaps between them are supposed and to be closed by extended doping. Band overlap conditions determine the phase diagram critical points. The supercarrier density varies with the disposition of the chemical potential and bands. Nodal and antinodal momentum regions are distinguished. In the case of hole doping the relevant regime lies near the top of the oxygen band. Illustrative calculations have been made using a mean-field multiband Hamiltonian. Manifestations of various gaps and pairing strength characteristics on the doping level are discussed. A nonmonotonic dependence of the critical coherence length is calculated. The coherence of noncritical mode is also investigated. The supercarrier effective mass diminishes moderately out of underdoping. The penetration depth curve is of the observed type. The isotope effect on supercarrier density is predicted. In the case of electron doping the events concentrate near the bottom of the upper Hubbard band. The gross features of the phase diagram with two pseudogaps remind the hole doping case. The pairing strength and the phase coherence develop simultaneously. The agreement of the results of our model calculations with experimental findings suggests that multiband pairing is an essential aspect of cuprate superconductivity.

1. Introduction

Cuprate high-temperature superconductivity is induced by doping. Both hole- and electron-doped systems are known. Doping destroys antiferromagnetic order and metallizes the sample. Its electronic and structural constitutions undergo essential reconstruction by strong correlation effects. This comprises the nonrigid electron spectrum as well as the lattice on the nanostructural level up to phase separation (at hole doping). One general approach considers cuprate superconductors as two-component systems with itinerant and “defect (polaronic)” interacting partners [1-5].

It can be expected that this multicomponent nature of doped cuprates will be reflected in the low energy spectra determined by the minimal quasiparticle excitation energies. At present there is a consensus [6] that cuprates are two-gap systems with at least one superconducting gap and the mysterious [7,8] pseudogap. The spectroscopy of cuprates has passed a long way of development with essential improvements. Some important reliable results have been obtained only recently. There remained the question about the number of observable superconducting gaps. Various investigations pointed to the presence of more than one gap [9-13]. A direct measurement of two coexisting superconducting gaps was reported recently in [14]. The extraction of a true superconducting gap from the background [15] is also a hot result.
The nature of the pairing interaction in cuprate superconductors remains elusive for the present time. Several approaches have been put forward. Various multiband schemes exploiting the advantages connected with interband pairing must be mentioned, see [16-20] for review. Interband pairing may support high transition temperatures by repulsive coupling of bands resonating at the Fermi energy. The nature of the combining electron bands is a special problem without a conclusive answer, so far.

In agreement with the two-component scenario there is experimental and theoretical evidence that for both types of doped cuprates a new “defect” band is created near the Fermi energy [21-31]. The lattice-phonon subsystem shows an analogous build-up of new vibration branches under doping [32]. Structural distortions of various nature [32-35] enter essentially into the physics of cuprate superconductors.

In a theoretical paper the “defect” carriers have been included first seemingly in [36]. The approach with minibands created by the striped phase separation has been developed in [37]. The recent state of the multiband applications to cuprate superconductivity can, e.g., be found in [5,18-20,38,39]. An approach to multiband scenario has developed by the authors in [40-44]. The present contribution summarizes a set of recent results obtained by this model.

2. Model assumptions

Our aim has been to develop a tractable multiband model, so simple as possible, to describe the high-\( T_c \) superconductivity of a “typical” cuprate which includes the accepted knowledge on various characteristic properties and features. A comparison of the results obtained using model assumptions with experiment could, at least, support (or contradict) the basic content of the theoretical scheme.

The basic assumption of our model is the presence of an interband pairing channel between the itinerant electron band and defect band components created by doping. The latter account for the different participation of the \((\pi,0)\)-hot and \((\pi/2,\pi/2)\)-cold regions of the momentum space. In this manner, the doping process introduces besides the carriers also a new (non BCS) pairing channel acting in the CuO\(_2\) planes.

This general scheme implies different electron structure components and different sublattices for hole and electron doping. In case of holes it is the energy region near the top of the oxygen band between the Hubbard components. In the electron doping case the relevant regime lies near the bottom of the upper Hubbard band (UHB).

