MULTIBAND MODEL OF CUPRATE SUPERCONDUCTIVITY

NIKOLAI KRISTOFFEL* and PAVEL RUBIN†

Institute of Physics, University of Tartu, Riia 142, 51014 Tartu, Estonia

*kolja@ft.tartu.ee
†rubin@ft.tartu.ee

TEET ÖRD
Institute of Physics, University of Tartu, Tähe 4, 51010 Tartu, Estonia
teed.ord@ut.ee

Received 7 April 2008

A minimal model for the description of cuprate superconductor characteristics on doping scale (hole and electron) is developed. The leading interband pairing channel couples an itinerant band and defect states created by doping. Bare gaps between them are supposed and become closed by extended doping. Band overlap conditions determine special points in the phase diagram. Nodal and antinodal momentum regions are distinguished. Illustrative calculations have been made using a mean-field pair-transfer multiband Hamiltonian and corresponding free-energy expansions. The results are self-consistent and demonstrate that the elaborated approach is able to reproduce characteristic features of cuprate superconductors as, e.g., the doping dependence of $T_c$, superconducting gaps and pseudogaps, supercarrier density and effective mass, coherence length and penetration depth, critical magnetic fields and some other properties. Interband pairing scheme is suggested to be an essential aspect of cuprate superconductivity.

Keywords: Cuprates; multiband model; phase diagram; doping; gaps.

1. Introduction

Cuprate superconductivity\cite{1-3} mechanism still remains elusive at present. It seemed to the authors that it will be of sense to develop a tractable model, as simple as possible, to describe the high-temperature superconductivity characteristics of a “typical” cuprate on the whole doping scale. As a basis, the accepted general knowledge on various properties and features in cuprates must be used. A comparison of the theoretical results obtained using the model background with wide experimental data could, at least, support or contradict the supposed superconductivity mechanism. A model multiband (multigap) approach of this trend has been started in Refs. 4–6 and developed in Refs. 7–12.

5299
Cuprate superconductivity is induced by the necessary doping. The latter introduces carriers into the basic charge-transfer insulator, destroys the antiferromagnetic order, and metallizes the material. The detailed scenario of the changes in the electron structure at weak dopings is not very clear, e.g., the building of ferrons\(^{13}\) around the doped holes, etc. Cuprates are strongly correlated systems and it is expected that their electron spectrum remains by no means rigid under doping.\(^{14-17}\) Such behavior is confirmed by extended experimental findings, i.e., the Fermi surface of cuprates evolves with doping.\(^{17-25}\) At underdoping, it is traced by “Fermi arcs”\(^{25}\) indicating the presence of carriers\(^{23}\) in the nodal momentum space region around the \((\pi/2, \pi/2)\) type points of the Brillouin zone. Extended doping leads to the formation of another Fermi sheet in the antinodal \((\pi, 0)\) type region until a common Fermi surface is formed.\(^{26}\) Then the Fermi-liquid like behavior becomes restored. Correspondingly, a theoretical approach to cuprate superconductivity must use an electron spectrum created and evolving with doping.\(^{4,5}\)

The essential creative effect of doping in the electron structure of the superconductivity playground CuO\(_2\) plane consists in the appearance of a new “defect” (polaronic) electron band in the charge-transfer gap between the upper (UHB) and lower (LHB) Cu Hubbard bands. It has been shown in early theoretical papers\(^{14-16}\) and confirmed in various investigations.\(^{17,20,23,27-32}\) This new band lies in the Fermi energy region which differs for hole and electron doping. In the first case, the defect band lies near the top of the (mainly) oxygen band. For electron doping, it is the region near the bottom of the UHB. These comparable dispositions occupy different energy regions and are realized on different crystal sublattices.

The defect band can be ascribed to the part of the material bearing doped holes. The structure of doped cuprates has been found to be inhomogeneous on the nanoscale accompanied by the electronic phase separation.\(^{33}\) Static or dynamic stripes, tweed patterns, granularities, etc. have been identified in the distorted CuO\(_2\) planes, see Refs. 34–39. In the phonon spectrum, a comparable (defect band) doping caused splitting of the LO-branch happens.\(^{37}\)

In summary, various data indicate that itinerant and “defect” type carriers are functioning in the physics of cuprate superconductivity. A corresponding two-component scenario has been formulated for cuprate superconductors.\(^{2,36,40-42}\) One concludes that doped cuprates are multiband systems in the actual Fermi-energy region. The hole-poor material can be considered as supporting the itinerant band. The distorted material bearing the effective doped carriers introduces defect states.

Diverse experimental methods have been elaborated and continuously improved to obtain reliable results on the quasiparticle excitations and the spectral gaps. There are numerous experimental appointments that cuprates are at least two-gap systems\(^{22,25,43-46}\) (a pseudogap plus a superconducting gap). The indications of two superconducting gaps have also been obtained in Refs. 47–51 referring to the multiband nature of the cuprate superconductivity. A distinct revelation of two coexisting superconducting gaps\(^{52}\) and the demonstration of the presence of two gaps in the same spectral region\(^{25}\) are quite recent results. The extraction of a true
superconducting gap from the background\cite{53} and identification of the well-defined Fermi surface at underdoping\cite{54} are also examples of hot results.

It is natural to apply for a multicomponent and multiband superconductor the corresponding theoretical approach incorporating the interband coupling. Such mechanism is known as considerable time\cite{55,56}, however, its advantages\cite{57} have not been exploited enough. The central advantage consists of the opening of the interband pairing channel in a multiband system. It can support high transition temperatures by (repulsive) coupling of bands resonating at the Fermi energy. Multiband approaches have been approved for cuprate superconductors from the beginning, (see for review Refs. 58–61). However, the nature of combining bands has often remained unclear or without special justification. A first approach incorporating “defect” carriers has been suggested seemingly in Ref. 62. The background of minibands created by the striped phase separation has been used in Ref. 27. A deeper understanding of the role of topological resonances for $T_c$ amplification\cite{60,61,63,64} and also the first distinct two superconducting gap system MgB$_2$ (see e.g., Refs. 65–68) have stimulated the interest to multiband models. It continues in applications to cuprates\cite{4–12,29,41,69–76} and other novel natural and artificial systems.

The present paper summarizes the results obtained using the model multiband approach of the authors. It uses an electron spectrum evolving with doping which incorporates an itinerant band and two defect system subbands. The leading pairing interaction is supposed to be the pair transfer between the itinerant and defect states.

2. Model Assumptions: Hole Doping

The actual normal state electronic spectrum of a hole-doped cuprate will include the (mainly) oxygen itinerant valence band ($\gamma$) and the defect subbands $\alpha$ and $\beta$ representing the ($\pi,0$) and ($\pi/2, \pi/2$) regions of the 2D momentum space correspondingly. These antinodal (hot) and nodal (cold) regions show different functionality in cuprate superconductivity.\cite{22} The valence band states are taken to lie between the energy zero and the cutoff ($-D$) and are normalized to $(1-c)$. At this $c$ characterizes the hole concentration introduced by doping. The defect subbands are created over the top of the valence band with the weight of states $c/2$. This choice accounts for the fact that the charge-transfer gap diminishes with doping.\cite{77}

At moderate dopings, the defect system states are supposed to be gapped in respect of the itinerant band. This choice allows us to explain\cite{4,5} the presence of pseudogap excitations in cuprates, e.g., Refs. 22, 43–46, 78–81. A depletion of the excitation density around the Fermi energy (pseudogaps) is observed in both superconducting ($T < T_c$) and normal ($T > T_c$) states. As a result of wide discussions, the experimental data point preferably to the extrinsic (without immediate contact with the superconducting order) dispatch of the pseudogap opening, e.g., Refs. 44, 80, 82–85. Such approaches suppose normal state gaps of various origins, especially as being connected with competing orders coexisting with superconductivity. Our
supposed bare gaps associated with the perturbative nature of the doping serve an original external source for pseudogaps.\cite{4,5,86}

