An effective Hamiltonian and its phase diagram for $T'$-structure cuprates

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Abstract. We study the superconducting transition near the half-filling of electron-doped cuprates with the so-called $T'$-structure based on an effective two-band model using fluctuation-exchange approximation and solving the linearized Eliashberg equation. We find $d$-wave superconductivity even at the half-filling of this model when the energy difference between the upper Hubbard level of Cu $d_{x^2-y^2}$ orbitals and O 2p levels is less than about 1.5eV, which is plausible for the $T'$-type cuprates.

1. Introduction

It has long been considered that the phase diagrams of hole- and electron-doped cuprates were well-established; there exists antiferromagnetism (AF) around the half-filling of their phase diagram, and then $d$-wave superconductivity (dSC) emerges with carrier doping. In particular, on the phase diagram of the electron-doped cuprates such as Nd$_{2-x}$Ce$_x$CuO$_4$ (NCCO), which is of the so-called $T'$-structure cuprates, AF phase overwhelmingly appears in the underdoped region of $x < 0.14$ [1]. Tsukada et al. claimed that, however, thin films of the $T'$-structure cuprates exhibit superconductivity without chemical doping of electrons, only when excess oxygen in as-grown samples are properly removed [2]. This observation has been followed by several experimental studies based on $T'$-NCCO thin films [3], polycrystalline samples [4, 5], and even on single crystals [6].

Theoretically, however, it is rather inconceivable that dSC appears around the half-filling of the phase diagrams of the t-J or the strong coupling regime of the Hubbard model on a square lattice. Recently, Weber et al. have shown that the parent compounds of $T'$-cuprates do not have the Mott gap based on DFT+DMFT calculations [7], which means the charge-transfer gap commonly found in the T-cuprates are vanished. If this is the case, we should consider the superconducting transition of $T'$-cuprate based on the d-p model to treat the O 2p degrees of freedom explicitly.

Thus in this paper, we propose an effective two-band model for $T'$-structure electron-doped cuprates. This two-band model is derived from the d-p model essentially along with the idea of Zhang and Rice [8], but explicitly consists of Cu d-orbitals and symmetrically hybridized O 2p orbitals. We also study the phase diagram of this two-band model using fluctuation exchange...
approximation (FLEX). We find that the d-wave superconductivity appears even at the half-filling when the charge transfer gap is small enough.

2. model and formalism

We start with the d-p model or three band Hubbard model that consists of the O 2p-orbitals in the CuO$_2$ planes as well as the Cu 3d-orbitals, written as

$$
\mathcal{H}_{dp} = -t_{dp} \sum_{\langle i,j \rangle \sigma} (d_{i\sigma}^\dagger p_{j\sigma} + h.c.) - t_p \sum_{\langle j,j' \rangle \sigma} (p_{j\sigma}^\dagger p_{j'\sigma} + h.c.) + \Delta \sum_{j \sigma} n_{p,j\sigma} + U_d \sum_i n_{d,i\uparrow} n_{d,i\downarrow} \tag{1}
$$

where $d_{i\sigma}$ is an annihilation operator of a hole with spin $\sigma$ on the Cu $d_{x^2-y^2}$-orbital at site $i$, $p_{j\sigma}$ is that on the O 2p-σ-orbital at site $j$, and $\langle i, j \rangle$ means the summation runs over nearest-neighbor Cu-O bonds, while $\langle j, j' \rangle$ the nearest-neighbor O-O bonds in the CuO$_2$ plane. The number operators for d- and p-holes are defined as $n_{d,i\sigma} = d_{i\sigma}^\dagger d_{i\sigma}$ and $n_{p,j\sigma} = p_{j\sigma}^\dagger p_{j\sigma}$. The Coulomb repulsion on Cu site is represented as $U_d$, 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 2p and Cu 3d levels. We note here that the Coulomb repulsion on O site is omitted for simplicity.

Following the idea of Zhang and Rice [8, 9], we derive an effective Hamiltonian for the T'-type cuprates by a perturbative procedure, but this time, we explicitly keep active a part of the O 2p degrees of freedom because the energy difference between the upper Hubbard band and the O 2p level can be smaller than that of the T-structure cuprates. The detail of the derivation will be published elsewhere [10], here we roughly describe the steps which are important for the derivation. We consider the symmetric linear combination of the $\sigma$-orbitals surrounding a Cu, and then construct Wannier orbitals of oxygen holes localized around each Cu based on these combinations. Omitting the anti-symmetric linear combinations of the $\sigma$-orbitals, and also leaving the interaction terms as it is, now we obtain a two-band effective Hamiltonian given as

