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Cuprate superconductivity interband model with a doping-formed spectrum

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Abstract. The basic properties of cuprate superconductivity are analysed by using a descriptive interband model with the two-component electron spectrum determined by doping. Pair-transfer and vibronic interactions couple the itinerant and "defect" bands. The vibronic renormalization of gaps causes important effects. Two normal-state pseudogaps appear at underdoping as recently observed [17,18]. The pseudogap behaviour is extended beyond the underdoped region with the beginning of overlap of the band components. Various cuprate properties are analysed in a qualitative agreement with experiments.

PACS. 74.72.-h High-T_c compounds – 74.20.Mn Nonconventional mechanism Cuprate interband model

1 Introduction

Cuprate superconductivity has recently been widely discussed within the frame of the two-component scenario [1–3]. The itinerant valence band and a "defect-polaronic" subsystem associated with doped holes are the basic functional ingredients of this scenario. One can compare these with a mainly oxygen band between the Cu-dominated Hubbard components and a new distribution of defect states created by the doped holes at the upper part of this band. It seems to be natural to describe the superconductivity in such a perturbed charge-transfer insulator by a two-band mechanism ([4–8] and the references therein). An interband model of such trend has been presented in [7,8]. There the pairing is supposed to be a result of the pair-transfer interaction between the "band" components mentioned, with the pairs being formed by the particles of the same band. The evolution of the electronic spectrum with hole doping has been described by a simple postulative model. The major result of [7,8] consists in the demonstration of the natural appearance of the underdoped state pseudogap in the model used. Also, the observed peculiarities in the magnitude and the doping behaviour of the two superconducting gaps have been qualitatively reproduced.

It must be mentioned that the two-gap behaviour of cuprates can be considered according to [10] as "widely accepted". This serves as an essential support to the description of the superconductivity in these systems by a two-band model.

In [7,8] the normal-state pseudogap covered only the underdoped region. In fact, the pseudogap has been found to be a phenomenon persisting to larger dopings [10–12]. One possible generalization of the model of reference [7,8] consists in the account of the vibronic interaction between the electronic band partners involved. It is supported by the knowledge that the interband electron-phonon renormalization of the electron spectrum, as *e.g.* in the vibronic theory of ferroelectricity [13–15], can induce gap features. This can be compared with the pseudogap opening [16] and is expected to enrich the pseudogap behaviour found in [7,8]. The account of the vibronic interband interaction within the framework of [7,8] is the aim of the present work. As a result, the pseudogap behaviour is extended to optimal (and larger) dopings. At the same time two underdoped state pseudogaps of a different nature (electronic and vibronic) and magnitude appear in the theory. Two underdoped state pseudogaps have been found experimentally in the recent investigations [17,18].

2 The basic model

We start with the description of the model [7,8] and its consequences. Numerous experimental (including ARPES) investigations and theoretical conclusions state that with the hole doping a new electronic band is developing near the Fermi energy of cuprates [18–27]. In the absence of doping the latter coincides with the top of the valence band. A progressive doping merges the defect band with the itinerant one.

In [7,8], the itinerant band (b) extends in energy from $\xi_b = -D$ to $\xi_b(\max) = 0$ with the number of states normalized to $1-c$. Here c represents the doped hole concentration, to be scaled for a given case. The defect band (a) created by doping develops its width with doping above

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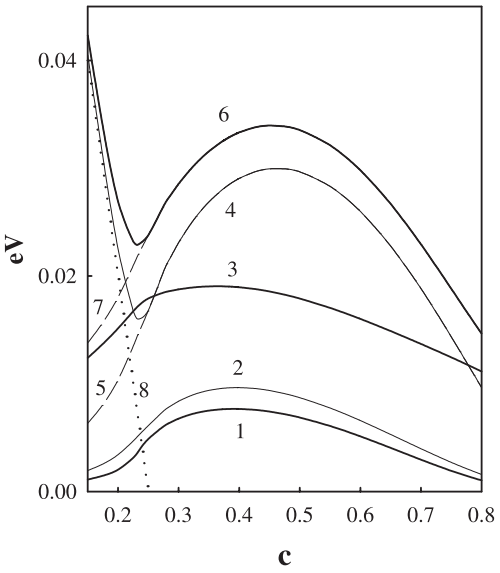