The phenomenon of the pseudogaps becomes quenched with extended doping, i.e., the bare gaps must close. We suppose that the defect band bottoms evolve down to the itinerant band top having energies \( d_1 - \alpha c \) and \( d_2 - \beta c \). The overlap with the \( \gamma \)-band is reached for the \( \alpha \)- and \( \beta \)-components correspondingly at \( c_{\alpha} = d_1 \alpha^{-1} \) and \( c_{\beta} = d_2 \beta^{-1} \). At these critical concentrations, the bare gaps close. In this manner the band overlap conditions determine the original source of the phase diagram critical points. The choice \( c_{\beta} < c_{\alpha} \) means that the lowest doping-created states are of nodal nature, as observed.\cite{20,23}

According to the present model, the constant 2\( D \) band densities read

\[
\rho_\alpha = (2\alpha)^{-1}, \quad \rho_\beta = (2\beta)^{-1}, \quad \rho_\gamma = (1 - c)D^{-1}.
\]

The closure of the bare energy gaps between the defect and itinerant states with extended doping correlates with the observed intimate relationship between the pseudogap and the semiconductor properties of underdoped cuprates.\cite{85,87,88}

We distinguish the following four qualitatively different regions of the doping.

(i) \( c_0 > c > c_\beta \). Here, the chemical potential

\[
\mu_2 = \frac{d_2 - \beta c}{1 + 2\beta(1 - c)D^{-1}}
\]

is shifted into the valence band (cf. the Fermi arcs development in Ref. 25). The overlap of the narrow \( \beta \) band with the wide \( \gamma \) band leads to the formation of two Fermi surface sheets with a tendency for the appearance of a “flat band” component and a hole-like barrel sheet with lowering \( \mu \) (see Refs. 23, 89, 90). The upper limit of this extended underdoped domain, \( c_0 \), is determined by the condition \( d_1 - \alpha c_0 = \mu_2(c_0) \).

(ii) \( c_1 > c > c_0 \). In such a situation, the role of the antinodal defect region is enhanced and the chemical potential

\[
\mu_3 = \frac{\alpha d_2 + \beta d_1 - 2\alpha \beta c}{\alpha + \beta + 2\alpha \beta(1 - c)D^{-1}}
\]

intersects all the three overlapping bands. Superconducting transition temperature as a function of doping passes through a maximum in this region. The limiting concentration \( c_1 \) is determined by the condition \( d_2 - \beta c_1 = \mu_3 \).

(iii) \( c > c_1 \). At extended overdoping, the chemical potential

\[
\mu_4 = \frac{d_1 - \alpha c}{1 - 2\alpha(1 - c)D^{-1}}
\]

falls out of the \( \beta \) band. The mixing of the band components in the doping process stimulates the Fermi liquid behavior of the carriers.
3. Theoretical Background with Interband Pairing

The general multiband Hamiltonian of a pair-transfer mediated superconductor reads

\[ H = H_0 + H_i = \sum_{\sigma, k, s} \epsilon_{\sigma}(k) a_{\sigma, k, s}^\dagger a_{\sigma, k, s} + \sum_{\sigma, \sigma'}^\prime \sum_{k, k'} q \times W(k, k') a_{\sigma, k}^\dagger a_{\sigma'(-k+q)}^\dagger a_{\sigma'(-k'+q)} a_{\sigma' k'} \].

(5)

Here, the electronic energies of band components (\(\sigma\)) are counted from the chemical potential \(\epsilon_{\sigma} = \xi_{\sigma} - \mu\). Usual designations for spins (s) and electron operators are used. The Cooper pairs with the momentum \(q\) are built up from the particles of the same band. The interband coupling constant \(W\) represents our central assumption that the leading pairing interaction in cuprates is realized by the pair transfer between the itinerant and defect subsystems. Superconductivity is then mutually induced in interacting components. The corresponding coupling allows contributions of exchange type Coulombic (\(U\)) and electron–phonon nature (\(V\)) regardless of repulsive or attractive sign of \(W = U + V\). Note that the interband electron–phonon constant \(V_{\sigma \sigma'}\) differs essentially\(^{59}\) from the one describing the Debye-region restricted attraction in the one-band case.

Inclusion of the intraband interactions does not change the qualitative physics described by (5) and is here neglected with the argument of smaller effective momentum volume capacity and known incapability to guarantee the cuprate high \(T_c\)-s. However, note that in suitable multiband cases, e.g., MgB\(_2\) the intraband phonon pairing channels can contribute decisively.\(^{66}\) The necessary condition for the prevailing pairing by interband interaction in a two-component system reads\(^{59}\)

\[ W^2 - U_1 U_2 > 0, \]

(6)

where \(U_2\) stands for intraband Coulombic contributions.

The superconductivity energetic characteristics will be calculated using the mean-field Hamiltonian corresponding to (5) and adapted to the model proposed

\[ H = \sum_{\sigma, k, s} \epsilon_{\sigma}(k) a_{\sigma, k, s}^\dagger a_{\sigma, k, s} + \sum_{k} \Delta_\gamma(k) [a_{\gamma - k}^\dagger a_{\gamma - k} + a_{\gamma - k}^\dagger] \]

\[ - \sum_{k, \tau}^\tau \Delta_\tau(k) [a_{\tau - k}^\dagger a_{\tau - k} + a_{\tau - k}^\dagger]. \]

(7)

Here \(\sigma = \alpha, \beta, \gamma; \tau = \alpha, \beta\) and \(\sum^\tau\) means the integration with the densities (\(\rho_{\alpha, \beta}\)) of states of the defect bands in the corresponding energy intervals. The superconducting gap order parameters are defined as

\[ \Delta_\gamma(q) = 2 \sum_{k, \tau}^\tau W(q, k) \langle a_{\gamma - k}^\dagger a_{\tau - k} \rangle, \]

\[ \Delta_\tau(q) = 2 \sum_{k} W(q, k) \langle a_{\gamma - k}^\dagger a_{\gamma - k} \rangle. \]

(8)
The operator (7) can be simply diagonalized, e.g., by the Green's function method and with the use of constant $W$ one arrives at the coupled gap system \( \Delta_\gamma = W \sum_{k, \tau} \Delta_\gamma(k) E_{\gamma}^{-1}(k) \frac{E_{\gamma}(k)}{2\Theta} \)

\[ \Delta_\tau = W \sum_k \Delta_\gamma(k) E_{\gamma}^{-1}(k) \frac{E_{\gamma}(k)}{2\Theta}. \]

Here, the Bogolyubov quasiparticle energies appear in the usual form \( E_\sigma(k) = \pm \sqrt{\epsilon_\sigma^2(k) + \Delta_\sigma^2(k)} \).

