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Application of the interband model to the dependence of the superconducting critical temperature on the carrier concentration for Bi-2212 and Y-123 cuprates

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Abstract. The dependences of T_c on the additional hole concentrations (n_h) in $YBa_2Cu_3O_{7-y}$ and $Bi_2Sr_2CaCu_2O_{8+\delta}$ cuprates have been calculated in the framework of the two-band model. The phase space for the pair-transfer scattering between the overlapping bands is governed by the position of the chemical potential. The characteristic bell-like curves for $T_c(n_h)$ agree with experiment for both of the systems mentioned. The fitting of the theory with experimental data shows one of the participating hole bands to be narrow, as expected from two-component scenarios of high-T_c superconductivity. The chemical potential shift with doping for Bi-2212 agrees with the observed one.

1. Introduction

It is of fundamental importance to explain the doping dependence of the superconducting properties of cuprate high-T_c systems. In the present contribution, the dependences of the superconducting transition temperature (T_c) on the concentrations of additional holes (n_h) in Bi-2212 and Y-123 have been calculated. We use a version of the two-band model proposed for high-T_c superconductivity in [1–4]. Our results for La-214 are given in [2] and a preliminary consideration of Y-123 in [3]. In our model, the pairing interaction between the participating bands is repulsive. Pairs built from carriers of the same band are scattered between bands by the Coulomb and electron–phonon interactions. This interband interaction leads to intraband pairing. The intraband Coulomb and electron–phonon interactions essentially cancel in the region around the Fermi surface [4].

Our model shares features with various other ones. The first considerations concerning the description of superconductivity in transition metals should be mentioned [5–8]. In the context of high-T_c superconductivity, the idea of an interband mechanism has been developed in various realizations by a number of groups [9–18].

There are a number of data indicating participation of several bands in the high-T_c superconductivity mechanism. In Y-123 these relate presumably to planes and chains. Two bands are found to intersect the Fermi level in Bi-2212 [19]. In $Bi_2Sr_2CaCu_2O_{8+\delta}$ the BiO-plane bands seem to be coupled to the CuO-plane bands [20]. Recent microwave measurements of the complex conductivity in the superconducting state of $YBa_2Cu_3O_{7-y}$ have revealed the two-gap nature of the superconductivity order parameter [21], in accordance with the two-band model.

However, the detailed nature of the participating bands remains in our view unexplained. This does not prevent us from handling the present problem. When considering the aniso-

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tropy of the order parameter and its possible symmetry change with n_h [22], the precise nature of the bands becomes crucial.

A general and natural basis for the applications of two-band models to high-T_c systems seems to be provided by the recently developed two-component scenario [23, 24] of high-T_c superconductivity. Time-resolved (femtosecond) spectroscopy and transient photoconductivity measurements have revealed the participation of coexisting band-type itinerant and localized-type (polaronic) carriers in the physics of high-T_c superconductors. These two types of carrier and the corresponding energy bands could possibly be connected with the striped structure [25, 26] of the superconductivity playground CuO_2 planes.

2. The model

We start with the following Hamiltonian for the high-T_c superconductor [1, 4]:

$$H = \sum_{\sigma,\boldsymbol{k},s} \tilde{\epsilon}_\sigma(\boldsymbol{k}) a^+_{\sigma\boldsymbol{k}s} a_{\sigma\boldsymbol{k}s} + 2\sum_{\boldsymbol{k},\boldsymbol{k}'} W(\boldsymbol{k},\boldsymbol{k})[a^+_{1\boldsymbol{k}\uparrow} a^+_{1-\boldsymbol{k}\downarrow} a_{2-\boldsymbol{k}'\downarrow} a_{2\boldsymbol{k}'\uparrow} + a^+_{2\boldsymbol{k}\uparrow} a^+_{2-\boldsymbol{k}\downarrow} a_{1-\boldsymbol{k}'\downarrow} a_{1\boldsymbol{k}'\uparrow}]. \tag{1}$$

Here $\tilde{\epsilon}_\sigma(\boldsymbol{k}) = \epsilon_\sigma(\boldsymbol{k}) - \mu$; the $\epsilon_\sigma(\boldsymbol{k})$ are the energies of the electrons in the bands $\sigma = 1, 2$; μ is the chemical potential; $\boldsymbol{k}$ is the quasi-wave-vector; $s = \uparrow, \downarrow$ are the spin projections; and the a^+ are the creation operators for electrons. The constant of the interband interaction $W = U + V_{12}$, where U is the interband Coulomb interaction and V_{12} is the corresponding contribution from the electron–phonon interaction.