The presence of pseudogaps [7,8] is in our model accounted for by an “external” source – bare gaps between the itinerant and defect states. In the multiband schemes there can be band components present not intersected by the chemical potential (\( \mu \)). These bands create pseudogap type excitations which survive in the normal state [40]. Extended doping restores the Fermi-liquid type behaviour with a mixed carrier family [45]. The pseudogaps continue to distinct critical points [8] where in the normal state insulator to metal transitions are observed [46,47]. Therefore the defect bands edges are supposed to reach the overlap with the itinerant band by progressive doping (linear shift for hole and quadratic for the electron doping case).

Band component overlaps generate the characteristic points in the phase diagram. A pseudogap continues behind such critical doping as the superconducting gap of the same subsystem. At this pseudogaps do not represent the pairing strength and do not compete with the superconductivity.

The supercarrier density (\( n_s \)) and the transition temperature are determined by the variable pairing conditions on the nonrigid spectrum according to the disposition of bands and chemical potential \( \mu \). The density of supercarriers does not equal the doped carriers concentration in multiband approaches. Accordingly the isotope effect on supercarrier concentration has been predicted [47] in contrast with widely expected absence.

Our calculations have been made using a multiband mean-field Hamiltonian with pairs build-up from particles of the same band [41]. The interband pairing strength is described by a constant. Intraband pairing has not been included. The thermodynamic characteristics have been obtained using
a calculated multiband free energy expansion of the Ginzburg-Landau type [43,44,48]. Plausible parameter sets have been proposed for numerical calculations and fixed on the “Tc and gaps level” so that the thermodynamic characteristics have been obtained without adjustments. Absence of disconformities in the scales of different calculated characteristics points to the inner consistency of the physics being modeled.

3. Results and discussion. Hole doping

We start with the calculated energetic characteristics of a hole-doped cuprate in Fig.1. The maximal Tc corresponds to the overlap of all band components intersected by $\mu$, $n_s$ follows the same trend. The Uemura type [49] sublinear relation at low dopings ($p$) with the following “boomerang” has been obtained. The bare gaps are not reflected in $n_s$ because of the interband nature of the pairing.

Theoretically two pseudogaps are possible, as found for some compounds [50-53]. The large pseudogap $\Delta_l$ extends until moderate overdoping and continues further as the defect superconducting gap $\Delta_\alpha$, cf. [54]. Behind $p_\alpha$ the manifestation of both superconducting gaps is expected. Note the $\Delta_l$-$\Delta_\gamma$ crossing, i.e. the energy scales of the pseudogap and the superconducting gap being rather different at underdoping can become further comparable. These gaps are noncompeting and belong to different subsystems. At low temperatures a pseudogap can not manifest on dopings where it will be found in the normal state. The normal state (pseudo)gap energy extrapolates to zero at the critical point, cf. [55]. Spectrally $\Delta_l$ is related to the hump-feature [54]. In this manner the nodal superconductivity coexists with incoherent antinodal excitations. The small pseudogap is known to be connected with the larger superconducting gap [50,51] as seen in Fig.1. However $\Delta_\alpha$ can be missing if the cold defect subsystem borns ungapped. Its presence is essential to help build up of $T_c$ on the way to optimal doping. This system contributes also decisively into the maximum of the c-axis second critical field $H_{c2}(0)$ dependence. The BCS universality of $\Delta_\alpha/(kT_c)^{-1}$ relations are found to be violated.

The strength of the pairing and the phase coherence develop and vanish simultaneously as seen in Fig.2. Experimental investigations confirm this finding [56,57]. Our two-component model is
described by two order parameters with critical and noncritical behaviour at $T_c$. The critical one (Fig.2) determines both superconducting gaps. Its fluctuations are damped exponentially in space. The doping dependence of $\xi_0$ calculated in [43,58] is in agreement with recent experimental results [59]. The noncritical fluctuation mode with zero equilibrium value corresponds to a periodic spatial wave with fluctuating relative phase of the two condensates [43,48], cf. [60]. Its imaginary characteristic length is remarkable at underdoping.