At \( T_c \) according to (9), the gaps \( \Delta_\sigma \) tend simultaneously to zero. For \( W > 0 \) two \( s \)-type order parameters (it is taken \( \Delta_\alpha = \Delta_\beta \)) appear with opposite signs. Equation (7) is written in the form to have positive \( s \). The supercarrier density is given by

\[ n_s = \frac{1}{2} \left[ \sum_k \Delta_\gamma^2(k) E_{\gamma}^2(k) \frac{E_{\gamma}(k)}{2\Theta} + \sum_k \Delta_\tau^2(k) E_{\tau}^2(k) \frac{E_{\tau}(k)}{2\Theta} \right]. \]

Not all the carriers become paired at \( T = 0 \) as in the one-band BCS scheme. The paired carrier number density \( N_s \) is given by \( N_s = n_s p N_0 \), where \( p \) is the hole doping concentration. The latter enters the theoretical scheme through \( \mu \), \( \rho_\gamma \), and the limits of integration. The condensation energy is represented by the thermodynamic critical field as

\[ H_{c0} = \sqrt{4\pi[(\rho_\alpha + \rho_\beta)(\Delta_\alpha^2 + \rho_\gamma \Delta_\gamma^2)]}. \]

4. Low-Energy Excitations

The low-energy excitation spectrum is reorganized in doped materials. The present multiband model superconductor can naturally manifest superconducting gaps and pseudogaps. The nature of these excitations is determined by the variable position of the chemical potential over the complex band scheme. A pseudogap appears as a minimal quasiparticle excitation energy of a component band not intersected by \( \mu \). \( \xi_\sigma \) is the superconducting gap. In the normal state the pseudogap survives as \( |\xi_\sigma - \mu| \). When an impact (e.g., doping) reorganizes the spectral relations so that \( \xi_\sigma = \mu \) becomes possible (\( \mu \) enters \( \sigma \)-band), the pseudogap transforms into the superconducting gap on such characteristic points of the phase diagram. A pseudogap continues behind this critical doping as the superconducting gap of the same subsystem. It does not represent the pairing strength and does not compete with the superconductivity. However, the pseudogap is not also a precursor of a superconducting gap on the energetic scale. It does not transform into the superconducting gap at \( T < T_c \) (cf. Refs. 82 and 85). Changes in the spectral contribution of the pseudogap with the temperature are expected to be small (cf. Refs. 81 and 82). The temperature of the existence of a
"pseudogap phase" must be interpreted as the energy scale necessary to overcome the pseudogap. In the model under consideration, one finds at heavy underdoping $c < c_\beta$ the following charge channel excitation gaps:

$$E_{\alpha}(\text{min}) = \Delta_i = [(d_1 - \alpha c - \mu_1)^2 + \Delta_\alpha^2]^{1/2},$$

$$E_{\beta}(\text{min}) = \Delta_\beta = \Delta_\alpha,$$

$$E_\gamma(\text{min}) = \Delta_s = [\mu_1^2 + \Delta_s^2].$$

It means that one has two pseudogaps: $\Delta_i$ (the large) and $\Delta_s$ observable in the nodal and antinodal spectral windows correspondingly. In the case where the $\beta$-subsystem states have born as ungapped, there will only be one (defect subsystem) pseudogap. The $\beta$-system superconducting gap of the nodal neighborhood can be exhausted by the extended account of the $d$-wave symmetry by multiplying $\Delta_\beta = \Delta_\alpha$ with the corresponding symmetry function restricting it to the nodal diagonal direction neighborhood. However, the participation of the nodal subsystem as the whole in the interband pairing is essential for the buildup of $T_c$ on the route to optimal doping.

In the case of two $s$-like order parameters, the two-band model with interband repulsion leads to two superconducting gaps of opposite signs. Pure $d$ and $s$, or mixed $d$--$s$ ordering symmetries are allowed in the two-band model according to the doping level and temperature. Extreme dopings favor separated $s$ and $d$ superconducting gap symmetries (cf. Ref. 94).

With extended doping at $c > c_\beta$, but $c < c_0$, $E_\gamma(\text{min})$ becomes represented by $\Delta_\gamma$, as $\xi = \mu$ can be satisfied — the small pseudogap is smoothly transformed into the itinerant superconducting gap which resides in the nodal window. The large pseudogap occupies at this the antinodal window. Its regime extends until $c \geq c_0$ is reached. The optimal doping is expected to appear near $c_0$ where all three-band components resonate with the Fermi energy and the multiband prerequisite to reach high transition temperatures becomes fulfilled. At overdoping $c > c_0$, the spectrum is expected to be determined by both superconducting gaps $\Delta_\gamma$ and $\Delta_\alpha$.

### 5. Calculated Gaps and Supercarrier Density

Illustrative calculations of cuprate pairing characteristics have been made with a plausible parameter set: $D = 2$; $d_1 = 0.3$ (according to Ref. 95); $d_2 = 0.1$; $\alpha = 0.66$; $\beta = 0.33$; and $W = 0.28$ (eV). The scale of the hole doping concentration ($p$) has been fixed by the choice $p = 0.28c$ which exposes the maximal $T_{cm} = 125$ K at the commonly pointed value $p = 0.16$. At this $p_\beta = 0.085$, $p_\alpha = 0.13$; $p_0 = 0.16$.

The bell-like behavior of the transition temperature (Fig. 1), as also of the supercarrier density in Fig. 2, is determined by the variable pairing conditions on the nonrigid spectrum according to the disposition of band components and the chemical potential. Such kind of $T_c$ behavior is well-known in two-band super-
conductivity and the destroyed profitable interband pairing conditions serve as a natural explanation of $T_c$ quenching at overdoping (cf. Ref. 83). The supercarrier number density is given by the multiple $n_s p$ and it can diminish with increasing $p$. Experimentally, it has been found$^{23}$ that the effective density of superconducting electrons is reduced as compared with the nominal carrier number density even in the overdoped region. There are no signs of bare fermionic gaps in $n_s(0)$ due to the interband nature of the pairing. The calculated order of the relation $N(\text{paired})$ to $N(\text{total})$ as $n_s p^{-1}$ agrees with the experimental estimations $\approx 0.2$ for various cuprate superconductors.$^{96}$ The Uemura-plot$^{97}$ calculated according to the present model shows a sublinear segment connecting $n_s$ and $T_c$ at underdoping and the following boomerang.

The calculated gaps at $T = 0$ (superconducting state) are also given in Fig. 1. The normal state (pseudo)gaps are seen in Fig. 2. The expected common manifestation of two underdoped state pseudogaps seems to be established for some La and Bi cuprates.$^{98-101}$ One can follow the smooth transformation of the small pseudogap into the larger superconducting gap (at $p_\beta$) in Fig. 1, as found in Refs. 20, 98 and 102. The large pseudogap extends to nearly optimal doping; experimentally, one sees it until slight overdoping.$^{43,44,82}$ At the second critical point $p_0$ the larger pseudogap transforms into the defect system superconducting gap as has been found also in Refs. 82 and 102. On intermediate dopings, the $\alpha$-defect system pseudogap and the itinerant superconducting gap appear together (cf. Refs. 25, 53, 103 and 104). According to the extent of the phase separation, one can attribute these gaps to different real space regions. The manifestation of $\Delta_\gamma$ in the nodal spectral window and of $\Delta_i$ in the antinodal one agrees with the observations.$^{43,82,105}$ Spectrally, one

Fig. 1. (1) The large pseudogap $\Delta_i$; (2) the small pseudogap $\Delta_s$; (3) the itinerant superconducting gap $\Delta_\gamma$; (4) the defect system superconducting gap $\Delta_\alpha$; (5) $T_c$. $p_\beta = 0.085$, $p_\alpha = 0.13$; $p_0 = 0.16$. 
Fig. 2. The doping dependences of supercarrier density $n_s(0)$ (1) dimensionless; (2) $T_c$; (3) the large and (4) the small normal state gap.

relates $\Delta_1$ to the hump feature. Accordingly, the nodal superconductivity coexists with the incoherent antinodal excitations. Eventually, the hump is shifted to larger energies with reduced dopings and it remains preserved for $T > T_c$.

The crossing of $\Delta_1$ and $\Delta_\gamma$ must be noted (cf. Ref. 82), i.e., the pseudogap and superconducting gap energy scales being very different at underdoping can become further comparable (cf. Ref. 107). The manifestation of a superconducting gap on a given doping can be substituted by the normal state gap for $T > T_c$ in this region. The normal state (pseudo)gap energy extrapolates to zero at a critical point (see Fig. 2 and cf. Ref. 85). It means that at low temperatures, a pseudogap cannot manifest itself on dopings where it will be found in the normal state. Behind $p_0$ at overdoping, the spectrum is expected to be determined by both superconducting gaps $\Delta_\alpha, \gamma$. Distinguishing of these two gaps spectrally can be complicated. The Fermi energy intersects the electron spectrum parts headed by different band components at different wave vectors and the larger gap can remain masked. The subsystem to which the smaller gap belongs can add spectral weight to the larger spectral hole, etc.

