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The behavior of superconducting gaps in a two-band model of HTSC

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The carrier concentration and temperature dependences of superconducting gaps are calculated for $La_{2-x}Sr_xCuO_4$ and $Y_1Ba_2Cu_3O_{7-y}$ in a two-band model. The ratios $2|\Delta_{1,2}(0)|/k_BT_c$ show peculiarities as a function of the carrier concentration. Temperature dependences of superconducting gaps are of the BCS type.

One of the directions in the theory of high-temperature superconductivity (HTSC) is the elaboration of many-band models of superconductivity (e.g., reviews [1,2]). In Refs. 3, an interband model of HTSC, according to which the Cooper pairing of holes (electrons) occurs on repulsive interband interaction (dominating Coulombic one) has been proposed. The model takes into account essential features of the electronic structure of 123, 214 and related systems: the two-dimensionality of the spectra of active bands and the crossing of several electronic bands by the Fermi surface in a metallic phase. There are clear experimental [4,5] and theoretical [6–10] indications about this.

The theory allows an explanation of the dependence of the superconducting transition temperature T_c on doping for $La_{2-x}Sr_xCuO_{4+\delta}$ and on oxygen content for $Y_1Ba_2Cu_3O_{7-y}$. Also, some thermodynamic and other properties of these compounds have been explained [2].

In this paper we consider temperature and carrier dependences of superconducting gaps for $La_{2-x}Sr_xCuO_{4+\delta}$ and $Y_1Ba_2Cu_3O_{7-y}$ in a two-band model of [3].

The corresponding Hamiltonian is taken in the form

$$H = \sum_{\sigma,\mathbf{k},s} \tilde{\varepsilon}_\sigma(\mathbf{k}) a^+_{\sigma\mathbf{k}s} a_{\sigma\mathbf{k}s} + $$

$$+ 2\sum_{\sigma,\sigma'}{}' \sum_{\mathbf{k},\mathbf{k}'} W(\mathbf{k},\mathbf{k}') a^+_{\sigma\mathbf{k}\uparrow} a^+_{\sigma-\mathbf{k}\downarrow} a_{\sigma'-\mathbf{k}'\downarrow} a_{\sigma'\mathbf{k}'\uparrow} \quad (1)$$

Here $\tilde{\varepsilon}_\sigma(\mathbf{k}) = \varepsilon_\sigma(\mathbf{k}) - \mu$: $\varepsilon_\sigma(\mathbf{k})$ are the energies of electrons in the bands $\sigma = 1, 2$; μ is the chemical potential; a^+ are the creation operators of electrons; W is the interband interaction constant.

The mean-field nonequilibrium free energy of this model has been obtained in [11]:

$$F(\delta_1, \delta_2) = \sum_\sigma \left\{ \sum_{\mathbf{k}} \left[\tilde{\varepsilon}_\sigma(\mathbf{k}) - 2k_BT \ln \left(2 \operatorname{ch} \frac{E_\sigma(\mathbf{k})}{2k_BT} \right) \right] + \right.$$

$$\left. + |\delta_\sigma|^2 \eta_\sigma(|\delta_\sigma|, T) \right\} - W\eta_1(|\delta_1|, T)\eta_2(|\delta_2|, T) \times$$

$$\times (\delta_1^*\delta_2 + \delta_1\delta_2^*) , \quad (2)$$

where

$$\eta_\sigma(|\delta_\sigma|, T) = \sum_{\mathbf{k}} (E_\sigma(\mathbf{k}))^{-1} \operatorname{th} \frac{E_\sigma(\mathbf{k})}{2k_BT} , \quad (3)$$

$$E_\sigma(\mathbf{k}) = \left[\tilde{\varepsilon}^2_\sigma(\mathbf{k}) + |\delta_\sigma|^2 \right]^{1/2} . \quad (4)$$

The quantities δ_σ are order parameters whose equilibrium values $\delta_{\sigma 0} = \Delta_\sigma$ (the superconducting gaps) found by minimization of free energy, are determined by a system of equations

$$\begin{cases} \Delta_1 = \Delta_2 \eta_2(\Delta_2, T) W , \\ \Delta_2 = \Delta_1 \eta_1(\Delta_1, T) W . \end{cases} \quad (5)$$

To calculate the superconducting gaps we approximate the hole energy bands ($m_{1,2} > 0$),

$$\begin{cases} \varepsilon_1(\mathbf{k}) = -\dfrac{\hbar^2}{2m_1}(k_x^2 + k_y^2) , \\ \varepsilon_2(\mathbf{k}) = -E_0 - \dfrac{\hbar^2}{2m_2}(k_x^2 + k_y^2) . \end{cases} \quad (6)$$

Here $\mathbf{k}$ is measured, e.g., for $La_{2-x}Sr_xCuO_4$ system, from the corresponding symmetry point (X; S) of the

