Superconductivity in the underdoped region of the T’-structure cuprates based on an effective two-band model

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Abstract. Electronic states in the underdoped (including non-doped) region of the so-called T’-structure cuprates are studied based on the d-p model and a newly proposed effective two-band model for those compounds. We find d-wave superconducting transition for both models when the charge transfer gap is small enough which is consistent with the recent experimental results for the properly reduced NCO films etc. We also show that the two-band model gives almost similar result for the superconducting transition temperature and the static spin susceptibility with those obtained in the d-p model, which implies the two-band model can give a good description of the T’-cuprates.

1. Introduction

Recently, growing attention has been paid to the reconstruction of the phase diagram of the T’-structure cuprates, that is, the so-called electron-doped curates. Several experimental studies have shown that the T’-type cuprates exhibit superconductivity with very low or without chemical carrier doping, only when excess oxygen which inevitably exists in as-grown samples are properly removed[1-8].

Theoretically, we have studied the superconducting transition around the underdoped region of these compounds based on an effective two-band model[9], which can be derived from the d-p model essentially along with the idea of Zhang and Rice[10], but explicitly consists of Cu d-orbitals and symmetrically hybridized O 2p-orbitals. Thus, the two-band model can be regarded as a simplified version of the d-p model. By applying the fluctuation-exchange approximation (FLEX)[11-12], we have found that the d-wave superconductivity appears around the underdoped region, and even at the non-doped point with one hole per Cu site, when the charge transfer gap Δ = U_d − Δ_p is small enough, where U_d is the on-site Coulomb repulsion on Cu site, and Δ_p is the energy difference between the O 2p and Cu 3d levels.

Although our theoretical results are qualitatively in agreement with the experimental observations for the T’-cuprates, the validity of the two-band model has not been assessed in detail. Thus the next question we must consider is whether the non-doped dSC is found even in the d-p model or not. In this paper, we study the superconducting transition at the non-doped point with one-hole per Cu site based on the d-p model, and compare the results such
as dispersion relations, $T_c$’s, and spin susceptibilities with those obtained using the two-band model.

2. Model and formalism

The Hamiltonian of the $d$-$p$ model is written as

$$
\mathcal{H}_{dp} = -t_{dp} \sum_{\langle i,j \rangle \sigma} (d^\dagger_{i\sigma} p_{j\sigma} + h.c.) - t_p \sum_{\langle j,j' \rangle \sigma} (p^\dagger_{j\sigma} p_{j'\sigma} + h.c.) + \Delta \sum_{j\sigma} n_{p,j\sigma} + U_d \sum_i n_{d,i\uparrow} n_{d,i\downarrow}
$$

in the standard notation, where $d_{i\sigma}$ and $p_{j\sigma}$ are annihilation operators of holes with spin $\sigma$ on the Cu 3$d_{x^2-y^2}$-orbital at site $i$ and on the O 2$p_{\sigma}$-orbital at site $j$, respectively. $t_{dp}$ and $t_p$ are amplitudes of the nearest-neighbor Cu-O and O-O hopping integral, respectively. $U_d$ is the Coulomb repulsion on Cu site $i$, and $\Delta = U_d - \Delta_p$ is the lowest excitation energy in the localized limit, where $\Delta_p$ is the energy difference between the O 2$p$ and Cu 3$d$ levels.

An effective two-band model for the T’-structure cuprates derived by following the idea of Zhang-Rice[10]. We keep the symmetrically hybridized O 2$p$-band and omit the anti-symmetric hybridized one. The two-band model is written as,

$$
\mathcal{H}^{\text{eff}} = \sum_{k\sigma} \varepsilon_p(k) d^\dagger_{k\sigma} p_{k\sigma} + \sum_{k\sigma} t_{dp} t_{k} (d^\dagger_{k\sigma} p_{k\sigma} + h.c.) + \frac{U_d}{N_L} \sum_{k,k',q} d^\dagger_{k+q\uparrow} d^\dagger_{k'q\downarrow} d_{k'q\downarrow} d_{k\uparrow}
$$

where

$$
\varepsilon_p(k) = \left\{ \Delta - 32t_p \frac{1}{t_k^2} \sin^2 \left( \frac{k_x}{2} \right) \sin^2 \left( \frac{k_y}{2} \right) \right\},
$$

$$
t_k = 2 \left\{ \sin^2 \left( \frac{k_x}{2} \right) + \sin^2 \left( \frac{k_y}{2} \right) \right\}^{1/2},
$$

$d_{k\sigma}$ and $p_{k\sigma}^{(s)}$ are the Fourier transforms of the annihilation operators for the holes with spin $\sigma$ on the $d$- and symmetrized $p$-orbitals, respectively, and $N_L$ is the number of atoms in the crystal.