The quenching of superconducting gaps with rising temperature and their common vanishing at $T_c$ is of the “usual” type. For the illustration, the $n_s(T)$ dependence is given in Fig. 3 for $p = 0.14$. The characteristic ratios of superconducting gaps to $T_c$ are of non-BCS universality. $2\Delta_\gamma / \Theta_c$ is nonmonotonic in $p$, whereas the smaller $2\Delta_\alpha / \Theta_c$ diminishes with enhanced doping over the scale.

The nonrigid behavior of the electron spectrum with doping introduces into the present model special concentrations where the band components begin overlap. The bare gaps become closed and the corresponding defect subsystem will be metallized. Insulator to metal transitions are expected on these concentrations as
observed. At that, the metallization of the nodal defect-liquid is reached at $p_\beta$. On much smaller dopings the formation of doped hole ferrons can be supposed. The defect bands act then as a bath of uncompensated spins, whereas the itinerant band preserves antiferromagnetic fluctuations. This is comparable with the situation in the (bi)polaron theory. Possibly a way for analogous explaining of underdoped state magnetic effects lies here. It must be noted that bands overlap regulated by doping opens the way for the participation of carriers of the nature (sign) not being introduced by doping (cf. Ref. 54). With extended dopings the Fermi surface must look more and more electron-like with peripheral hole pockets according to the overlapping band dispersion image. For smaller dopings than $p_0$ the antinodal particles remain insulating, the nodal ones being metallic. Further, a mixed carrier liquid is formed; the itinerant and defect subsystem lose their individuality. The contribution of the antinodal momentum region grows here essentially as observed.

As result, the general trends and events on the hole-doped cuprate superconductors phase diagram can be explained by the present model with multiband nonrigid gapped spectrum.

6. The Free Energy Functional

The investigation of thermodynamic characteristics of cuprate superconductors using the present model needs the derivation of the long-wavelength expansion of the free energy for a two component superconductor with the leading pair-transfer interaction. We define the effective interaction Hamiltonian

$$H_\lambda = W \sum_{\sigma k q} (\lambda_{\sigma q} \tilde{a}_{\sigma k} ^+ \tilde{a}_{\sigma k} + \text{h.c.})$$

(14)
and divide the full Hamiltonian (5) into parts as

\[ H = H_1 + H_2, \quad H_1 = H_0 + H_\lambda, \quad H_2 = -H_\lambda + H_i. \]  

(15)

The fluctuating superconducting order parameters bear the index \( \mathbf{q} \) of the total momentum of an electron pair.

The mean-field free energy of \( H \) reads according to Bogolyubov

\[ F = -k_B T + \ln Z(H_1) + \langle H_2 \rangle_{H_1}, \]  

\[ Z(H_1) = Sp \exp \left(-\frac{H_1}{k_B T} \right), \]  

(16)

(17)

where \( \langle \cdot \rangle_{H_1} \) means the average with respect to \( H_1 \). Near the phase transition temperature the free energy (16) will be expanded as \( F = F_0 + F_2 + F_4 \), where \( F_0 = -k_B T \ln Z(H_0), \) \( F_2 \sim \lambda^2, \) \( F_4 \sim \lambda^4 \). Whereas we will consider only the long-wave fluctuations of \( \lambda_\sigma \), the coefficients in \( F_4 \) can be taken at \( \mathbf{q} = 0 \) and the fourth-order contribution \( F_4 \) can be written down according to the analogy with the corresponding terms in the homogeneous free energy expansion. So, in fact, we have to find only \( F_2 \) in the case \( \mathbf{q} \neq 0 \).

To obtain \( F_2 \), we will use the unitary transformation \( \hat{A} = U^{-1} A U, U = \exp(iS) \) with

\[ S = iW \sum_{\sigma \mathbf{k} \mathbf{q}} \left[ \frac{a_{\sigma \mathbf{k}}^+ a_{\sigma \mathbf{q} - \mathbf{k}}^+}{\epsilon_\sigma(\mathbf{k}) + \epsilon_\sigma(\mathbf{k} - \mathbf{q})} \lambda_{\sigma \mathbf{q}} + \text{h.c.} \right] \]  

(18)

which leads in the second-order approximation to the expression

\[ \hat{H}_1 \approx H_0 + i \frac{1}{2} [H_\lambda, S]. \]  

(19)

By means of this transformation, one can find

\[ Z(H_1) \approx Z \left(H_0 + \frac{i}{2} [H_\lambda, S]\right) \approx Z(H_0) \left[1 + \frac{|W|}{2k_B T} \sum_{\sigma \mathbf{q}} |\lambda_{\sigma \mathbf{q}}|^2 \eta_{\sigma \mathbf{q}}(T) \right], \]  

\[ \sum_{\mathbf{k}} \langle a_{\sigma \mathbf{k} + \mathbf{q}} a_{\sigma \mathbf{k}} \rangle_{H_1} \approx -\frac{w}{2} \lambda_{\sigma \mathbf{q}} \eta_{\sigma \mathbf{q}}(T), \]  

(20)

(21)

where \( w = \text{sgn}(W) \) and

\[ \eta_{\sigma \mathbf{q}}(T) = \frac{|W|}{2} \sum_{\mathbf{k}} (\epsilon_\sigma(\mathbf{k}) + \epsilon_\sigma(\mathbf{k} - \mathbf{q}))^{-1} \left[ \frac{\epsilon_\sigma(\mathbf{k})}{2k_B T} + \tanh \frac{\epsilon_\sigma(\mathbf{k} - \mathbf{q})}{2k_B T} \right]. \]  

(22)

As a result, we have factorizing \( \langle H_2 \rangle_{H_1} \)

\[ F_2 = \frac{|W|}{2} \sum_{\mathbf{q}} \left[ \sum_{\sigma} \eta_{\sigma \mathbf{q}}(T) |\lambda_{\sigma \mathbf{q}}|^2 + \frac{w}{2} \eta_{1 \mathbf{q}}(T) \eta_{2 \mathbf{q}}(T) (\lambda_{1 \mathbf{q}} \lambda_{2 \mathbf{q}}^* + \lambda_{1 \mathbf{q}}^* \lambda_{2 \mathbf{q}}) \right]. \]  

(23)

The coefficient (22) will be expressed near \( T = T_c \) (\( \tau = (T - T_c) T_c^{-1} \)) and \( \mathbf{q} = 0 \) as

\[ \eta_{\sigma \mathbf{q}}(T) = \eta_{\sigma 0}(\theta_c) - \alpha_\sigma \tau - \sum_{i,j} B_{\sigma ij} q_i q_j, \]  

(24)
where \((\theta_c = k_B T_c)\)

\[
\alpha_{\sigma} = \frac{|W|}{2\theta_c} \sum_k \cosh^{-2} \frac{\xi_{\sigma}(k)}{2\theta_c}
\]  

(25)

and \(B_{\sigma}\) is given by a complicated formula for which an approximate expression will be presented later. The linear terms \(\sim q_i\) in Eq. (24) are absent in connection with the approximation

\[
\xi_{\sigma}(k) = E_{0\sigma} \pm \sum_i \frac{\hbar^2 k_i^2}{2m_{\sigma i}}
\]  

(26)

for the band energies with \(m_{\sigma i} > 0\).

