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I.3

MODELLING CUPRATE GAPS IN A COMPOSITE TWO-BAND MODEL

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Abstract: A simple model to cover the two-component scenario of cuprate superconductivity is developed. Interband pairing interaction acts between itinerant and defect states created by doping. Two defect system subbands correspond to "hot" and "cold" regions of the momentum space. Superconductivity energetic characteristics vs doping are compared to experimental findings. Transformations of two pseudogaps into superconducting and normal state gaps can be traced. Doping concentrations where the band components begin to overlap determine essential borders on the phase diagram. Qualitative agreement with observations is present including the effect of photodoping.

Key words: Cuprate; Two-band Model; Gaps

1. INTRODUCTION

Pair transfer interaction between the states of an electron system components can cause the gauge symmetry breaking realized in superconductivity. This circumstance forms the basis of the two-band model of superconductivity known already during a considerable time [1,2]. The basic advantage of such approaches consists in the possibility to reach pairing by a repulsive interband interaction which operates in a considerable volume of the momentum space. An electronic energy scale is

correspondingly introduced into determination of the transition temperature. Further elaborations have been remained without distinct bases of applications until the high-T_c cuprate superconductivity has been discovered. Under numerous approaches looking for the basic mechanism of this event the two-band approaches have been used as one of the possible channels. The nature of the electron band components used has been variable (for review see e.g. [3-5]).

The progress in experimental investigations has revealed some coupled general properties of cuprates which are connected with the necessary doping treatment. First, the structure of doped cuprates has been found to be essentially inhomogeneous on the nanoscale (stripes, tweed patterns, granularity) with the associated electronic phase separation [6-12] in the CuO_2 planes. At the same time it has been found that the hole doping creates a new band of defect-states in the cuprate charge-transfer gap [13-24]. Various data have indicated the functioning of itinerant and "defect"-type carriers in the basic physics of cuprate superconductivity. A corresponding "two-component" scenario [25-27] has been formulated. The hole-poor material can be considered as remaining the source for the itinerant band and the part of the distorted material bearing doped holes as creating the defect-band. The application of two-band models in the frame of the two-component scenario becomes natural. Such kind of approaches are strongly supported by the recent tunneling and angle resolved photoemission spectroscopy data [28,29], which have revealed the two-gap behaviour of cuprates. As a minimum it means the presence of a pseudogap plus a superconductivity gap [30], or two pseudogaps and a superconductivity gap [31-35].

However, meantime the new superconductor MgB_2 [36] has been discovered, which shows a clear two-gap behaviour [37]. Two-band models have been applied to MgB_2 [38-39] and at present this system is addressed as the reigning representative of the two-band superconductivity.

Concerning the cuprates it is now clear that a nonrigid basic electron spectrum must be used. Doping creates not only carriers but prepares the whole background (incorporating also structural changes) for the appearance of superconductivity. Under corresponding approaches there are ones which take as the basis a narrow defect (bipolaron) band above the itinerant band [23,40-48], or stripe-induced minibands [11,42].

It seems that a self-consistent scheme of cuprate multigap properties over the phase diagram incorporating the essence of numerous experimental investigations is yet missing. The statements about the relations and coexistence of various gaps for different doping regions and energy scales are partly controversial. In such a situation elaboration of a simple and easily

tractable model for the calculation of cuprate energetic characteristics with the following projection of results on the experimental data can make sense. Correspondingly, in [45,46] a model for the evolution of the cuprate electron spectrum under hole doping has been postulated. The central result of the model has been the natural explanation of the underdoped state pseudogap by the narrowing gap between the defect and itinerant band states. This model has been extended by the account of interband vibronic interaction [46,47]. It allowed to extend the pseudogap behaviour behind the optimal doping as observed [48].

Structurally the defect subsystem is anisotropic and it is manifested in differences of gap characteristics measured for various regions of the momentum space [18,28,29,49]. The well-expressed pseudogap is connected with the neighbourhood of the "hot" (π, 0)-type points in the Brillouin zone. The spectrum at (π, π)-type "cold" points seems to be nongapped, as in the *d*-wave concept [50].

In what follows we present a generalization of [45,46] by introducing two subbands to distinguish the role of "hot" and "cold" regions of the defect-system spectrum, cf. [43].