$$
\mathcal{H}^{\text{eff}} = \sum_{k\sigma} \varepsilon_p(k) p_{k\sigma}^\dagger p_{k\sigma} + \sum_{k\sigma} t_{dp} t_k (d_{k\sigma}^\dagger p_{k\sigma} + h.c.) + \frac{U_d}{N_L} \sum_{k,k',q} d_{k+q,\uparrow}^\dagger d_{k',-q,\downarrow}^\dagger d_{k',\downarrow} d_{k,\uparrow} \tag{2}
$$

where

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

$$
t_k = 2 \left\{ \sin^2 \left( \frac{k_x}{2} \right) + \sin^2 \left( \frac{k_y}{2} \right) \right\}^{1/2}, \tag{3}
$$

$N_L$ is the number of sites, and $p_{k\sigma}^\dagger$ is the annihilation operator of the Bloch state of symmetrized Wannier orbitals [9].

Here we carry out the FLEX calculation to the present two-band model to obtain the Green’s function renormalized by the many-body self-energy correction. The effective interaction for singlet pairing is obtained by taking account of the contributions from bubble and ladder diagrams in the self-energy, as $V^{(2)}(k-k') = U_d + \frac{2}{3} U_d^2 \chi_d^{(s)}(k-k') - \frac{1}{2} U_d^2 \chi_d^{(c)}(k-k')$, where the
spin and charge susceptibilities for the d-orbital $\chi_d^{(s)}$ and $\chi_d^{(c)}$. Then we substitute the Green’s function to linearized Eliashberg equation

$$\phi(k, i\epsilon_n) = -\frac{T}{N_L} \sum_{k', m} V^{(2)}(k - k', i\epsilon_n - i\epsilon_m)G_d(k', i\epsilon_m)G_d(-k', -i\epsilon_m)\phi(k' i\epsilon_m)$$  \hspace{1cm} (4)$$

to evaluate the transition temperature.

3. Results

As we mentioned in the Introduction, the charge-transfer gap can be vanished in the T’-cuprates. Thus we should assume that the excitation energy parameter $\Delta$ in the Hamiltonian (1) and (2) is rather small as estimated for T-cuprates ($\Delta = 2-4$ eV). Here we take $\Delta = 1.43$ eV, and also 2.6 eV for comparison. We also take $U_d = 6.5$ eV for the present calculations. For FLEX calculation, we take up to 64 $k$-point meshes, and up to 8192 Matsubara frequencies for $\Delta = 1.43$ eV, while 4096 for 2.6 eV.

First, we look at the $q$-dependences of the static susceptibility $\chi(q, 0)$ just above $T_c$ for several electron doping concentrations in the two-band model. Figure 1 shows $\chi(q, 0)$ for (a) $\Delta = 2.6$ eV (T-cuprates) and (b) $\Delta = 1.43$ eV (T’-cuprates). We can clearly see in Fig. 1 (a) that an antiferromagnetic peak is found at $\delta = 0.16$, and then the peak split into two incommensurate peaks with increasing $\delta$. This is consistent with the experimental observations in ref. [1], and also previous theoretical studies for T-cuprates [11, 12]. In contrast, when $\Delta = 1.43$ eV (for T’-cuprates), the peak structure found at $(\pi, \pi)$ in Fig. 1 (b) holds for $0 < \delta < 0.08$.

Next, we show the phase diagram for the two-band model in Fig. 2. We find that d-wave superconducting state appears in the overdoped region ($0.16 < \delta < 0.22$) for $\Delta = 2.6$ eV, while in the underdoped region ($0 < \delta < 0.11$) for $\Delta = 1.43$ eV. $T_c$’s for $\Delta = 1.43$ eV are lower than those for $\Delta = 2.6$ eV, however, it is worth noting here that the $T_c$ at the half-filling is not very low, which is consistent with the recent experimental results for T’-cuprates [2, 3, 4, 6].
\[\Delta = 1.43 \text{eV} \quad \Delta = 2.6 \text{eV}\]

**Figure 2.** $T_c$ of the effective two-band model for $\Delta = 1.43 \text{eV}$ and $2.6 \text{eV}$ as functions of electron doping concentration $\delta$.

## 4. Summary and discussions

In this paper, we have found that the $d$-wave superconducting state appears in the low electron-doping region, and even at the half-filling, of the effective two-band model derived from the $d$-p model when the energy level difference between the upper Hubbard level of Cu and O 2p level is smaller than 1.5 eV. This result is consistent with the recent experimental observations for T’-cuprates. The detailed information about the two-band model and the nature of the superconducting state will be reported in the forthcoming paper [10].

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