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Material-parameter dependence of superconductivity in high-temperature cuprates

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Abstract

We show that there is an interesting correlation between material parameters and critical temperature $T_c$ in cuprate high temperature superconductors. Our analysis is based on the d-p model, that is, the three-band Hubbard model including d and p orbitals explicitly. This model contains many parameters; the transfer integrals $t_{dp}$ and $t_{pp}$, the energy levels $\varepsilon_p$ and $\varepsilon_d$, and the Coulomb interaction parameters $U_d$ and $U_p$. Our main results are the following: (a) $T_c$ increases as $\varepsilon_p - \varepsilon_d$ is increased for $U_p = 0$, (2) $T_c$ is lowered with increase of $U_p$ when $\varepsilon_p - \varepsilon_d > 0$, (3) $T_c$ is increased with increase of $U_p$ when $\varepsilon_p - \varepsilon_d < 0$, (4) $T_c$ has a minimum at near $\varepsilon_p - \varepsilon_d = 0$ as a function of $\varepsilon_p - \varepsilon_d$ when $U_d$ and $U_p$ are comparable, (5) $U_d$ induces $d_{x^2-y^2}$ pairing while $U_p$ induces $d_{xy}$ pairing, (6) $T_c$ has a peak as a function of $t_{pp}$. The results imply that $T_c$ will increase if we can suppress $U_p$. The role of $U_p$ is consistent with the experimental tendency that $T_c$ increases as the relative ratio of the hole density at oxygen site to that at copper site is increased, which means that when $U_p$ increases, the number of p holes is decreased and $T_c$ is also decreased.

Keywords: high-temperature superconductivity; band parameter; interaction parameter; gap equation; material dependence

1. Introduction

The study of high-temperature superconductivity has been addressed extensively since the discovery of cuprate superconductors [1]. It is primarily important to clarify electronic states in the CuO$_2$ plane [2-5]. Electron
correlation is important in cuprates [6-13] and relationship between material parameters and critical temperature \( T_c \) is also significant in the study of cuprate high temperature superconductors. There are two kinds of material parameters. The first one is related to the band structure and the Fermi surface; they are transfer integrals \( t_{dp} \), \( t_{pq} \) and the levels of d and p electrons. The \( t_{dp} \) is the transfer integral between nearest d and p orbitals in the CuO\(_2\) plane, and \( t_{pq} \) is that between nearest p orbitals. The other is concerning with the strength of interactions such as the Coulomb interactions, \( U_d \) and \( U_p \), and the electron-phonon interaction. In our previous studies, the transfer integrals play an important role to stabilize superconductivity and striped states [7-13] as well as to obtain a finite bulk limit of the superconducting condensation energy [14,15].

There are experimentally known correlation between material parameters and \( T_c \). For example, \( T_c \) increases as the relative ratio of hole density at O site against that at Cu site is increased [16]. This indicates that doping hole carrier at O site is more favorable for higher \( T_c \). The hole carrier density is determined by the relative level difference \( \varepsilon_p - \varepsilon_d \) and Coulomb interactions \( U_d \) and \( U_p \). Thus, \( T_c \) would crucially depend on these parameters.

The purpose of this paper is to show relationships between \( T_c \) and material parameters on the basis of the d-p model in the CuO\(_2\) plane. We investigate the gap equation that is derived for the effective interaction in terms of \( U_d \) and \( U_p \). We use a weak-coupling formulation to solve the gap equation and show correlation between \( T_c \) and material parameters.