The integration in the momentum space is supposed to be performed from \(0\) to \(c\) for an electron band and from \(c\) to \(0\) for a hole band. For constant densities of states \((\rho_\sigma)\) and supposing that \(|\Gamma - \mu| > \theta_c\), with \(\mu\) inside of the integration limits, one obtains

\[
\eta_{\sigma} = |W|\rho_\sigma \ln \frac{|\Gamma_{0\sigma} - \mu|}{(\pi\theta_c)^2} \frac{|\Gamma_{c\sigma} - \mu|}{(2\gamma)^2},
\]  

(27)

\[
\alpha_{\sigma} = 2|W|\rho_\sigma,
\]  

(28)

\[
\sum_{i,j} B_{\sigma ij} q_i q_j = \beta_{\sigma} \sum_i \frac{\hbar^2 q_i^2}{4m_{\sigma i}},
\]  

(29)

\[
\beta_{\sigma} = \frac{7\zeta(3)|W|\rho_\sigma|\mu - E_{0\sigma}|}{2(\pi\theta_c)^2},
\]  

(30)

where \(\gamma \approx 1.78\) and \(\zeta(3) \approx 1.2\). Note that \(|\mu - E_{0\sigma}|\) determines the Fermi energy in the corresponding band. In the case if \(\mu\) lies out of the integration limits

\[
\eta_{\sigma} = |W|\rho_\sigma \ln \left| \frac{\Gamma_{c\sigma} - \mu}{\Gamma_{0\sigma} - \mu} \right|, \quad \alpha_{\sigma} = \beta_{\sigma} = 0.
\]  

(31)

Analogous formula can be found also for \(\mu\) coincidence with one of the integration limits.

On the basis of Eqs. (24) and (29), \(F_2\) takes the following form:

\[
F_2 = \frac{|W|}{2} \sum_q \left\{ \sum_{\sigma} \left[ \eta_{\sigma} - \alpha_{\sigma} \tau - \beta_{\sigma} \sum_i \frac{\hbar^2 q_i^2}{4m_{\sigma i}} \right] |\lambda_{\sigma q}|^2 
\]

\[
+ \frac{w}{2} \left[ 4 - (\eta_1 \alpha_2 + \eta_2 \alpha_1) \tau - \eta_1 \beta_2 \sum_i \frac{\hbar^2 q_i^2}{4m_{2i}} - \eta_2 \beta_1 \sum_i \frac{\hbar^2 q_i^2}{4m_{1i}} \right] 
\]

\[
\times (\lambda_{1q}^* \lambda_{2q} + \lambda_{1q}^* \lambda_{3q}) \right\}. 
\]  

(32)
After the Fourier transformation to the coordinate space, the approximate expression for the second-order contribution to the free energy reads

\[
F_2 = \frac{|W|}{2V} \int dr \left\{ \sum_{\sigma} \left[ (\eta_\sigma - \alpha_{\sigma}\tau)|\lambda_\sigma(r)|^2 - \beta_\sigma \sum_i \frac{\hbar^2}{4m_{\sigma i}} \left| \left( \nabla_i - \frac{2ie}{\hbar c} A_i \right) \lambda_\sigma(r) \right|^2 \right] \\
+ \frac{w}{2} \left[ 4 - (\eta_1\alpha_2 + \eta_2\alpha_1)\tau \right] |\lambda_1(r)\lambda_2^*(r) + \lambda_1^*(r)\lambda_2(r)| \\
- \sum_i \left( \eta_1\beta_2 \frac{\hbar^2}{4m_{2i}} + \eta_2\beta_1 \frac{\hbar^2}{4m_{1i}} \right) \\
\times \left( \left( \nabla_i - \frac{2ie}{\hbar c} A_i \right) \lambda_1(r) \left( \left( \nabla_i - \frac{2ie}{\hbar c} A_i \right) \lambda_2(r) \right)^* \\
+ \left( \left( \nabla_i - \frac{2ie}{\hbar c} A_i \right) \lambda_1(r) \right)^* \left( \left( \nabla_i - \frac{2ie}{\hbar c} A_i \right) \lambda_2(r) \right) \right] + \frac{(\text{rot} A)^2}{8\pi}, \right\}, \tag{33}
\]

where the vector potential $A$ takes care of the gauge invariance. This $F_2$ expression contains squared gradient terms, however, with opposite signs in comparison with the one band case. Products of gradient terms of different bands appear in (33).

For the fourth-order term, we have

\[
F_4 = -\frac{|W|}{2V} \int dr \left\{ \frac{3}{2} \sum_{\sigma} \nu_\sigma |\lambda_\sigma(r)|^4 + \frac{w}{2} \nu_1 \eta_2 |\lambda_1(r)|^2 \\
+ \nu_2 \eta_1 |\lambda_2(r)|^2 |\lambda_1(r)\lambda_2^*(r) + \lambda_1^*(r)\lambda_2(r)| \right\}. \tag{34}
\]

Here in the integration scheme described above

\[
\nu_\sigma = \frac{7\zeta(3)|W|^3\rho_\sigma}{(2\pi\theta_c)^2}, \tag{35}
\]

with $\mu$ inside of the integration limits. If $\mu$ lies out of the integration limits, $\nu_\sigma = 0$.

### 7. Equilibrium Equations of Band Order Parameters

Minimization of the free energy functional determined by Eqs. (33) and (34) leads to the system of equations for superconducting band order parameters:

\[
2w\lambda_1(r) + \left[ \frac{\eta_2}{\nu_\sigma} - \sum_i \frac{i\hbar\nabla_i - \frac{2e}{c} A_i}{4m_{2i}} \right] \left( \frac{2e}{c} A_i \right)^2 - \frac{\alpha_2\tau}{\nu_2} |\lambda_2(r)|^2 \right] \lambda_2(r) = 0, \tag{36}
\]

\[
2w\lambda_2(r) + \left[ \frac{\eta_1}{\nu_\sigma} - \sum_i \frac{i\hbar\nabla_i - \frac{2e}{c} A_i}{4m_{1i}} \right] \left( \frac{2e}{c} A_i \right)^2 - \frac{\alpha_1\tau}{\nu_1} |\lambda_1(r)|^2 \right] \lambda_1(r) = 0.
\]
The homogeneous solutions of these equations, \( \tilde{\lambda}_{1,2} \), are the following (\( A = 0 \) and \( T < T_c \))

\[ |\tilde{\lambda}_{1,2}|^2 = -\eta_2 \Xi \tau, \quad (37) \]

where

\[ \Xi = \eta_1 \alpha_2 + \eta_2 \alpha_1 \quad (38) \]

The superconducting gaps are proportional to \( \tilde{\lambda}_{1,2} \),

\[ \Delta_{1,2} = W \tilde{\lambda}_{1,2}, \quad (39) \]

and vanish simultaneously at \( T_c \).

8. Coherence Characteristics

The second-order contribution \( F_2 \) into free energy can be diagonalized by an orthogonal transformation

\[ \lambda_{1q} = \lambda_{rq} \cos \varphi_q + \lambda_{sq} \sin \varphi_q, \]

\[ \lambda_{2q} = -\lambda_{rq} \sin \varphi_q + \lambda_{sq} \cos \varphi_q, \quad (40) \]

with

\[ \tan \varphi_q = \frac{w \eta_2}{2} \left\{ -1 + [4(\eta_1 + \eta_2)]^{-1} \left[ (\eta_1^2 \alpha_2 - \eta_2^2 \alpha_1) \tau \right. \\
+ \sum_i (\eta_1^2 \beta_2 m_{21}^{-1} - \eta_2^2 \beta_1 m_{1i}^{-1}) \frac{\hbar^2 q_i^2}{4} \right] \} \]

\[ (41) \]

In terms of new variables,

\[ \psi_{s,r}(r) = \frac{1}{2} \sqrt{\frac{W}{V}} (\beta_1 + \beta_2) \sum_q \lambda_{s,rq} e^{iqr}, \quad (42) \]

we obtain

\[ F_2 = \int dr \left[ a_0 |\psi_s(r)|^2 + (a_0 - a_r) |\psi_r(r)|^2 + \sum_i \frac{\hbar^2}{4M_i} \left( \nabla_i - \frac{2ie}{\hbar c} A_i \right) |\psi_s(r)|^2 \right. \\
- \sum_i \frac{\hbar^2}{4M_i} \left( \nabla_i - \frac{2ie}{\hbar c} A_i \right) |\psi_r(r)|^2 + \frac{(\text{rot} A)^2}{8\pi} \right], \quad (43) \]

where

\[ a_0 = (\eta_1 + \eta_2)^2 u^{-1}, \quad (44) \]

\[ u = \frac{1}{2} (\eta_1 + \eta_2)(\beta_1 + \beta_2), \quad (45) \]
Here, the indices \( s \) and \( r \) refer to the words “soft” and “rigid.” The coefficient \( a_s \) changes its sign when temperature passes \( T_c \). On the contrary, the coefficient before \( j_r j_2 \) remains positive. The “soft” variable \( \psi_s \) plays the role of a driver for the phase transition.