2. THE MODEL

The itinerant (valence) band (γ) is taken to be lying between energies $\xi = -D$ and $\xi = 0$ with the number of states normalized to $1 - c$. Here c characterizes the doped hole concentration and must be scaled for a given case. The defect bands (α; β) created by doping occupy the energy intervals $d_1 - \alpha c$ and $d_2 - \beta c$ correspondingly with the weight of states $c/2$. The $2D$ densities of states read $\rho_\alpha = (2\alpha)^{-1}$; $\rho_\beta = (2\beta)^{-1}$; $\rho_\gamma = (1-c)D^{-1}$. By doping the β and γ-band join at $c_\beta = d_2\beta^{-1}$ and a common overlapping energy distribution of all the bands is reached at $c_\alpha = d_2\alpha^{-1}$. The α-band is attributed to the "hot" region. At $c < c_\beta$ the chemical potential $\mu = d_2 - \beta c$ is connected with the "cold" β band. For $c > c_\beta$, $\mu = (d_2 - \beta c)\,[1 + 2\beta(1 - c)D^{-1}]^{-1}$ intersects both (β; γ) bands. Further for $c \geq c_0$ ($d_1 - \alpha c_0 = \mu$) one finds $\mu = [\alpha d_2 + \beta d_1 - 2\alpha\beta c][\alpha + \beta + (1-c)2\alpha\beta D^{-1}]^{-1}$ which intersects all the three overlapping bands.

Superconductivity characteristics will be calculated supposing the interband transfer of pairs formed from the particles of the same band

according to the mean-field Hamiltonian

$$H = \sum_{\sigma\vec{k}s} \in_{\sigma}(\vec{k})\alpha^{+}_{\sigma\vec{k}s}\alpha_{\sigma\vec{k}s} + \sum_{\vec{k}} \Delta\gamma(\vec{k})[\alpha_{\gamma\vec{k}\uparrow}\alpha_{\gamma-\vec{k}\downarrow} + \alpha^{+}_{\gamma-\vec{k}\downarrow}\alpha^{+}_{\gamma\vec{k}\uparrow}] - \sum_{\vec{k},\sigma'} \Delta\sigma'(\vec{k})[\alpha_{\sigma'\vec{k}\uparrow}\alpha_{\sigma'-\vec{k}\downarrow} + \alpha^{+}_{\sigma'-\vec{k}\downarrow}\alpha^{+}_{\sigma'\vec{k}\uparrow}] \quad (1)$$

Here $\in_{\sigma} = \xi_{\sigma} - \mu, \sigma = \alpha, \beta, \gamma$, $\sigma' = \alpha, \beta$, usual designation for spins (s) and electron operators apply. The superconductivity order parameters are defined as

$$\Delta\gamma(\vec{q}) = 2\sum_{\vec{k},\sigma'} W(\vec{q},\vec{k})\langle\alpha_{\sigma'\vec{k}\uparrow}\alpha_{\sigma'-\vec{k}\downarrow}\rangle$$
$$\Delta\sigma'(\vec{q}) = 2\sum_{\vec{k}} W(\vec{q},\vec{k})\langle\alpha_{\gamma-\vec{k}\downarrow}\alpha_{\gamma\vec{k}\uparrow}\rangle \quad (2)$$

The interband interaction constant $W > 0$ corresponds to repulsion with possible electronic and electron-phonon contributions. The quasiparticle energies read $E_{\alpha}(\vec{k}) = \sqrt{\in^2_{\sigma}(\vec{k}) + \Delta^2_{\sigma}(\vec{k})}$. In what follows the momentum dependences will be accounted for only by the $\alpha-\beta$ differentation at a constant W (different energy intervals for (α,β) in gap-equation integrals). It is taken $\Delta_{\alpha} = \Delta_{\beta}$. At T_c, $\Delta_{\alpha,\gamma} \to 0$ simultaneously. For $W > 0$ two s-type order parameters appear with opposite signs [3]; expr. (1) uses positive $\Delta_{\alpha,\gamma}$.

3. THE GAPS AND RELATIONS BETWEEN THEM

Now we look on the minimal excitation energies of the quasiparticles which reflect the presence of gaps in the charge-excitation-channel of the superconductor.

In the low underdoping region for $c < c_{\beta}$

$$E_{\alpha}(min) = \Delta_l = \sqrt{(d_1 - \alpha c - \mu)^2 + \Delta^2_{\alpha}}$$
$$E_{\beta}(min) = \Delta_{\alpha}$$
$$E_{\gamma}(min) = \Delta_s = \sqrt{\mu^2 + \Delta^2_{\gamma}} \quad (3)$$

It is seen that in the normal state Δ_l and Δ_s survive and can be interpreted as the large and small pseudogap. Passing on to the optimal doping ($c \geq c_\beta$, $c < c_0$) the small pseudogap transforms into the itinerant superconducting gap. For $c \geq_s c_0$ the large pseudogap becomes also quenched and is smoothly transformed to the defect system ($\Delta_\alpha < \Delta_\gamma$) superconducting gap.