Fig. 1. Dependences on doping in the superconducting state. $1-T_c$, $8-\mu$. Superconductivity gaps and the pseudogap with the corresponding vibronically renormalized partners: $2-\Delta_a$; $3-\tilde{\Delta}_a$; $5-\Delta_b$; $7-\tilde{\Delta}_b$; $4-\Delta_p$; $6-\tilde{\Delta}_p$.

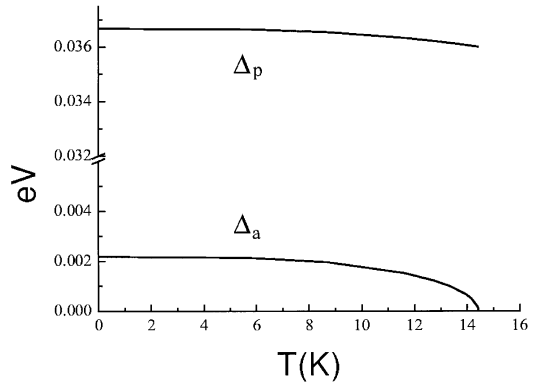

Fig. 2. The temperature-dependent underdoped state ($c = 0.16$; $c_0 = 0.25$) pseudogap Δ_p and the a-band superconductivity gap.

the b band from d to $d - \alpha c$ possessing the weight of states c. A positive d corresponds to a reduction in the charge-transfer gap by doping [3]. In the absence of doping the b-band is filled and the a-band is missing. A progressive doping leads to the overlap of bands at $c_0 = d/\alpha$. For a two-dimensional system (CuO_2 planes) $\rho_a = \alpha^{-1}$, $\rho_b = (1-c)D^{-1}$.

Papers [7,8] deal with two nondispersive order parameters. Some recent works [3,28–30] reveal an extended s-wave-type cuprate superconductivity ordering in contrast to the widely proposed d-type, *cf.* [31]. One notes that a change of the order parameter symmetry with doping and temperature can appear [11,32–35]. The description of the anisotropy of the pairing with two s-type order parameters cannot be excluded either. The point is that in the case of a repulsive interband coupling the two gap parameters appear with different signs [36]. In [7,8] the quasiparticle energies take the usual form $E_{a,b} = \sqrt{\epsilon_{a,b}^2 + \Delta_{a,b}^2}$, where the band energies are $\xi_{a,b} = \epsilon_{a,b} + \mu$ and $\Delta_{a,b}$ represents the superconductivity gaps. In a coupled two-band system these gaps close simultaneously at T_c.

The chemical potential $\mu = d - \alpha c$ for $\mu \geq 0$ and $\mu = (d - \alpha c)[1 + (1-c)\alpha D^{-1}]^{-1}$ for $\mu \leq 0$. Positive values of μ-s lie beyond the bands overlap. This is known to correspond to underdoping [6]. The minimal excitation energy of an underdoped superconductor is $\Delta_p = \sqrt{\mu^2 + \Delta_b^2}$ and should be interpreted as a pseudogap. It decreases nearly linearly with doping ($\mu \gg \Delta_b$ for $c < c_0$). For overlapping bands ($\mu \leq 0$) the minimal E_b is determined by the superconducting gap Δ_b to which Δ_p smoothly transforms. In an underdoped normal state Δ_p remains in the form of $|d - \alpha c|$, *i.e.* it shows the basic property of a pseudogap. The concentration c_0 determines the under/optimal doping line. At $c > c_0$ there are two "usual" superconducting gaps which do not survive for the case $T > T_c$ in [7,8]. With underdoping only Δ_a vanishes for $T > T_c$, while for $T < T_c$ the superconductivity gap Δ_a and the pseudogap Δ_p coexist.