2. Hamiltonian and gap equation

The model is the Hamiltonian that contains d and p electrons [7,8,17]:

\[
H = \varepsilon_d \sum_{\alpha \sigma} d_{\alpha \sigma}^\dagger d_{\alpha \sigma} + \varepsilon_p \sum_{\alpha \sigma} \left( p_{\alpha + \frac{\pi}{2}, \sigma}^\dagger p_{\alpha - \frac{\pi}{2}, \sigma} + p_{\alpha - \frac{\pi}{2}, \sigma}^\dagger p_{\alpha + \frac{\pi}{2}, \sigma} \right) \\
+ t_{dp} \sum_{\alpha \sigma} \left[ d_{\alpha \sigma}^\dagger \left( p_{\alpha + \frac{\pi}{2}, \sigma} + p_{\alpha - \frac{\pi}{2}, \sigma} - p_{\alpha - \frac{\pi}{2}, \sigma} - p_{\alpha + \frac{\pi}{2}, \sigma} \right) \right] + h.c. \\
+ t_{pp} \sum_{\alpha \sigma} \left( p_{\alpha + \frac{\pi}{2}, \sigma} p_{\alpha - \frac{\pi}{2}, \sigma} - p_{\alpha - \frac{\pi}{2}, \sigma} p_{\alpha + \frac{\pi}{2}, \sigma} - p_{\alpha - \frac{\pi}{2}, \sigma} p_{\alpha + \frac{\pi}{2}, \sigma} + p_{\alpha + \frac{\pi}{2}, \sigma} p_{\alpha - \frac{\pi}{2}, \sigma} \right) + h.c. \\
+ U_d \sum_i n_{i,\alpha}^d n_{i,\bar{\alpha}}^d + U_p \sum_i \left( n_{i,\sigma}^p n_{i,\bar{\sigma}}^p + n_{i,\sigma}^p n_{i,\bar{\sigma}}^p \right)
\]

where \( n_{i,\alpha}^d \) and \( n_{i,\bar{\alpha}}^p \) (\( \mu = x, y \)) are number operators for d and p electrons, respectively. \( U_d \) and \( U_p \) indicate the Coulomb interaction for d and p electrons, respectively. We examine the doped case within the hole picture where the lowest band is occupied up to the Fermi energy \( \mu \). The non-interacting part is written as

\[
H_0 = \sum_{k\alpha} \left( d_{\alpha \sigma}^\dagger p_{\alpha \sigma}^\dagger \right) \begin{pmatrix}
\varepsilon_d - \mu & \varepsilon_{d\alpha} & \varepsilon_{y\alpha} \\
-\varepsilon_{d\alpha} & \varepsilon_p - \mu & \varepsilon_{p\alpha} \\
-\varepsilon_{y\alpha} & -\varepsilon_{p\alpha} & \varepsilon_p - \mu
\end{pmatrix} \begin{pmatrix}
d_{\alpha \sigma} \\
p_{\alpha \sigma} \\
p_{\alpha \sigma}
\end{pmatrix}
\]

where \( \varepsilon_{d\alpha} = 2t_{dp} \sin(k_x/2), \varepsilon_{y\alpha} = 2t_{dp} \sin(k_y/2) \) and \( \varepsilon_{p\alpha} = -(4t_{pp} \sin(k_x/2) \sin(k_y/2)) \). \( p_{\alpha \sigma} \) and \( d_{\alpha \sigma} \) are Fourier transforms of \( p_{\alpha + \frac{\pi}{2}, \sigma} \) and \( d_{\alpha \sigma} \), respectively. The eigenvectors of this matrix give the corresponding weights of d and p electrons.

The gap equation was derived by means of the perturbation theory in terms of \( U_d \) [18,19,20]. The inclusion of \( U_p \) is recently achieved to give the effective interaction [21]:

\[
V_{kk'} = \frac{1}{N} \sum_{p\rho} \sum_{p' \rho'} \frac{f_p^{\rho} - f_{p'}^{\rho'}}{\varepsilon_p(p) - \varepsilon_p(k + k' + p)} \sum_{\rho' = \rho, \rho'} U_{\rho \rho'}(p) z_{\rho'}(k + k' + p) z_{\rho'}(k)
\]