Here we show the noninteracting dispersion relations of the energy band in which the Fermi energy lies for both models in Fig. 1. It should be noted here that these dispersion relations are depicted in the hole picture. We can see that these two models have very similar dispersion relations all over the Brillouin zone.

We note here that the Coulomb interaction is considered only within a $d$-orbital for brevity. We use the parameters of NCO[13]($t_{dp} = 1.18$eV, $t_p = 0.62$eV), but $\Delta$ is changed($\Delta = 1.65$eV$-1.80$eV) to take into account the effect of the excess oxygen in the T'-structure cuprates on both models. In order to obtain the renormalized Green’s function, we carry out the FLEX calculation to the $d$-$p$ model and the two-band model. The transition temperature is determined as the temperature which the linearized Eliashberg equation using the Green’s function,

$$
\phi(k, i\epsilon_n) = -\frac{T}{N_L} \sum_{k',m} V^{(2)}(k - k', i\epsilon_n - i\epsilon_m) G_d(k', i\epsilon_m) G_d(-k' - i\epsilon_m) \phi(k' i\epsilon_m)
$$

has a non-trivial solution, and we assume that the d-wave superconductivity is realized in the T’-structure cuprates. Here, the effective interaction for singlet pairing is obtained as $V^{(2)}(k - k') = U_d + \frac{3}{2} U_d^2 \chi_d^{(s)}(k - k') - \frac{1}{2} U_d^2 \chi_d^{(c)}(k - k')$, where the spin and charge susceptibilities for the d-orbital $\chi_d^{(s)}$ and $\chi_d^{(c)}$. In this paper, we employ 128×128 $k$-point and 16384 Matsubara frequencies.
3. Results and discussion

Let us look at first the superconducting transition temperatures $T_c$ for the $d$-$p$ and the two-band model as functions of the charge transfer gap $\Delta$ at the non-doped point with one hole per Cu site. We can clearly see that the both models describe the superconducting transition even at the non-doped point. The $\Delta$ dependences are qualitatively the same, but the $T_c$’s for the $d$-$p$ model is somewhat lower than those for the two-band model, except for one case ($\Delta = 1.8$eV). In any case, the superconducting transitions at the non-doped point is confirmed even in the $d$-$p$ model.

In the present calculation, when $\Delta \geq 1.85$eV, we have confirmed that the spin susceptibility diverges at higher temperatures than $T_c$’s shown in Fig. 2, implying the antiferromagnetic (AFM) phase transition. But the coexisting state of AFM and d-wave superconductivity may still be possible as a candidate for a lower-temperature phase or the ground state of the present system. Although it is not possible to figure out if this is the case within the present theoretical framework, we note here that it is interesting to study the stability of the coexisting state by using variational Monte Carlo simulations.

Figure 2. $T_c$ of the $d$-$p$ model and the two-band model for $t_{dp} = 1.18$eV, $t_p = 0.621$eV, $U_d = 5.0$eV, and $\Delta = 1.65 - 1.80$eV.
Next, we compare the $q$-dependences of the static spin susceptibility $\chi(q, 0)$ for both models for several $\Delta$'s at the same temperature $T = 0.005eV$ in Fig. 3. The antiferromagnetic peaks around the X point are found for both cases, and the height of these increases as $\Delta$ increases. The peaks for the $d$-$p$ model are, however, smaller than those for the two-band model, which is consistent with the results for $T_c$'s shown in Fig. 2.

Since the discovery of the cuprate superconductors, the $t$-$J$ model and the single band Hubbard model have been used to analyze the low-energy physics in the CuO$_2$ planes. Because of the extensive theoretical studies, it is known that these single-band models provide a reasonable description of the phase diagram of cuprate superconductors, in particular of the hole-doped cuprates with T'-structure. For the electron-doped cuprates with T''-structure, however, the O 2p degrees of freedom plays an important role as implied by the present results. Thus the three-band $d$-$p$ model, or the two-band $d$-$p$ model should be used to analyze such materials. In particular, because of the less degrees of freedom, we believe that the two-band model is more preferable when we further examine the phase diagram of the electron-doped cuprates by using laborious computational techniques for many-body problems[14].

![Figure 3. The static spin susceptibility $\chi^s(q, 0)$ of the $d$-$p$ model and the two-band model for $t_{dp} = 1.18eV$, $t_p = 0.621eV$, $U_d = 5.0eV$, and $\Delta = 1.75 - 1.65eV$.](image)

4. Summary
We have studied the superconducting transition of the T'-cuprates based on the $d$-$p$ model and the effective two-band model, and found that these two models describe the $d$-wave superconductivity at the non-doped point when the charge transfer gap is small enough. The two band model is found to give $T_c$'s, spin susceptibilities which are in satisfactory agreement with those for the $d$-$p$ model.

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