The results of [7] are partly illustrated in Figure 1. The $\Delta_p(\Delta_b)$ is characterized by a large gap/T_c ratio of a non-BCS universality over the whole doping scale. At $c < c_0$ this ratio is a decreasing function of c, while T_c is rising.

We also illustrate the dependences of Δ_p and Δ_a on temperature (for $c = 0.16$) in Figure 2, because these have not been presented in [7]. Δ_p diminishes slowly, whereas the Δ_a and Δ_b tend to zero in a traditional manner as $T \to T_c$.

The results of [7,8] correspond qualitatively to the experimental findings for cuprates [37–43]. Note that our c must be scaled when projecting the results on a typical cuprate. For the, say, Bi 2212 [41] the estimation $c(\text{real}) \approx 0.4c$ can be taken.

There are various findings pointing to the existence of a critical doping concentration (c_k) in cuprates [24], where the properties of the system change markedly. The pseudogap is sometimes said to become unobservable or suppressed in magnitude when passing the c_k-border. In the absence of superconductivity an insulator-metal transition can be expected at c_k. Such a c_k is of utmost importance in the quantum critical point scenario [24,44,45], which incorporates also some typical elements of the two-gap scheme. It is tempting to relate c_k to c_0, *i.e.* to the band-overlap reached with progressive doping. However, it is known that c_k is located in a slightly overdoped region, which is not the case for c_0 in [7,8].

3 Vibronic interaction included

The presence of two closely-related electronic bands opens also a coupling channel to phonons through vibronic mixing. This can lead to the softening of the active vibration branch accompanied by the renormalization of the

electron spectrum [13]. The lattice distortion or the corresponding fluctuations can induce contributions to the band-gap [46,47]. Such an effect known for ferroelectrics can be compared with the vibronically-induced pseudogap behaviour in superconductors [16].

The essential role of the interband electron-phonon coupling in cuprates is indicated experimentally by the data of phonon frequency anomalies at the onset of superconductivity [48]. There have been a number of theoretical papers using the interband electron-phonon interaction (with rigid electron spectra, however) to explain various structural effects and as a source for pseudogap formation. Some recent papers [49–51] with the references therein can be consulted in this aspect.

Under various lattice effects a structural distortion (dimpling) of CuO_2 planes with the enhancement of Cu-O distances [52–56] is of interest in the context of the present paper. The striped phase separation [12,58–62] (static or dynamic [57]) of the doped CuO_2 plane incorporates this transition. There has been an attempt [63] to describe this by using the electron spectrum behaviour postulated in [7,8]. One can ascribe the defect band (a) to the part of the striped material bearing the doped holes and the band b, to the slightly disturbed itinerant background preserving the antiferromagnetic fluctuations.

Paper [63] investigated the interband vibronic effect by using the spectrum of [7] to follow the phonon softening in the whole doping region (a previous paper is [64]). The self-energy factor of the phonon frequency renormalization has a sharp maximum (smoothed by the onset of superconducticity) at c_0. Experimentally the enhanced phonon softening has been observed at just this under/optimal border [65], where also the CuO_2 plane structural transition appears [52,53].

We use here the scheme of [7] and the results of [63] to look for the vibronic contribution to the behaviour of the actual gaps. The following linearized Hamiltonian is used:

