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 $\epsilon_p$ and $\epsilon_d$, and the Coulomb interaction parameters $U_d$ and $U_p$. Our main results are the following: (a) $T_c$ increases as $\epsilon_p - \epsilon_d$ is increased for $U_p = 0$, (2) $T_c$ is lowered with increase of $U_p$ when $\epsilon_p - \epsilon_d > 0$, (3) $T_c$ is increased with increase of $U_p$ when $\epsilon_p - \epsilon_d < 0$, (4) $T_c$ has a minimum at near $\epsilon_p - \epsilon_d = 0$ as a function of $\epsilon_p - \epsilon_d$ 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.

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 $t_{dp}$ and $t_{pp}$ 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 $t_{pp}$ 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 $\epsilon_p-\epsilon_d$ 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]:

$$
H = \varepsilon_d \sum_{i\alpha} d^\dagger_{i\alpha} d_{i\alpha} + \varepsilon_p \sum_{i\sigma} \left( p^\dagger_{i+\frac{1}{2},\sigma} p_{i+\frac{1}{2},\sigma} + p^\dagger_{i+\frac{1}{2},\sigma} p_{i+\frac{1}{2},\sigma} \right) + t_{dp} \sum_{i\sigma} \left[ d^\dagger_{i\sigma} \left( p_{i+\frac{1}{2},\sigma} + p_{i-\frac{1}{2},\sigma} - p_{i-\frac{1}{2},\sigma} - p_{i+\frac{1}{2},\sigma} \right) + h.c. \right] + t_{pp} \sum_{i\sigma} \left[ p^\dagger_{i+\frac{1}{2},\sigma} p_{i+\frac{1}{2},\sigma} - p^\dagger_{i+\frac{1}{2},\sigma} p_{i-\frac{1}{2},\sigma} - p^\dagger_{i-\frac{1}{2},\sigma} p_{i+\frac{1}{2},\sigma} + p^\dagger_{i-\frac{1}{2},\sigma} p_{i-\frac{1}{2},\sigma} + h.c. \right] + U_d \sum_{i} n^d_{i+\frac{1}{2}} n^d_{i-\frac{1}{2}} + U_p \sum_{i} \left( n^p_{i+\frac{1}{2}} n^p_{i+\frac{1}{2}} + n^p_{i-\frac{1}{2}} n^p_{i-\frac{1}{2}} \right),
$$

where $n^d_{i\sigma}$ and $n^p_{i\sigma}$ ($\mu=x, y$) 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

$$
H_0 = \sum_{k\sigma} \left( d^\dagger_{i\sigma} p^\dagger_{i\sigma} \right) \begin{pmatrix} \epsilon_d - \mu & \epsilon_{dk} & \epsilon_{jk} \\ -\epsilon_{dk} & \epsilon_p - \mu & \epsilon_{pk} \\ -\epsilon_{jk} & -\epsilon_{pk} & \epsilon_p - \mu \end{pmatrix} \begin{pmatrix} d_{i\sigma} \\ p_{i\sigma} \end{pmatrix},
$$

where $\epsilon_{dk} = 2t_{dp}\sin(k_y/2)$, $\epsilon_{jk} = 2t_{dp}\sin(k_y/2)$ and $\epsilon_{pk} = -4t_{pp}\sin(k_y/2)\sin(k_y/2)$. $p_{d\sigma}$ and $d_{d\sigma}$ are Fourier transforms of $p_{i+\frac{1}{2},\sigma}$ and $d_{i\sigma}$, 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]:

$$
V_{kk'} = \frac{1}{N} \sum_{p}\frac{f^d_p - f^p_p}{\varepsilon^d_p(p) - \varepsilon^p_p(k + k' + p)} \left| \sum_{\mu=d,p} \sum_{p'} U_{i\sigma} z^\mu_{p'}(k') z^\mu_{i\sigma}(k + k' + p) \right|^2,
$$

where $f^\mu_p$ is the Fermi integral for p electrons.
where \( e_f(k) \) is the dispersion relation of the \( \alpha \)-th band \((\alpha = 0, 1, 2) \) and \( f_i^\alpha \) 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 \( U_p = U_{px} = U_{py} \). \( \epsilon^\alpha = (\epsilon^\alpha_{px}, \epsilon^\alpha_{py}, \epsilon^\alpha_{py}) \) indicates the eigenvector of the non-interacting Hamiltonian matrix shown above. Our gap equation is

\[
\Delta_i = -\frac{1}{N} \sum_{k} V_{i}^k \frac{\Delta_k}{2E_k},
\]

where \( \Delta_k \) is the gap function and \( E_k = \sqrt{\epsilon_k^2 + \Delta_k^2} \) for \( \xi_k = \epsilon_k^0 - \mu \).

3. Results and Discussion

The magnitude of the gap function is obtained as \( \Delta = \exp(-2t_{dp}/xU_d^2) \) 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 \( t_{dp} = 0 \) 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 \( t_{dp} \) 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 \( t_{dp} = 0 \) 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 $\epsilon_p-\epsilon_d$ is increased for $U_p=0$, (2) $T_c$ is lowered with increase of $U_p$ when $\epsilon_p-\epsilon_d>0$, (3) $T_c$ is increased with increase of $U_p$ when $\epsilon_p-\epsilon_d<0$, (4) $T_c$ has a minimum at near $\epsilon_p-\epsilon_d=0$ as a function of $\epsilon_p-\epsilon_d$ 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 $t_{pp}$.

Acknowledgements

We thank J. Kondo for useful discussions.

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