Concerning the manifestation of various gaps of the model, the E_γ excitations become attributed to the "hot" spectrum. The "cold" spectrum is usually considered as nongapped [28,49]. If one takes account of this by multiplying the defect subsystem Δ_α by a d-wave symmetry factor, the cold spectrum becomes empty. At $c < c_\beta$ the appearance of two pseudogaps is expected. In the basic optimal doping region ($c \geq c_\beta$, $c < c_0$) the spectrum involves the large pseudogap and the superconducting gap Δ_γ. At heavier overdoping $c > c_0$ the spectrum is expected to contain two superconductivity gaps – the defect Δ_α manifested by additional spectral weight inside of Δ_γ. Such kind of the phase diagram is in qualitative agreement with the results found experimentally.

In spite of that the majority of gap manifestations appears in the "hot" spectrum, the "cold" electrons act essentially in building up superconductivity. Beyond c_β the cold subband acts as the necessary overlapping partner to achieve a high T_c by the interband mechanism. The presence of pseudogaps in the present model is reduced to the creation of a multicomponent electron liquid by doping.

4. ILLUSTRATION AND DISCUSSION

The illustrative calculation of cuprate energetic characteristics on the doping scale (Fig.1) has been made with a plausible set of parameters: $D = 2$; $d_1 = 0.3$; $d_2 = 0.1$; $\alpha = 0.66$; $\beta = 0.33$ and $W = 0.28$(eV). The maximal $T_c = 125$ K is reached for $c = 0.57$ and $c_\alpha = 0.45$; $c_\beta = 0.30$; $c_0 = 0.57$. A scaling for a typical cuprate hole doping has been made through $p = 0.4\,c$. The large pseudogap Δ_l is extended until the moderate overdoping in agreement with observations [17,50-52]. Further it is smoothly transformed into the defect system superconducting gap. This agrees with the experimental result [53]. The manifestation of both superconductivity gaps expected at $c > c_0$ (of two Fermi surfaces) is often debated. However, the common Fermi surface is

then intersected by the band components at different wave vectors and the large Δ_γ can remain masked. At intermediate dopings the large pseudogap and the superconducting gap appear and cross close to the optimal doping, as found experimentally [52]. Δ_l and Δ_γ are connected with different but non competing order parameters of defect and itinerant subsystems. Spectrally Δ_l must be related to the hump-feature. Eventually it remains preserved for $T > T_c$ (insert in Fig.1) at the dopings where T_c is optimized [52] and it is shifted to larger energies with reduced doping [54].

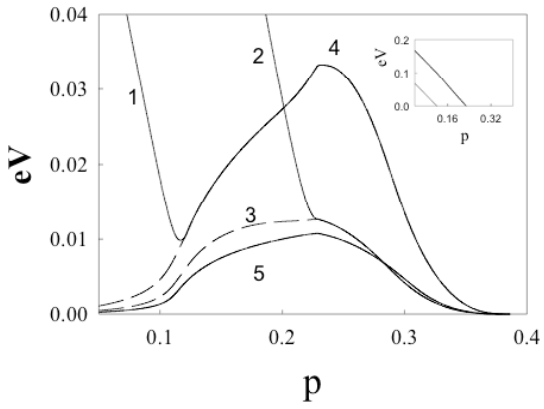

Figure I:3:1. Energetic characteristics of a mode cuprate on the doping scale. 1 – the underdoped state small pseudogap Δ_s; 2 – the large pseudogap Δ_l; 3 – the defect system superconducting gap Δ_α; 4 – the itinerant system superconducting gap Δ_γ 5 – T_c. The insert shows normal state gaps. $p_\alpha = 0{:}18$; $p_\beta = 0{:}12$; $p_0 = 0{:}23$; $p(T_{cm}) = 0{:}23$]

The common manifestation of two underdoped state pseudogaps is expected theoretically. This has been recently established experimentally for the Laand Bi-cuprates [31-35]. The small pseudogap is known to develop smoothly from the larger superconducting gap [18,31,32]. That is comparable with the transformation $\Delta_s \leftrightarrow \Delta_\gamma$ at c_β.

In Fig.2 the calculated Uemura type plot [22] is given. It is considered as universally characteristic for cuprates.