\( k \in \Delta \cup \Delta \), \( \rho \in \{d, p\} \), \( \rho' \in \{d, p\} \), \( \Delta \subseteq \mathbb{R} \), and \( \mathbb{R} \) denotes the set of all real numbers.
where $e_i(k)$ is the dispersion relation of the $\alpha$th band ($\alpha = 0, 1, 2$) and $f_k^{\alpha}$ is the Fermi distribution function. We adopt that $\alpha = 0$ indicates the lowest band which gives a dominant contribution. The subscript $i$ mean $d, p_x$ and $p_y$ components where we set $U_p = U_{px} = U_{py}$. $x^n = (e^{\alpha}_{d}, e^{\alpha}_{px}, e^{\alpha}_{py})$ indicates the eigenvector of the non-interacting Hamiltonian matrix shown above. Our gap equation is

$$\Delta_k = \frac{1}{N} \sum_i V_{ii} \frac{\Delta_k}{2E_k},$$

where $\Delta_k$ is the gap function and $E_k = \sqrt{\xi_k^2 + \Delta_k^2}$ for $\xi_k = e_k - \mu$.

3. Results and Discussion

The magnitude of the gap function is obtained as $\Delta = \exp(-2t_{dp}^2/\pi U_p^2)$ in the weak-coupling formulation [22, 23] where we take $t_{dp}$ as an energy unit. The exponent $x$ indicates the strength of superconductivity. We first show the result for $U_p = 0$. With increase of $\Delta_{dp} = e_p - e_d$, the exponent $x$, namely $T_c$, increases quickly as seen in Fig.1 where $x$ is shown as a function of $\Delta_{dp}$ using $t_{pp} = 0$ and $U_p = 0$ at the hole carrier density $n_h = 0.13$.

The gap functions are specified by one of irreducible representations of the square lattice. We have five irreducible representations $A_1, A_2, B_1, B_2$ and $E$ [22]. The $d_{x^2-y^2}$ symmetry is in $B_1$ and $d_{xy}$ symmetry is in $B_2$. The Fig.1 implies that $d_{x^2-y^2}$ pairing symmetry is realized for all the $\Delta_{dp}$ when $U_p = 0$. The Fig.2 shows $x$ as a function of $t_{pp}$ where a sharp peak indicates a peak of the density of states due to the van Hove singularity.

Next we examine the effect of $U_p$. The Fig.3 shows $x$ vs $U_p / U_d$ for $\Delta_{dp} = e_p - e_d = 3$ and $t_{pp} = 0$ at the doped hole density $n_h = 0.13$. This obviously indicates that $T_c$ decreases as $U_p$ is increased, that is, $U_p$ suppresses $T_c$. This is because the pairing symmetries induced by $U_d$ and $U_p$ are different from each other. This means that $T_c$ will increase if we can suppress $U_p$. Hence, when $U_p > 0$, $U_p$ induces $d_{xy}$-symmetry paired state. In fact, when $U_p = U_d$, $d_{x^2-y^2}$ pairing state changes into $d_{xy}$ state as $\Delta_{dp}$ is reduced from positive to negative values as shown in Fig.4. Here we mention that in this figure, $x$ of $A_1$ pairing state is very close to that of $d_{xy}$. We also found that $T_c$ is increased with increase of $U_p$ when $e_p - e_d < 0$. Lastly, we note that the role of $U_p$ is consistent with the experiment concerning relationship between $T_c$ and the relative ratio of hole density at O site to that at Cu site [16, 21]. This is because we have lower $T_c$ and lower p-hole density when $U_p$ grows large.
As a summary, we have investigated material-parameter dependence of $T_c$. We summarize as follows: (a) $T_c$ increases as $\varepsilon_p - \varepsilon_d$ is increased for $U_d = 0$, (2) $T_c$ is lowered with increase of $U_p$ when $\varepsilon_p - \varepsilon_d > 0$, (3) $T_c$ is increased with increase of $U_p$ when $\varepsilon_p - \varepsilon_d < 0$, (4) $T_c$ has a minimum at near $\varepsilon_p - \varepsilon_d = 0$ as a function of $\varepsilon_p - \varepsilon_d$ when $U_d$ and $U_p$ are comparable, (5) $U_d$ induces $d_{x^2-y^2}$ pairing while $U_p$ induces $d_{xy}$ pairing, (6) $T_c$ has a peak as a function of $t_{pp}$.

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