On the basis of Eqs. (37), (40), and (42), one can find the homogeneous equilibrium values of \( \psi_{s,r} \) if \( T < T_c \),

\[
|\tilde{\psi}_s|^2 = \frac{|W|}{2V} (\beta_1 + \beta_2)(|\lambda_1|^2 + |\lambda_2|^2) = -\frac{|W|}{2V} u \Xi \tau
\]  

and

\[
|\tilde{\psi}_r|^2 = 0.
\]

If \( T > T_c \), we have \( \tilde{\psi}_s = \tilde{\psi}_r = 0 \). Therefore, the superconducting gaps are determined only by \( \tilde{\psi}_s \).

Minimization of the second-order contribution of the free energy (43) leaves us with the following linearized independent equations for \( \psi_{s,r} \), respectively:

\[
\left[ \sum_i \frac{\hbar^2}{4M_{si}} \left( \nabla_i - \frac{2ie}{\hbar c} A_i \right)^2 - a_s \tau \right] \psi_s(\mathbf{r}) = 0,
\]

\[
\left[ \sum_i \frac{-\hbar^2}{4M_{ri}} \left( \nabla_i - \frac{2ie}{\hbar c} A_i \right)^2 - a_o + a_r \tau \right] \psi_r(\mathbf{r}) = 0.
\]

Consequently, the squared coherence lengths, associated with \( \psi_s \) and \( \psi_r \), are given by

\[
\xi_{ss}^2 = \frac{\hbar^2}{4M_{si} a_s \tau},
\]

\[
\xi_{rr}^2 = \frac{-\hbar^2}{4M_{ri}(a_o - a_r \tau)}.
\]

As the result, the spatial behavior of superconducting order parameters are governed by two different coherence scales. The \( \xi_s \) acts as an Ornstein–Zernicke type critical coherence length known for one-band systems and diverging at \( T \to T_c \). The other one, \( \xi_r \), behaves noncritically and as an imaginary quantity characterizes obviously a periodic spatial coherence wave.

Similarly, the damping of the order parameters fluctuations of a two-band superconductor with interband pairing is characterized by a critical and a noncritical
relaxation channel. The relaxation times connected with these channels reveal correspondingly critical and noncritical dependencies on temperature.

The discussion of the nature of the spatial periodic fluctuation structure characterized by the rigid coherence length $\xi_r$ with weak dependence on temperature remains out of the scope of the present paper. Note that Leggett has shown that two-band superconductors possess, besides the usual amplitude Goldstone type excitation mode, another one, which operates with the difference of the phases of the two superfluids. If one associates $\psi_r$ with the Leggett mode, it can then be supposed to behave noncritically near the phase transition point. It will be tempting to attribute the parameter $\xi_r$ to the recently observed pair density wave without phase coherence. Then, probably, $\xi_r$, characterizes the average distance between the pairs (without phase coherence in the normal state). One can find that $\xi_r$ as a function of doping falls off by leaving the underdoped region of actual $T_c - s$. In this case, the pair distribution density becomes more homogeneous (cf. Ref. 116). As the result, in multiband case the spatial distribution of superconducting characteristics must not necessarily stem from the granularity of the superconducting material.

9. Cuprate Coherence Length, Supercarrier Effective Mass, and Penetration Depth

According to (54) in our model, we characterize the CuO$_2$ plane coherence length ($\xi_{ab}$) by the quantity

$$\xi_{0}^2 = \tau \xi_{s}^2 = \frac{\hbar^2}{4} \frac{(\eta_{a} + \eta_{b})\beta_{a}m_{a}^{-1} + \eta_{b}(\beta_{a}m_{a}^{-1} + \beta_{b}m_{b}^{-1})}{(\eta_{a} + \eta_{b})\alpha_{a} + \eta_{b}(\alpha_{a} + \alpha_{b})},$$

(56)

The bare effective masses of the bands are expressed through the densities of states $m_i = 2\pi\hbar^2\rho_i V^{-1}$ with $V$ being the plaquette area in the CuO$_2$ plane. The calculated $\xi_0$ over the whole doping region together with the dependence of the thermodynamic critical field representing the condensation energy is given in Fig. 4. The order of $\xi_0$ of some tens of Å in the actual region agrees with the values given in the literature. This points to certain self-consistency of the present theoretical scheme concerning the results of Sec. 5.

The theoretical valley-profile like $\xi_0(p)$ curve agrees in its general behavior well with the essential recent experimental result covering the whole doping scale. The points in Fig. 4 represent the results of Ref. 118 scaled to the theoretical curve. At extreme dopings it grows faster in comparison with the indication of the experiment. The dependence of $\xi_0$ must be qualified as an expected result: weakly coupled pairs must have larger spatial extensions. The behavior of $H_{c0}$ repeats the dependence of $T_c$ and $n_s$ and projecting it on $\xi_0$ leads one with the conclusion that in the present model, the strength of the pairing and the phase coherence develop and vanish simultaneously in accordance with the conclusions of the recent experimental investigations on cuprates. The common trend of the
condensation energy and of the superconducting gap has been followed in Ref. 125. Note that the overdoped regime corresponds to higher carrier concentrations but to smaller supercarrier density. Theoretical doping dependence of the $c$-axis second critical magnetic field ($T = 0$) $H_{c2} = \Phi(2\pi\xi_0^2)^{-1}$ is given in Fig. 5. It also shows a well-expressed maximum corresponding to the effective contribution of the nodal subsystem after the overlap concentration $p_\beta$ is passed.

The paired carrier effective mass $m_{ab}$ has been calculated according to (48) as

$$m_{ab} = \frac{1}{2} \frac{(\eta_\alpha + \eta_\beta + \eta_\gamma)\beta_\alpha + \beta_\beta + \beta_\gamma}{(\eta_\alpha + \eta_\beta)\beta_\gamma m_\gamma^{-1} + \eta_\gamma(\beta_\alpha m_\alpha^{-1} + \beta_\beta m_\beta^{-1})}.$$  \hspace{1cm} (57)

Its theoretical dependence on the whole doping scale $^8$ is given in Fig. 6 where $m_{ab} = x m_0$ ($m_0$ is the free electron mass) diminishes in the whole doping region.

Fig. 4. The critical plane coherence length and the thermodynamic critical field (dashed, $T = 0$). ■ scaled results of Ref. 118.

Fig. 5. The $c$-axis second critical magnetic field versus doping.
Out of the extremely underdoped region, this decrease is not fast and a rough estimation \( x \sim 3 \), as often supposed, seems to be acceptable. The recent experimental result\(^{126}\) disposes \( m_{ab} \) to be constant. Our large values of \( x \) at the origin reduce to large effective mass of the narrowest defect \( \beta \)-band. Starting from \( p_\beta \), the contribution of wide valence band carriers is added. The kink near \( p_0 \) corresponds to the simultaneous action of the \( \alpha-\beta \) carriers. The supercarrier effective mass reflects the structure of the electron spectrum and reproduces the trend of the carrier collective toward the normal Fermi liquid behavior with doping in cuprate.