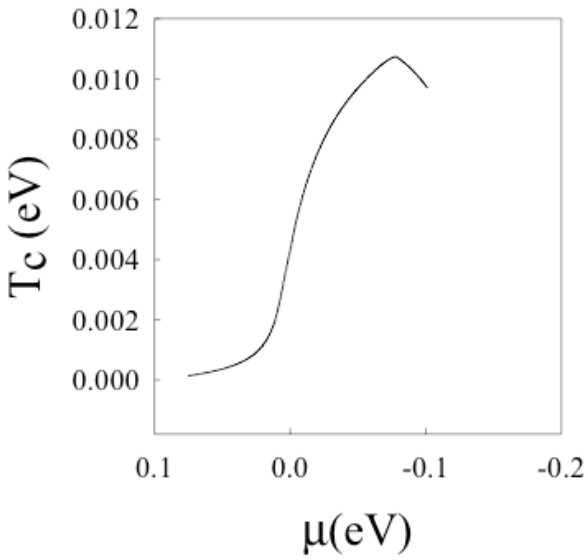

Figure I:3:2. Transition temperature vs. chemical potential for a model cuprate (an Uemura type plot).

The nonrigid dynamics of the electron spectrum with doping as characteristic for the present model points to special concentrations where the band components begin to overlap. A special critical doping region on the cuprate phase diagram where the properties of the electron liquid change essentially is well known [15,16,55]. This is of utmost importance in quantum critical point scenarios [15,42]. The (large) pseudogap is lost when passing this c_k border. It is tempting to relate c_k to c_0. Then the progressive doping is expected to restart the Fermi-liquid behaviour (cf. [15,16]) by building up a mixed electronic system of overlapping defect and itinerant bands. It appears when the bottom edge of the hot defect states lowers so that μ intersects all three bands. The Fermi surface becomes more and more electron-like and the difference between the itinerant and defect subsystem is washed up. Experiments on the normal state [55] show that a quantum metal-insulator transition appears at c_k. For smaller dopings the hot quasiparticles become insulating whereas the cold quasiparticles remain metallic. This is the same story which follows from the present model.

In the last paragraph we demonstrate that the present model is able to reproduce also the experimental findings on the photodoping effect.

5. PHOTODOPING EFFECT

Investigations of the photodoping effect in $YBa_2Cu_3O_{6+x}$ [56,57] and $Tl_2Ba_2CaCu_2O_8$ [58] have revealed an increase of T_c. On the contrary, for $Bi_2Sr_2CaCu_2O_{8+\delta}$ a photoinduced depression of T_c has been found [59]. These cases differ seemingly by the localization of the photoelectrons. In the case of Y-123 the photoelectrons become localized out of the CuO_2 planes. In the present model it is characterized by the simple substitution $c \rightarrow c + x$. It means that the sign of the photodoping effect is determined by dT_c/dc. For $YBa_2Cu_3O_{6+\delta}$ it gives the enhancement of T_c for compositions from $\delta = 0.4$ to $\delta = 1$. The experimental $\Delta T_c(\delta)$ curve of [57] is roughly reproduced by the left part of the theoretical curve in Fig.3 with $c \sim \delta/2$.

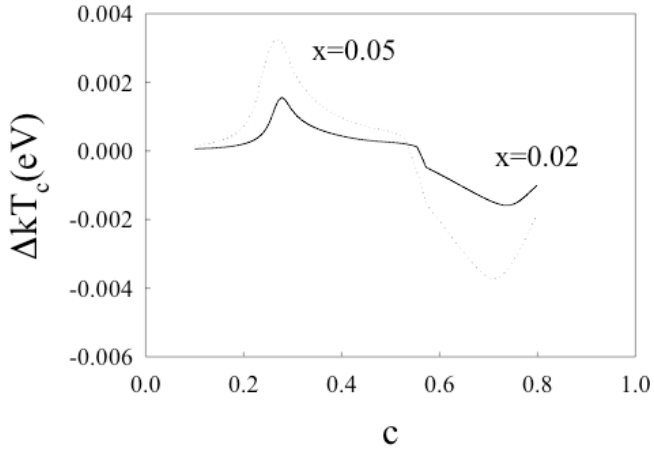

Figure I:3:3. The photoinduced shift of T_c for the case of photoelectrons localized out of the CuO_2 planes.

6. CONCLUSION

The present simple and partly postulative model seems to be able to reproduce the observed behaviour of the cuprate energetic characteristics. The possible coexistence of pseudogap with the superconducting gap of the other partner subsystem has been demonstrated. The transformation of the

pseudogap into the superconducting gap of the own subsystem by extended doping can appear. The pseudogap and the normal state gap are connected by the quenching of the superconducting gap contribution. These relations are reduced to the multicomponent nature of the cuprate electron spectrum reorganized by doping.

The results following from the present model (it must not be taken too literally) seem to point to the plausible nature of its basic content. A wide freedom remains to its improvement in various aspects.

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