Furthermore, we need the free energy of our model (see also [27]). We rewrite Hamiltonian (1) in the form

$$H = H_0 + H_1 \tag{2}$$

where

$$H_0 = \sum_{\sigma,\boldsymbol{k},s} \tilde{\epsilon}_\sigma(\boldsymbol{k}) a^+_{\sigma\boldsymbol{k}s} a_{\sigma\boldsymbol{k}s} + \sum_{\sigma,\boldsymbol{k}} (-1)^\sigma (\delta_\sigma a^+_{\sigma\boldsymbol{k}\uparrow} a^+_{\sigma-\boldsymbol{k}\downarrow} + \delta^*_\sigma a_{\sigma-\boldsymbol{k}\downarrow} a_{\sigma\boldsymbol{k}\uparrow}) \tag{3}$$

$$H_1 = -\sum_{\sigma,\boldsymbol{k}} (-1)^\sigma [\delta_\sigma a^+_{\sigma\boldsymbol{k}\uparrow} a^+_{\sigma-\boldsymbol{k}\downarrow} + \delta^*_\sigma a_{\sigma-\boldsymbol{k}\downarrow} a_{\sigma\boldsymbol{k}\uparrow}] + 2W \sum_{\sigma,\sigma'}{}' \sum_{\boldsymbol{k},\boldsymbol{k}'} a^+_{\sigma\boldsymbol{k}\uparrow} a^+_{\sigma-\boldsymbol{k}\downarrow} a_{\sigma'-\boldsymbol{k}'\downarrow} a_{\sigma'\boldsymbol{k}'\uparrow}. \tag{4}$$

Interband scatterings operate over large regions of the $\boldsymbol{k}$-space; however, the coupling constant W is further supposed to be independent of the wave vector $\boldsymbol{k}$ for simplicity, because we do not go into the detailed nature of the order parameters here. In (3) and (4) the δ_σ are at this point the formal order parameters, whose equilibrium values must be found by minimization of the model free energy. Taking into account the relation

$$F_{\text{exact}} \leqslant F(H_0) + \langle H_1 \rangle_{H_0}$$

we write the free energy F in the mean-field approximation as

$$F = F(H_0) + \langle H_1 \rangle_{H_0}$$

where

$$F(H_0) = \sum_{\sigma,\boldsymbol{k}} [\tilde{\epsilon}_\sigma(\boldsymbol{k}) - 2k_B T \ln(2\cosh(E_\sigma(\boldsymbol{k})/2k_B T))] \tag{5}$$

$$E_\sigma(\boldsymbol{k}) = [\tilde{\epsilon}^2_\sigma(\boldsymbol{k}) + |\delta_\sigma|^2]^{1/2} \tag{6}$$

$$\langle H_1\rangle_{H_0} = -\sum_{\sigma,\boldsymbol{k}}(-1)^{\sigma}(\delta_\sigma\langle a^+_{\sigma\boldsymbol{k}\uparrow}a^+_{\sigma-\boldsymbol{k}\downarrow}\rangle_{H_0} + \delta^*_\sigma\langle a_{\sigma-\boldsymbol{k}\downarrow}a_{\sigma\boldsymbol{k}\uparrow}\rangle_{H_0}) + 2W\sum_{\sigma,\sigma'}{}'\sum_{\boldsymbol{k},\boldsymbol{k}'}\langle a^+_{\sigma\boldsymbol{k}\uparrow}a^+_{\sigma-\boldsymbol{k}\downarrow}\rangle_{H_0}\langle a_{\sigma'-\boldsymbol{k}'\downarrow}a_{\sigma'\boldsymbol{k}'\uparrow}\rangle_{H_0}. \tag{7}$$

Since

$$\langle a_{\sigma-\boldsymbol{k}\downarrow}a_{\sigma\boldsymbol{k}\uparrow}\rangle_{H_0} = (-1)^{\sigma+1}\frac{\delta_\sigma\tanh(E_\sigma(\boldsymbol{k})/2k_BT)}{2E_\sigma(\boldsymbol{k})} \tag{8}$$

it was found [27] that

$$F = \sum_\sigma\left\{\sum_{\boldsymbol{k}}[\tilde{\epsilon}_\sigma(\boldsymbol{k}) - 2k_BT\ln(2\cosh(E_\sigma(\boldsymbol{k})/2k_BT))] + |\delta_\sigma|^2\eta_\sigma(|\delta_\sigma|,T)\right\} - \frac{W}{2}\eta_1(|\delta_1|,T)\eta_2(|\delta_2|,T)(\delta_1^*\delta_2+\delta_1\delta_2^*) \tag{9}$$