The plane penetration depth is expressed as

\[
\lambda = \sqrt{\frac{m_{ab}e^2}{4\pi e^2 N_s}}.
\]  

(58)

The quantity \( \lambda^{-2} \), which is proportional to \( n_s(0)px^{-1} \) determines the behavior of the superfluid stiffness. This dependence is shown in Fig. 7. The presence of the
maximum on this curve (in slightly overdoped region) is driven by the behavior of 
\( n_s(0) \). It dominates over the supercarrier effective mass changes and the increase 
of normal state carrier number with extended (over)doping. The calculated doping 
dependence of \( \lambda^{-2} \) is in agreement with the experimental findings in Refs. 121 and 
122, also by its order of magnitude.

10. The Isotope Effect

A trend of the isotope (O\(^{16} \rightarrow \)O\(^{18} \)) effect exponent (\( \alpha \) for \( T_c \)) to enhance with 
lowering transition temperature and vice versa appeared to be characteristic for 
cuprates.\(^{4,127-129} \) Correspondingly, one asks about the relative contribution of the 
electron–phonon interaction (intra- and interband) into the cuprate pairing mech-
anism. In the framework of multiband superconductivity with interband pairing, 
the unexpected behavior of \( \alpha \) can be simply explained\(^{59,130} \) (see also Refs. 61, 
131–133). Furthermore, a moderate electron–phonon contribution into interband 
\( W \) does not necessarily mean a small isotope effect.\(^{59,130} \) This circumstance is 
connected with the mass dependence of the effective interelectronic coupling by 
phonons of frequency \( \omega \)

\[
V_{\sigma\sigma'}(\mathbf{k}, \mathbf{k}') = \frac{|g_{\sigma\sigma'}(\mathbf{k} - \mathbf{k}')|^2 \hbar \omega(\mathbf{k} - \mathbf{k}')}{[\epsilon_{\sigma}(\mathbf{k}) - \epsilon_{\sigma'}(\mathbf{k}')]^2 - [\hbar \omega(\mathbf{k} - \mathbf{k}')]^2} \tag{59}
\]

in the interband case. The attractive part of (59) does not depend on \( M \) in both 
intra- and interband (\( \sigma = \sigma' \)) and interband (\( \sigma \neq \sigma' \)) cases because \( g = \sqrt{\hbar/2M\omega_D} \) with 
\( \omega_D \sim M^{1/2} \). In the BCS theory, the mass \( M \) attributed to the effective vibrations 
enters only through the Debye integration borders. However, in a large part of 
momentum space where \( \hbar \omega \) can be neglected in comparison with \( |\epsilon_{\sigma} - \epsilon_{\sigma'}| \), one 
has \( V \sim M^{-1} \). This interband repulsive coupling \( V_{\sigma\sigma'} \sim M^{-1} \) can immediately 
participate in pairing.

The isotope effect characteristic exponents are defined as

\[
\alpha_{X_i} = \frac{d \ln X}{d \ln M} C_i, \tag{60}
\]

where \( X \) designates the physical quantity under consideration and \( i \) specifies the 
atomic mass (\( M_i \)) undertaken to be isotopically substituted. The effective vibration 
mass (\( M \)) can be a complicated function of the masses of the atoms in the unit cell. 
This is accounted by \( C_i = d \ln M(d \ln M_i)^{-1} \). Further, \( \alpha_n \) will correspond to the 
supercarrier density \( n_s \); \( \alpha_m \) to supercarrier effective mass; \( \alpha_\lambda \) to the penetration 
depth; and \( \alpha_\rho \) to the superfluid stiffness. One has

\[
\alpha_m \alpha_n^{-1} = \frac{T_c}{m_{ab}} \frac{dm_{ab}}{dT_c}, \quad \alpha_\lambda = \frac{1}{2} (\alpha_m - \alpha_n), \quad \alpha_\rho = -2 \alpha_\lambda. \tag{61}
\]

In the case of dominating interband pairing, leaving out \( C_i \), and designating by 
\( Z = VW^{-1} \) the relative electron–phonon contribution into the interband pairing

\[
\alpha_X = Z \frac{W}{X} \frac{dX}{dW}. \tag{62}
\]
Recently, the investigations of isotope effects concentrated on $\lambda^{-2}$ as superfluid stiffness.\textsuperscript{128,129} This quantity depends on supercarrier number density $N_s$ and paired carrier effective mass through the factor $N_s m_{ab}^{-1}$. In the conventional BCS theory, $N_s$ is usually interpreted as the total carrier density. Correspondingly, one often interprets $\alpha_\lambda$ ignoring the $\alpha_n$ contribution because the number of the normal state carriers does not change by isotopic substitution (see Ref. 135). In the multiband case with interband pairing the isotope effect on $N_s$ must appear, as has been predicted in Ref. 134. According to the mechanism driving $n_s$, only a part of normal state carriers will be paired even at $T = 0$.

The transition temperature and supercarrier density isotope effect exponents have been calculated numerically. The interband interaction constant $W$ has been varied according to (62) and the necessary derivatives have been determined from the doping dependence curves.

The calculated $\alpha_n$ curve corresponding to $Z = 0.05$ is shown in Fig. 8. The decrease of $\alpha$ with increasing $T_c$ is illustrated. One can conclude that even a contribution of some percent from the electron–phonon interaction to the interband pairing channel can lead to “normal valued” transition temperature isotope exponents. This can be understood from the approximate formulae for $T_c$ of the present approach (see Ref. 59). The experimental doping dependence of $\alpha$ in cuprates has been approximated in Ref. 135 by the expression $\alpha = 0.25 T_c T_{cm}^{-1} \sqrt{1 - T_c T_{cm}}$ ($T_{cm}$ is the maximal value of $T_c$) for the underdoped region. Our result is compared with this curve in Fig. 9 and is exposed as being too slow. One source for this discrepancy can be the dependence of $z$ on doping. The enhancement of the electron–phonon relative contribution into $W$ with progressive underdoping can improve the result.

The calculation supports the presence of the predicted isotope effect in the supercarrier density.\textsuperscript{134} It behaves analogously to $\alpha(p)$ because the $n_s$ and $T_c$ bell-like doping dependencies have the same origin.

![Fig. 8. The supercarrier density isotope effect exponent versus hole doping.](image-url)
Fig. 9. Theoretical $\alpha$ (full line) compared with the averaged experimental data\textsuperscript{135} at underdoping.

Fig. 10. The supercarrier effective mass isotope effect exponent versus doping.

The paired carrier effective mass isotope effect exponent dependence on doping is shown in Fig. 10. The negative values of $\alpha_m$ at underdoping agree with the observed trend find from superfluid stiffness data supposing the absence of the contribution from the paired carrier density.\textsuperscript{128,129} Theoretical absolute values of $\alpha_m$ are small as compared with $\alpha_n$ which is in the same order as $\alpha$. As the result, the overall negative isotope exponent of the plane ($T = 0$) penetration depth is determined by dominating $\alpha_n$. The theoretical $\alpha_\lambda(p)$ curve is given in Fig. 11. Its behavior and observed order of magnitude are also determined by the isotope effect in the paired carrier density overwhelming the paired carrier effective mass contribution. Experimentally, the superfluid density oxygen isotope effect exponent is estimated to be around 0.5. A representative value of $\alpha_\lambda$ from Fig. 11 leaves one for $\alpha_\rho = -2\alpha_\lambda$ in this scale.
11. Model Scenario for Electron-Doped Cuprates

In the case of the electron doping, the defect states are built up near the bottom of the UHB ($\beta$). The leading pairing interaction is supposed to be the pair transfer between the defect antinodal ($\alpha_1$) and nodal ($\alpha_2$) defect subbands and the UHB\cite{112} (see also Refs. 21 and 136). The total number of states is normalized to one (including the LHB $\gamma$) and the doping concentration for one Cu site and one spin is $c$. At half-filling ($c = 0$) the spectral weight of Hubbard bands (of width $\Delta d$) is $1/2$. With extended electron doping it diminishes\cite{16} to $(1/2 - c)$. The loosed weight $2c$ is divided between defect subbands equally.