$$H = \sum_{\boldsymbol{k}\sigma} \epsilon_a(\boldsymbol{k}) a^+_{\boldsymbol{k}\sigma} a_{\boldsymbol{k}\sigma} + \sum_{\boldsymbol{k}\sigma} \epsilon_a(\boldsymbol{k})\epsilon_b(\boldsymbol{k}) b^+_{\boldsymbol{k}\sigma} b_{\boldsymbol{k}\sigma} + \Delta_a \sum_{\boldsymbol{k}} \left[a_{\boldsymbol{k}\uparrow} a_{-\boldsymbol{k}\downarrow} + a^+_{-\boldsymbol{k}\downarrow} a^+_{\boldsymbol{k}\uparrow} \right] - \Delta_b \sum_{\boldsymbol{k}} \left[b_{\boldsymbol{k}\uparrow} b_{-\boldsymbol{k}\downarrow} + b^+_{-\boldsymbol{k}\downarrow} b^+_{\boldsymbol{k}\uparrow} \right] + VQ \sum_{\boldsymbol{k}\sigma} \left[a^+_{\boldsymbol{k}\sigma} b_{\boldsymbol{k}\sigma} + b^+_{\boldsymbol{k}\sigma} a_{\boldsymbol{k}\sigma} \right]. \tag{1}$$

Here the band energies are defined as $\xi = \epsilon + \mu$; σ and the arrows designate spins. The following two superconductive interaction terms describe the scattering (intensity W) of the intraband pairs between the bands. The superconducting gap order parameters are defined as

$$\Delta_a(\boldsymbol{q}) = 2 \sum_{\boldsymbol{k}} W(\boldsymbol{q},\boldsymbol{k}) \langle b_{\boldsymbol{k}\uparrow} b_{-\boldsymbol{k}\downarrow} \rangle \tag{2}$$

$$\Delta_b(\boldsymbol{q}) = 2 \sum_{\boldsymbol{k}} W(\boldsymbol{q},\boldsymbol{k}) \langle a_{-\boldsymbol{k}\downarrow} a_{\boldsymbol{k}\uparrow} \rangle .$$

The last term in (1) describes the vibronic hybridization of the bands a and b with the coupling constant V. The phonon coordinate Q stands for the whole averaged active vibration branch. The quasiparticle energies read

$$E^2_{\pm}(\boldsymbol{k}) = \frac{1}{2}\Big\{ \epsilon^2_{a\boldsymbol{k}} + \Delta^2_a + \epsilon^2_{b\boldsymbol{k}} + \Delta^2_b + 2V^2Q^2 \pm \Big([(\epsilon^2_{a\boldsymbol{k}} + \Delta^2_a) - (\epsilon^2_{b\boldsymbol{k}} + \Delta^2_b)]^2 + 4V^2Q^2[(\epsilon^2_{a\boldsymbol{k}} + \epsilon^2_{b\boldsymbol{k}})(\Delta_a + \Delta_b)^2] \Big)^{1/2} \Big\} . \tag{3}$$

This spectrum is renormalized in both the superconducting and normal phases.

The minimal excitation energy of the band b quasiparticle defines the renormalized pseudogap

$$\tilde{\Delta}_p = \sqrt{\mu^2 + \tilde{\Delta}^2_b}\ \mu \geq 0$$
$$\tilde{\Delta}_p = \tilde{\Delta}_b \qquad \mu \leq 0,$$

where

$$\tilde{\Delta}^2_b = \Delta^2_b + V^2Q^2_0 \tag{4}$$

is the renormalized superconductivity b-gap. For the normal phase ($\Delta_{a,b} = 0$)

$$\tilde{\Delta}_p = \sqrt{\mu^2 + V^2Q^2_0}\ \mu \geq 0$$
$$\tilde{\Delta}_p = |VQ_0| \qquad \mu \leq 0.$$

In the expressions (4–6), Q_0 stands for the lattice distortion of a realized structural transition or for $\sqrt{Q^2}$ in the case of a fluctuating softened phonon branch. The method of calculating Q_0 for a given case is described in [13]. We will use here the amplitude $|VQ_0| = 0.01$ eV for the illustrations and the doping dependence of the phonon destabilization factor (proportional to the second-order self-energy) defined and calculated in [63] for the dependence of $Q_0(c)$.