where

$$\eta_\sigma(|\delta_\sigma|,T) = \sum_{\boldsymbol{k}}\frac{\tanh(E_\sigma(\boldsymbol{k})/2k_BT)}{E_\sigma(\boldsymbol{k})} \qquad E_\sigma(\boldsymbol{k}) = [\tilde{\epsilon}^2_\sigma(\boldsymbol{k}) + |\delta_\sigma|^2]^{1/2}. \tag{10}$$

With no loss of generality, we further consider the δ_σ as real quantities. The superconducting state is stable independently of the sign of W [27].

From the free energy (9), the system of equations for the order parameters (the equilibrium values of the δs) follows:

$$\Delta_1 = \frac{1}{2}W\rho_2\Delta_2\int_{\Gamma_3-\zeta}^{\Gamma_4-\zeta}\frac{\mathrm{d}E}{\sqrt{E^2+\Delta_2^2}}\tanh\frac{\sqrt{E^2+\Delta_2^2}}{2k_BT}$$
$$\Delta_2 = \frac{1}{2}W\rho_1\Delta_1\int_{\Gamma_1-\zeta}^{\Gamma_2-\zeta}\frac{\mathrm{d}E}{\sqrt{E^2+\Delta_1^2}}\tanh\frac{\sqrt{E^2+\Delta_1^2}}{2k_BT}. \tag{11}$$

The equation

$$\kappa F(\Gamma_1-\zeta,\Gamma_2-\zeta)F(\Gamma_3-\zeta,\Gamma_4-\zeta) = 1 \tag{12}$$

corresponding to $\Delta_{1,2}(T_c) = 0$ determines the superconducting transition temperature according to (11). Here

$$F(\Gamma_\sigma-\zeta,\Gamma_{\sigma'}-\zeta) = \int_{\Gamma_\sigma-\zeta}^{\Gamma_{\sigma'}-\zeta}\frac{\mathrm{d}E}{E}\tanh\frac{E}{2k_BT_c} \tag{13}$$

$$\kappa = \frac{1}{4}W^2\rho_1\rho_2. \tag{14}$$

It is supposed that the limits of integration in equation (13) for the higher band ($\sigma = 1$) are $\{-\Gamma_1,-\Gamma_2\}$ and that those for the lower one ($\sigma = 2$) are $\{-\Gamma_3,-\Gamma_4\}$. To calculate the superconducting transition temperature, we use approximate two-dimensional parabolic hole energy bands ($m_{1,2} > 0$):

$$\epsilon_1(\boldsymbol{k}) = -\frac{\hbar^2}{2m_1}(k_x^2+k_y^2) \qquad \epsilon_2(\boldsymbol{k}) = -E_0 - \frac{\hbar^2}{2m_2}(k_x^2+k_y^2). \tag{15}$$

Here $\boldsymbol{k}$ is measured from the corresponding symmetric point (e.g. S) of the Brillouin zone, and there are correspondingly n such 'valleys'. The density of states for the cylindrical isoenergetic surface is as follows:

$$\rho_{1,2} = \frac{v k_z m_{1,2} n}{2\pi^2 \hbar^2} \tag{16}$$

where v is the unit-cell volume, $k_z = \pi/a$, and $n = 4$ [20]. In the optimally doped superconductor, as follows from the two-band model [4], the chemical potential for the holes $\zeta = -\mu$ crosses both overlapping bands. Correspondingly, $\Gamma_1 = 0$ fixes the top energy of the higher band of width E_1, $\Gamma_3 = E_0$, where $-E_0$ is the top energy of the lower band, and the cut-off energy $-E_c$ determines $\Gamma_2 = \Gamma_4 = E_c$. For $E_0 < \zeta < E_c$, the superconducting transition temperature T_c, on the basis of (12) and (15), equals

$$k_B T_c = 1.14[\zeta(\zeta - E_0)]^{1/4}(E_c - \zeta)^{1/2} \exp\left[-\frac{1}{2}\left(\frac{1}{4}\ln^2\frac{\zeta}{\zeta - E_0} + \kappa^{-1}\right)^{1/2}\right]. \tag{17}$$

The formula (17) corresponds predominantly to the optimally doped superconductor (the common region of the two bands). The moving of the chemical potential ζ leads to a change of the phase space for scattering of electron pairs (holes) between the bands, and, correspondingly, to the curve for $T_c(\zeta)$ with a maximum. The changes of the chemical potential caused by doping are measured here from the half-filling of the higher band.