The ($\alpha_1$) band bottom is shifted by $d$ over the ($\alpha_2$) band bottom as energy zero. The $\beta$-band bottom is fixed at $d_1$. The defect band tops must be shifted towards the UHB with extended doping by the same arguments as in the case of hole doping. As suggested by the pseudogap,\cite{137} energy dependencies given in Refs. 138 and 139 we have chosen quadratic evolving of ($\alpha_1$) and ($\alpha_2$) top energies as $(d + \alpha c^2)$ and $(\alpha c^2)$ correspondingly. The defect subbands densities of states $\rho_{\alpha}(1, 2) = (\alpha c)^{-1}$ rise with doping, and of the Hubbard components $\rho_{\beta, \gamma} = (1/2 - c)(\Delta d)^{-1}$ diminish.

At the critical concentration $c_0 = [(d_1 - d)/\alpha^{-1}]^{1/2}$ the $\alpha_1$-$\beta$ gap closes. For $c < c_0$, $\mu_1 = d + \alpha c^2$ remains connected with the upper defect subband in accordance with the conclusion in Refs. 140 and 141 that at low dopings electrons occupy the antinodal region. For $c \geq c_0$ ($c < c_x$) the $\alpha_1$ and $\beta$ bands overlap, being both intersected by $\mu_2 = (d + \alpha c^2 + d_1 \alpha c \rho_\beta)(1 + \alpha c \rho_\beta)^{-1}$. Experimentally, one can observe here a steep ($\alpha_1$) and a flat ($\beta$) energy dispersion.\cite{140} Behind $c_x$, $\mu_2(c_x) = \alpha c_x^2$, all three actual band components overlap and are intersected by $\mu_3$. Now, additional nodal spectral intensity is added and a mixed carrier liquid is formed. Experimentally, observed\cite{142} growing participation of hole type carriers with doping can be explained by the position of $\mu$ in the upper parts of defect subbands. The optimal interband pairing conditions near $c_x$ become destroyed by further doping.
At heavy underdoping \( c < c_0 \), two pseudogaps are expected. The \( \beta \)-band attributed
\[
\Delta_{p\beta} = \left[ (d_1 - d - \alpha c^2)^2 + \Delta_{\beta} \right]^{1/2}
\] (63)
is expected to appear in the antinodal, and the \( \alpha \)-2-band attributed
\[
\Delta_{p\alpha} = \left[ d^2 + \Delta_{\alpha}^2 \right]^{1/2}
\] (64)
in the nodal region. The normal state gap \( \Delta_{p\beta} \) closes at \( c_0 \); the separation of occupied and empty states vanishes indicating the destruction of the antiferromagnetic order. The smaller pseudogap starts to diminish for \( c > c_0 \) until \( c_x \) as
\[
\Delta_{p\alpha} = \left[ (\mu - \alpha c^2)^2 + \Delta_{\alpha}^2 \right]^{1/2}.
\] (65)
The superconducting gap \( \Delta_{\alpha} \) is expected to appear here in the antinodal spectral window. Beyond \( c_x \) the excitation spectrum is expected to be determined by both superconducting gaps \( \Delta_{\beta} \) and \( \Delta_{\alpha} \) (in the whole momentum window). By vanishing normal state gap \( |\mu - \alpha c^2| \) at \( c_x \), the AF order tracks also disappear in the nodal window.

12. Calculated Doping Dependencies for Electron Doping

For illustrative calculations of a model electron doped cuprate with \( T_c \sim 30 \) K near \( c = 0.15 \) in the domain between \( c = 0.07 \) and 0.3, the following set of parameters have been taken: \( d = 0.03; d_1 = 0.1; \Delta d = 1.0 \); and \( \alpha = 10 \) (eV). Then \( W = 0.175 \) eV leads to \( T_{cm} = 28 \) K at \( c = 0.15 \). At this, \( c_0 = 0.08 \) and \( c_x = 0.13 \).

Figure 12 shows the calculated \( T_c \), \( \mu \) and both pseudogaps on the doping scale. The transition temperature and the density of paired carriers show the “usual”

Fig. 12. \( T_c \) (1); \( \mu \) (2); the large (3) and the small (4) normal state (pseudo)gaps on electron doping scale. The inset shows the supercarrier density.
piked behavior with the drop behind $T_{cm}$ where, on the contrary, the number of doped carriers grows. A large pseudogap is well-known also for the electron-doped systems.\textsuperscript{22,44,46} However, there is possibly also an experimental indication of the manifestation of the second pseudogap\textsuperscript{138} predicted here and entering the superconducting domain. The chemical potential rises with electron doping as observed.\textsuperscript{96,143}

The calculated plane coherence length (seemingly a novel result) is of the same nonmonotonic nature as in the case of hole doping and of opposite behavior with the condensation energy as seen in Fig. 13. Note that the $\xi_0$ calculated without any further fittings reproduces the typical 200 Å value given\textsuperscript{96} for electron doped cuprates. This is roughly one order of magnitude larger in comparison with the

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure13}
\caption{The plane coherence length and the $T = 0$ thermodynamic critical field on the electron doping scale.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure14}
\caption{The excitation energies represented by pseudogap and superconducting gap components ($T = 0$): (1) $\Delta_{p\alpha}$ and $\Delta_{\alpha}$; (2) $\Delta_{p\beta}$ and $\Delta_{\beta}$.}
\end{figure}
case of hole doping and an expected result if one compares the typical transition temperatures.

Minimal quasiparticle excitation energies at $T = 0$ are shown in Fig. 14. The curve 1 joins on the doping scale the smaller pseudogap and the superconducting gap $\Delta_\alpha$ generated by the $\alpha 2$ defect system in the antinodal window. For $c > c_x$, $\Delta_n$ must appear in the whole momentum region by the cooperation of $\alpha 1$ and $\alpha 2$. The expected insulator–metal crossover at $c_x$ in the normal state can be attributed to an observed effect\textsuperscript{109} with the resistivity curve roughly comparable with $|\mu_2 - \alpha c^2|$ in Fig. 14 (4). The larger pseudogap transforms into the UHB associated superconducting gap at $c_0$. At $c > c_x$ the spectral response is expected to be covered by both superconducting gaps. The spectral hump\textsuperscript{140} must be associated with the larger gap. The gap relations $2\Delta_{\beta,\alpha}/\theta_c$ violate the BCS universality being approximately 4.8 and 2.6 for defect and UH bands, respectively.

It seems that these results are comparable with the properties of the not very thoroughly investigated electron doped cuprates.

The logistics of the interband pairing scheme creates comparable behavior of superconducting characteristics for both types of doping on different but resonating backgrounds.

13. Conclusion

A multiband superconductivity mechanism on nonrigid background seems correspond naturally to the complex and variable nature of the doped cuprates. Our calculated results on this way are self-consistent and show that the elaborated simple multiband approach is able to reproduce characteristic features of cuprate superconductors, e.g., the doping dependencies of $T_c$, superconducting gaps and pseudogaps, supercarrier density and effective mass, 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.

Acknowledgments

This work was supported by the Estonian Science Foundation Grant Nos. 6540 and 7296.

References

N. Kristoel, P. Rubin & T. Örd

73. H. Kamimura et al., Theory of Copper Oxide Superconductors (Springer, Berlin, 2005).
5326  N. Kristoel, P. Rubin & T. Órd