The superconducting gaps have been calculated by numerically solving (with the parameter values of [7]) the system

$$\Delta_a = W\Delta_b\rho_b \int_{-D-\mu}^{-\mu} \frac{\mathrm{d}E}{\sqrt{E^2+\Delta^2_b}} \mathrm{th}\frac{\sqrt{E^2+\Delta^2_b}}{2k_BT}$$
$$\Delta_b = W\Delta_a\rho_a \int_{d-\alpha c-\mu}^{d-\mu} \frac{\mathrm{d}E}{\sqrt{E^2+\Delta^2_a}} \mathrm{th}\frac{\sqrt{E^2+\Delta^2_a}}{2k_BT}.$$

The transition temperature follows as the solution to (7) with $\Delta_{a,b} = 0$.

The results for doping dependences of T_c, $\Delta_{a,b}$, $\tilde{\Delta}_{a,b}$, Δ_p and $\tilde{\Delta}_p$ are given in Figure 1 for the superconducting phase at $T = 0$. As compared to the missing vibronic interaction [7] one can see in Figure 1 only quantitative changes. However, for the normal phase the vibronic interaction introduces qualitative effects, as can be seen in

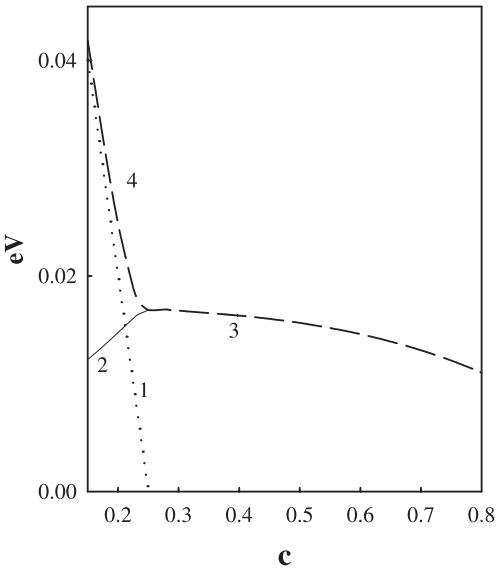

Fig. 3. Normal state pseudogaps *vs.* doping ($c_0 = 0.25$). 1 – μ; 2 and 3 – $|VQ_0| = 0.01$ eV; 4 – $\sqrt{\mu^2 + V^2Q_0^2}$.

Figure 3. Now a vibronically-induced pseudogap enters ($c_0 = 0.25$) the optimally- and over-doped region. The pseudogap covers the wide doping scale in agreement with recent experimental findings [10–12]. The interband effects considered vanish formally at $c = 1$, which is physically interpreted as a suppression effect with overdoping.

The second novel effect consists of the appearance of a second pseudogap $\tilde{\Delta}_a$ besides $\tilde{\Delta}_p$ on underdoping. It stems from the a-gap renormalization $\tilde{\Delta}_a^2 = \Delta_a^2 + V^2Q_0^2$. Two underdoped state pseudogaps have been found recently experimentally for Bi 2212 [17] in tunneling and for LSCO [18] in photoemission spectra.

As the result, the two-band model [7,8] with an interband vibronic interaction allows the qualitative elucidation of essential aspects of the pseudogap behaviour for cuprates.

4 Discussion

The two normal-state pseudogaps $\tilde{\Delta}_p$ and $\tilde{\Delta}_a$ correspond to the quasiparticle excitations of the two operating electron subsystems. On underdoping the corresponding energy scales are quite different: $\sqrt{\mu^2 + V^2Q_0^2}$ - of an electronic origin and large and $|VQ_0|$ – purely vibronic and small. The larger pseudogap is associated with the band under the chemical potential. On entering the optimally doped region the bands determine a common pseudogap $|VQ_0|$ of a vibronic nature. It can be considered as an analogue of a vibronically-induced dielectric gap [66]. A pure manifestation of the vibronic contribution in the normal state would presumably allow the estimation of the vibronic interaction constant.