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Brillouin zone and there are four such «valleys». In the quasi-two-dimensional case of the CuO_2 plane, the densities of states $\rho_{1,2} = \text{const}$, taken per spin. The quantity $W(\mathbf{k}, \mathbf{k}')$is supposed to be operative and constant in the energy intervals $\{-\Gamma_1, -\Gamma_2\}$ for the higher band ($\sigma = 1$) and $\{-\Gamma_3, -\Gamma_4\}$ for the lower one ($\sigma = 2$). It is assumed that $0 \le \Gamma_1 < \Gamma_3 < \Gamma_{2,4}$. Then from (5) one obtains the gaps satisfying the system.

$$\begin{cases} |\Delta_1| = \frac{1}{2} W\rho_2 |\Delta_2| \int\limits_{\Gamma_3-\zeta}^{\Gamma_4-\zeta} \frac{dE}{\sqrt{E^2 + |\Delta_2|^2}} \operatorname{th} \frac{\sqrt{E^2 + |\Delta_2|^2}}{2k_B T}, \\ |\Delta_2| = \frac{1}{2} W\rho_1 |\Delta_1| \int\limits_{\Gamma_1-\zeta}^{\Gamma_2-\zeta} \frac{dE}{\sqrt{E^2 + |\Delta_1|^2}} \operatorname{th} \frac{\sqrt{E^2 + |\Delta_1|^2}}{2k_B T}. \end{cases} \tag{7}$$

For $T = 0$ this system is simplified to

$$\begin{cases} |\Delta_1(0)| = \frac{1}{2} W\rho_2 |\Delta_2(0)| \ln \frac{\Gamma_4 - \zeta + [(\Gamma_4 - \zeta)^2 + |\Delta_2(0)|^2]^{1/2}}{\Gamma_3 - \zeta + [(\Gamma_3 - \zeta)^2 + |\Delta_2(0)|^2]^{1/2}}, \\ |\Delta_2(0)| = \frac{1}{2} W\rho_1 |\Delta_1(0)| \ln \frac{\Gamma_2 - \zeta + [(\Gamma_2 - \zeta)^2 + |\Delta_1(0)|^2]^{1/2}}{\Gamma_1 - \zeta + [(\Gamma_1 - \zeta)^2 + |\Delta_1(0)|^2]^{1/2}}. \end{cases} \tag{8}$$

The number of superconducting gaps is determined by the number of electron bands intersecting the Fermi level.

Now we calculate numerically the concentration and temperature dependences of superconducting gaps, taking $\Gamma_1 = 0$ (top energy of the higher band of the width E_1) and $\Gamma_3 = E_0$ ($-E_0$ being the top energy of the lower band); $\Gamma_2 = \Gamma_4 = E_c$ ($-E_c$ is the cut-off energy). We use the same parameter values of the theory as in [3,11], where the formulas for T_c are also given.

The expression connecting the concentration of holes in $La_{2-x}Sr_xCuO_{4+\delta}$ with the chemical potential $\zeta = -\mu$ is [3]

$$\zeta = \frac{n_h}{\rho_1} + \frac{1}{2} E_1 , \qquad \text{if } \zeta \le E_0 , \tag{9}$$

$$\zeta = \frac{n_h + \rho_2 E_0 + 1/2 \rho_1 E_1}{\rho_1 + \rho_2} , \text{ if } \zeta > E_0 . \tag{10}$$

Here n_h is the number of holes in CuO_2 planes per cell added by doping to pure La_2CuO_4. For $La_{2-x}Sr_xCuO_{4+\delta}$ density of state $\rho_1 = 1\,(\text{eV})^{-1}$, $\rho_2 = 2\,(\text{eV})^{-1}$, $E_1 = 4$ eV, $E_0 = 2.14$ eV, $E_c = 2.3$ eV and $W = 0.17$ eV. The calculated relations $2|\Delta_{1,2}(0)|/k_B T_c$ as a function of carrier concentration are given in Fig. 1. At $\zeta > E_0$, where the chemical potential begins to intersect both bands, this ratio increases with the rising number of holes for the first band; however, for the second band the behavior is reversed. At $\zeta < E_0$ (in a narrow region over T_c) there is only one superconducting gap Δ_1 with the BCS universality ($2|\Delta_1(0)|/k_B T_c = 3.5$).

One of the characteristic features of the model consists in $E_0 \neq 0$. This offers a richer relief on which ζ

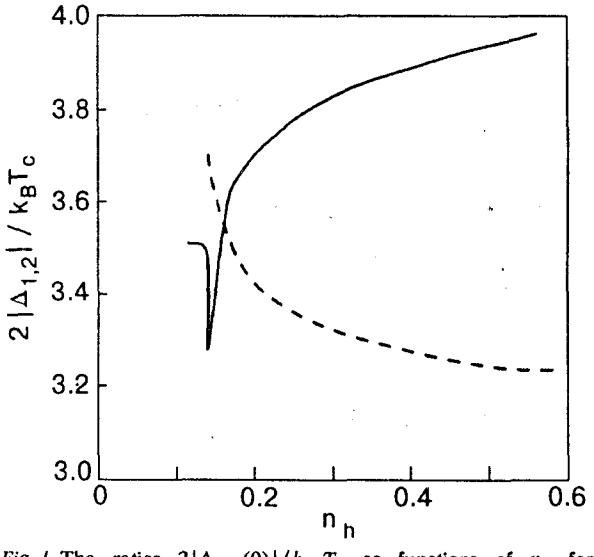

Fig. 1. The ratios $2|\Delta_{1,2}(0)|/k_B T_c$ as functions of n_h for $La_{2-x}Sr_xCuO_{4+\delta}$ 1st (——) and 2nd (– – –) bands.