3. Calculations of $T_c(n_h)$

The theory of [1, 4] was applied to obtain a description of the carrier concentration dependence of T_c for $La_{2-x}M_xCuO_4$ [2], and a good agreement with the experiment was achieved. In [3], for $YBa_2Cu_3O_{7-y}$, the dependence of T_c on y was considered using the semiempirical relation between y and the total number of holes per cell (p) in CuO_2 planes. In this work, we consider the dependence of T_c on n_h, the carrier concentration added by doping to the CuO_2 planes, for $Bi_2Sr_2CaCu_2O_{8+\delta}$ (both pure and impurity doped) and $YBa_2Cu_3O_{7-y}$.

Using the condition of electroneutrality, we obtain the equation for the chemical potential:

$$\rho_1[E_1 - k_B T \ln(1 + e^{-\zeta/k_B T})(1 + e^{E_1 - \zeta/k_B T})] + \rho_2\left(-E_0 + E_c + k_B T \ln\frac{(1 + e^{E_0 - \zeta/k_B T})}{(1 + e^{E_c - \zeta/k_B T})}\right) = p \tag{18}$$

where p is the total number of holes per cell. The relation connecting n_h and p reads $n_h = 2\,\Delta p = p - p_0$, where $p_0 = \rho_1(E_1/2)$. From (18) one finds

$$\zeta = \frac{n_h}{\rho_1} + \frac{1}{2}E_1 \qquad \text{if } E_0 - \zeta \gg k_B T \tag{19}$$

$$\zeta = (\rho_1 + \rho_2)^{-1}(n_h + \rho_2 E_0 + (1/2)\rho_1 E_1) \qquad \text{if } \zeta - E_0 \gg k_B T \text{ and } E_c - \zeta \gg k_B T \tag{20}$$

$$\zeta = \left(\frac{n_h}{\rho_1} + \frac{1}{2}E_1 - \frac{\rho_2}{\rho_1}k_B T \ln 2\right) \qquad \text{if } \zeta = E_0. \tag{21}$$

The dependences of $T_c(n_h)$ for pure Bi-2212, and for Bi-2212-Y, Tm and Bi-2212-Na, K (see figure 1; $\Delta p = n_h/2$) are calculated using equation (12) immediately. We use the following fitting parameters: $\rho_1 = 1.0$ eV^{-1}, $\rho_2 = 2.2$ eV^{-1}, $W = 0.22$ eV, $E_c = 2.33$ eV, $E_1 = 4.0$ eV, $E_0 = 2.18$ eV for pure Bi-2212, and $\rho_1 = 1.0$ eV^{-1}, $\rho_2 = 2.2$ eV^{-1},

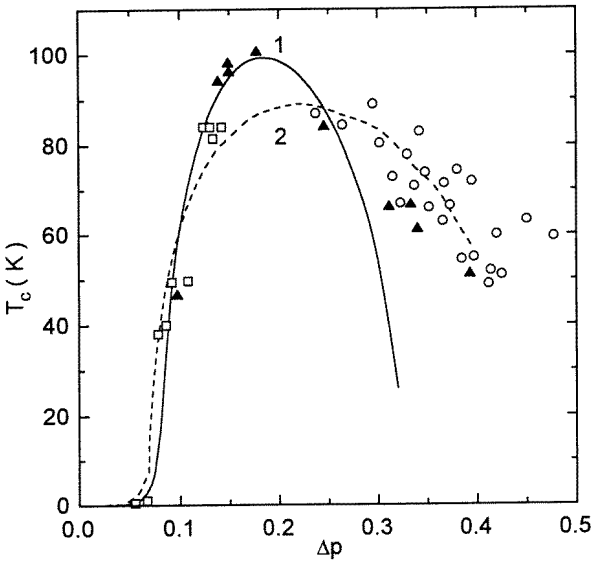

Figure 1. The theoretical dependences of T_c on the hole concentration Δp for pure Bi-2212 (line 1) and doped Bi-2212 (line 2) in comparison with the experimental data for pure Bi-2212 (triangles) [28], Bi-2212-Y, Tm (squares) [29] and Bi-2212-Na, K (circles) [29].