The doping dependence of supercarrier effective mass [44] is shown in Fig.3. Large $m_{ab}$ values at underdoping stem from the narrow “cold” band. As the contribution of the itinerant band is included $m_{ab}$ diminishes slowly. The recent experimental paper [61] disposes $m_{ab}$ to be constant. The superfluid stiffness represented by the quantity $\rho n_s N_0 m_{ab}^{-1}$ is also shown in Fig.3 ($T=0$, $pN_0$ is the normal state

![Figure 2](image1.png)

**Figure 2.** The critical plane coherence length $\xi_0$ and the thermodynamic critical field (dashed). $T=0$. Squares – scaled results of [59].

![Figure 3](image2.png)

**Figure 3.** The supercarrier effective mass $m_{ab}=x m_0$ (dashed) and the superfluid stiffness on the doping scale.
carrier density). In its behaviour, \( n_s \) dominates over \( m_{abh} \). Note that the maximum of the corresponding inverse penetration depth (squared) is shifted to higher dopings due to the rise of \( p \) at diminishing \( n_s \). The same has been seen experimentally [56,57,62]. The constant of the interband electron-phonon interaction depends on the active vibration mass. This enables to explain the peculiarities of the isotope effect in multiband superconductors (cuprates) until its existence also in the supercarrier density [63] (contrary to the one-band case).

4. Results and discussion. Electron doping

In the case of electron doping the participating band components are the UHB (\( \beta \)) and LHB (\( \gamma \)) plus the \( (\pi,0) \) and \( \left( \frac{\pi}{2}, \frac{\pi}{2} \right) \) regions associated defect subbands \( \alpha_1 \) and \( \alpha_2 \). The weight of the Hubbard bands decreases under electron doping as \( \left( 1 - \frac{1}{2^c} \right) \) and supplies (equally) the defect subbands [23] (c stands for one Cu and one spin). In this manner the doping process destroys the Hubbard bands and builds up a midgap state distribution. A phase separation is not expected here.

Figure 4 shows the transition temperature and pseudogap doping dependences. Maximal \( T_c \) is reached when both defect subbands overlap with the UHB. The larger pseudogap exists until the gap between the filled and empty states vanishes. This reflects the quenching of the antiferromagnetic order in the \( (\pi,0) \) window. The smaller pseudogap is driven by the \( \alpha_2 \) subband in the \( \left( \frac{\pi}{2}, \frac{\pi}{2} \right) \) window and can enter the superconductivity domain. Observation of two pseudogaps in electron-doped cuprates has been claimed [64].

![Figure 4](image_url)

**Figure 4.** The transitions in temperature (1), chemical potential (2), the large (3) and the small (4) normal state (pseudo)gaps on the electron doping scale. The insert shows the paired carrier density.
Figure 5 illustrates the behaviour of the excitation gaps in the superconducting state at $T=0$. The larger pseudogap transforms into the UHB superconducting gap $\Delta_\beta$ at the first critical point. The same happens with the smaller pseudogap and $\Delta_\alpha$ in the $\left(\frac{\pi}{2},\frac{\pi}{2}\right)$ window. Under the second critical point $\Delta_\alpha$ must be detectable only in the $(\pi,0)$ window, but behind it in both.

![Figure 5](image)

**Figure 5.** Excitation energies represented by pseudogap and superconducting components (electron doping, $T=0$). 1 – $\Delta_{\text{p}\alpha}$ and $\Delta_\alpha$; 2 – $\Delta_{\text{p}\beta}$ and $\Delta_\beta$.

The behaviour of the thermodynamic critical field and of the critical coherence length (calculated, seemingly, for the first time) is of the same nonmonotonic nature as in the case of the hole doping. The absolute value of $\xi_0$ in the electron case is an order of magnitude larger in the correlation with the smaller $T_c=28$ K. It seems that these results are comparable with the properties with the not very thoroughly investigated electron doped cuprates.

5. Conclusion

The logistic of the interband pairing scheme creates comparable behaviour of superconducting characteristics for both types of doping. The calculated results are self-consistent and show that the elaborated simple multiband approach is able to reproduce characteristic features of cuprate superconductors as e.g. the doping dependences of $T_c$, superconducting gaps and pseudogaps, supercarrier density, coherence and penetration length, critical magnetic fields and some other properties. We believe that an argument for the functioning of the interband pairing in the cuprate multiband high-temperature superconductivity is given by the present communication.

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