moves with a varying composition and leads to $2|\Delta_{1,2}(0)|/k_B T_c$ dependences on n_h of the observed nature. These dependences are connected with the changes of the volume of the phase space for inter-band pair-transfer scattering of electrons on the variation of ζ.

Approximate relations between the number of holes (carriers) p in CuO_2 planes and y of $Y_1Ba_2Cu_3O_{7-y}$ are given according to [3] as $p = 3.5 - 2y$ $(0.5 \le y \le 0.75)$; $p = 2.5$ $(0.25 \le y \le 0.5)$; $p = 3 - 2y$ $(0 \le y \le 0.25)$. The number of holes per cell equals $2\,(2 - y)$ and for $y = 0$ the number of additional holes $n_h = 1$. The chemical potential ζ is connected with p by the relations $\zeta = p\rho_1^{-1}$, $\zeta \le E_0$ and $\zeta = (\rho_1 + \rho_2)^{-1}(p + \rho_2 E_0)$, $\zeta > E_0$.

The adjustable values of parameters for $Y_1Ba_2Cu_3O_{7-y}$ are [3] $E_0 = 2$ eV, $E_c = 2.5$ eV, $\rho_1 = 1.2$ eV^{-1}, $\rho_2 = 2.2$ eV^{-1}, $W = 0.15$ eV. The calculated dependence of the gap Δ_1 on temperature and carrier concentration is shown in Fig. 2 (the dependences $|\Delta_2|$ on n_h and T are analogous). The dependences $2|\Delta_{1,2}(0)|/k_B T_c$ as a function of additional carriers per cell, n_h, and $\Delta_{1,2}(T)$ for 214 and 123 systems are similar and of the same nature.

Experimental spectra have revealed several gap features [12–17]. According to [12,13,17–20] there are two superconducting gaps in both systems under consideration. By measuring the surface impedance of epitaxial YBCO films in [17] a larger gap $(2|\Delta_1(0)|/k_B T_c \approx 5)$ associated with the CuO_2 planes and a smaller one $(2|\Delta_2(0)|/k_B T_c \approx 1)$ ascribed to chains have been found. These measurements agree qualitatively with our calculations (the two-band model used does not specify the origin of the bands).

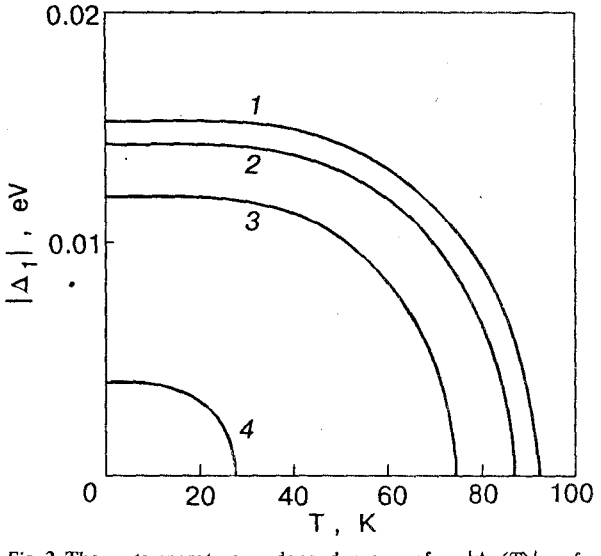

Fig. 2. The temperature dependence of $|\Delta_1(T)|$ for $Y_1Ba_2Cu_3O_{7-y}$ at various additional carrier concentrations n_h: 0.91 (*1*); 0.74 (*2*); 0.57 (*3*); 0.40 (*4*).

Recent experimental data [21] suggest that the order parameter (s) is anisotropic in some high T_c systems, while it appears to be approximately isotropic in others. The anisotropic data have been used to support a $d_{x^2-y^2}$ [21,22] or an extended s wave symmetry [23]. In two-band model there is the possibility for the jointed gap parameter belonging to different bands, and correspondingly to different sheets of the Fermi surface, to be of different signs in the case of repulsive driving interaction for the superconductivity [24]. On this way the deviation from the isotropic s wave behavior of the order parameter can be explained in our model, see also [25].

In connection with the dependences predicted here it seems to be of interest to measure the carrier and the temperature dependence of the gaps $\Delta_{1,2}$ and $2|\Delta_{1,2}(0)|/k_B T_c$ in $Y_1Ba_2Cu_3O_{7-y}$, $La_{2-x}Sr_xCuO_4$ and also related systems.

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