$W = 0.19$ eV, $E_c = 2.39$ eV, $E_1 = 4.0$ eV, $E_0 = 2.15$ eV for impurity-doped Bi-2212. The values of $\rho_{1,2}$ and E_1 that we used agree as regards order of magnitude with the theoretical estimations of [20].

As seen from figure 1, a good fitting of the experimental data [28, 29] with the theoretical curves can be achieved in both cases. The difference between the results for pure and impurity-doped Bi-2212 is mainly connected with the different values of W and the value of the width of the lower band $E_c - E_0$. Optimally doped pure Bi-2212, and Bi-2212-Y, Tm and Bi-2212-Na, K have $\Delta p = n_h/2 = 0.17$ and 0.22, respectively. As follows from figure 1, the dependences $T_c(n_h/2)$ for pure Bi-2212 and impurity-doped Bi-2212 are not reduced to the universal behaviour $T_c(n_h/2)/T_{cmax}(n_h/2)$ proposed in [30]. According to the equations (18)–(21), there is a downward chemical potential shift $\Delta\mu = 0.2$ eV when $n_h/2$ changes from 0 to 0.3, in agreement with $\Delta\mu = 0.15$–0.2 observed by photoemission spectroscopy for Bi-2212 [31].

For the Y-123 superconductor, we use the parameter values $\rho_1 = 0.9$ eV^{-1}, $\rho_2 = 2.2$ eV^{-1}, $W = 0.23$ eV, $E_c = 2.33$ eV, $E_1 = 4.0$ eV, and $E_0 = 2.18$ eV. The calculated dependence of T_c on Δp for Y-123, in comparison with the experimental data [28], is depicted in figure 2. The agreement is good.

From the comparison of the theory with the experiment, it follows that the lower participating band in Y-123 and Bi-2212 must be narrow: $E_c - E_0 \sim 0.15$ eV. So our calculation reveals the participation of a broad and a narrow (possibly corresponding to the localized carriers) band in the high-T_c superconductivity mechanism. The existence of the narrow band justifies the assumption that the interband coupling constant W can be treated as independent of $\boldsymbol{k}$.

Consideration of the isotope effect is outside the scope of the present contribution. We mention that for the La-214 system it has been investigated [4]. In the interband scattering, the Coulomb interaction (strong correlations) dominates, $U \gg V_{12}$. However, a small

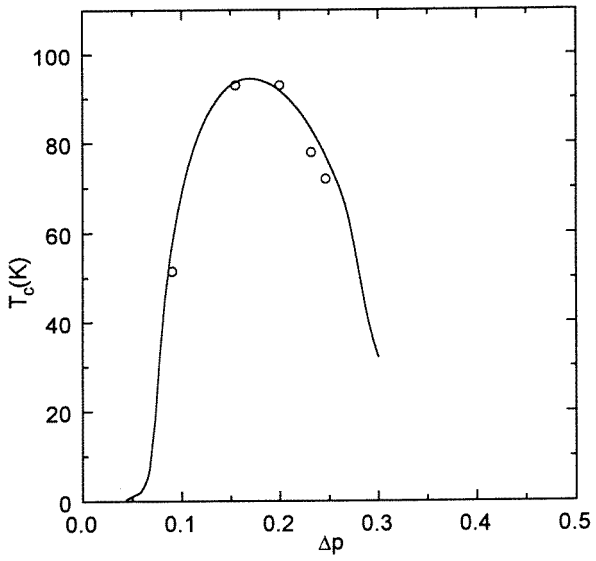

Figure 2. The theoretical dependence of T_c on the hole concentration Δp for Y-123 (solid line) in comparison with the experimental data (circles) [28].

(several %) contribution of the electron–phonon interaction can explain the behaviour of the isotope exponent as the doping varies. It is remarkable in the region of low values of T_c, but diminishes rapidly on entering the optimally doped region. As seen from (17), in the interband model the atomic-mass-dependent interband electron–phonon contribution V_{12} enters with the parameter (14) into the exponential factor of the expression for T_c.

4. Conclusion

In conclusion, it can be stated that the two-band model of high-T_c superconductivity is able to describe the dependence of the superconducting transition temperature on the carrier concentration for three representative systems, La-214 [2], Y-123, and Bi-2212, from a common viewpoint. The parameter set that we used also gives a chemical potential shift with doping in agreement with the observed one for Bi-2212. The present work reveals one of the bands participating in the pair-transfer interaction to be narrow. This supports a two-component scenario for the high-T_c superconductivity.

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