The larger normal-state pseudogap connected with the band b changes its nature when passing the under-over-doped border. Here, the same conclusions about the ratio $\tilde{\Delta}_p/k_BT_c$ can be made as in Section 2. The slow dependence of $\tilde{\Delta}_p$ on temperature with underdoping is confirmed by the experiment [39]. The temperature dependence $Q_0(T)$ can affect the behaviour of the gaps. This is equally true for the superconductivity order parameter fluctuations. The latter have also been considered as a possible origin of the pseudogap behaviour (for a review, see [67]). However, the consideration of these special problems (of most interest for the normal state beyond underdoping) is not an issue of the present discussion.

The intensive narrow density distribution of the defect band (a) remains associated with μ. This circumstance can be of importance for the explanation of the normal state peculiarities analogously to the van Hove singularity scenario [67].

A t-J model investigation [36] associated the density of the spin-polaron band pinned near the Fermi surface with the formation of the underdoped sample pseudogap. This interpretation is not far from the present one.

The evolution of the electronic spectrum in our model is expected to be accompanied by changes in the nature of the electron liquid and the properties connected to the Fermi-surface. In the case of small doped hole concentrations a formation of ferron-type defect complexes is expected [68] and the superconductivity is percolative [69]. Further doping with the formation of the defect band (a) leads to a metallization and a hole-like Fermi surface appears. When the defect band bottom enters the itinerant band it remains slightly under μ. The difference in the defect and itinerant band states will be suppressed. The Fermi surface becomes electron-like with hole pockets and is determined by the states of both bands. A progressive doping restores the Fermi liquid behaviour. These statements agree with the known properties of cuprate [10,22,23,70,71].

In the tunneling spectra of cuprates a characteristic peak-dip-hump structure has been revealed [41–43]. The present model associates the peak with the smaller ($\tilde{\Delta}_a$) and the hump with the larger pseudogap $\tilde{\Delta}_p$. The peak position of the quasiparticle densities $\rho_{a,b}|E|(E^2 - \Delta_{a,p}^2)^{-1/2}$ indicate the broadening of the hump and its shift to larger energies with a diminishing underdoping as has been observed [41]. The hump remains preserved in the normal state at the dopings, where T_c becomes optimized [72]. This corresponds directly to its association with $\tilde{\Delta}_p$. This way the peak-dip-hump structure reflects the superposition of two gaps.

In the case of an interband superconductivity the property $\rho_a > \rho_b$ leads to $\Delta_b > \Delta_a$. This circumstance can mask to some extent the observability of the itinerant band contribution to the Fermi surface in the case of larger dopings, *cf.* [26].

As was mentioned above, the defect band starts as a bath of uncompensated spins (hole ferron complexes). At the same time the antiferromagnetic itinerant subsystem acts as a singlet spin component. The nature and position of the bands with such a spin distribution is to some extent comparable with the situation proposed in the

bipolaron theory [21,73]. Presumably, this offers an analogous way for explaining the underdoped cuprate magnetic properties. It concerns especially the presence of a magnetic pseudogap [26,39,61] in the spin excitation channel. In such a case the charge-channel pseudogap considered here and the spin-(pseudo)gap will appear as a common result of the doped hole segregation, creating a two-band spectrum.

A cuprate complex electron system shows two relaxation times [74] of essentially different magnitudes. One of these shows a critical, and the other one, an uncritical behaviour at T_c. The latter depends weakly on temperature. It has been shown [75] that the presence of such two relaxation channels is a natural property of two-band superconductors. According to [75] the noncritical relaxation time is connected with the itinerant band pseudogap as observed. Also, the properties of the transition temperature isotope effect and its presence in the paired carrier effective mass [76,77] can be explained in the two-band model [6,78,79]. The pseudogap isotope effect [80] can be a further consequence of the interband electron-phonon interaction, since $V \sim M^{-1}$ (M – atomic mass of the active vibration), *cf.* [6]. At $T < T_c$ the isotope dependence of $\Delta_{a,b}$ through the corresponding vibronic contribution to W [6,78] must also be considered.

The results of the present discussion seem to point to a two-band scheme with a doping-determined spectrum as a plausible approach to a description of cuprate superconductivity.

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