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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 ε_p and ε_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_{x2-y2} 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.

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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

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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_{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 ε_p-ε_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]:

$$\begin{aligned} H &= \varepsilon_d \sum_{i\sigma} d^+_{i\sigma} d_{i\sigma} + \varepsilon_p \sum_{i\sigma} \left(p^+_{i+\hat{x}/2,\sigma} p_{i+\hat{x}/2,\sigma} + p^+_{i+\hat{y}/2,\sigma} p_{i+\hat{y}/2,\sigma} \right) \\ &+ t_{dp} \sum_{i\sigma} \left[d^+_{i\sigma} \left(p_{i+\hat{x}/2,\sigma} + p_{i+\hat{y}/2,\sigma} - p_{i-\hat{x}/2,\sigma} - p_{i-\hat{y}/2,\sigma} \right) + h.c. \right] \\ &+ t_{pp} \sum_{i\sigma} \left(p^+_{i+\hat{y}/2,\sigma} p_{i+\hat{x}/2,\sigma} - p^+_{i+\hat{y}/2,\sigma} p_{i-\hat{x}/2,\sigma} - p^+_{i-\hat{y}/2,\sigma} p_{i+\hat{x}/2,\sigma} + p^+_{i-\hat{y}/2,\sigma} p_{i-\hat{x}/2,\sigma} + h.c. \right) \\ &+ U_d \sum_i n^d_{i\uparrow} n^d_{i\downarrow} + U_p \sum_i \left(n^p_{i+\hat{x}/2\uparrow} n^p_{i+\hat{x}/2\downarrow} + n^p_{i+\hat{y}/2\uparrow} n^p_{i+\hat{y}/2\downarrow} \right) \end{aligned}, \tag{1}$$

where $n^d_{i\sigma}$ and $n^p_{i+\hat{\mu}/2\sigma}$ ($\mu=x, y$) 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 μ. The non-interacting part is written as

$$H_0 = \sum_{k\sigma} \left(d^+_{k\sigma} p^+_{xk\sigma} p^+_{yk\sigma} \right) \begin{pmatrix} \varepsilon_d - \mu & \varepsilon_{xk} & \varepsilon_{yk} \\ -\varepsilon_{xk} & \varepsilon_p - \mu & \varepsilon_{pk} \\ -\varepsilon_{yk} & \varepsilon_{pk} & \varepsilon_p - \mu \end{pmatrix} \begin{pmatrix} d_{k\sigma} \\ p_{xk\sigma} \\ p_{yk\sigma} \end{pmatrix}, \tag{2}$$

where $\varepsilon_{xk} = 2it_{dp}\sin(k_x/2)$, $\varepsilon_{yk} = 2it_{dp}\sin(k_y/2)$ and $\varepsilon_{pk} = -4t_{pp}\sin(k_x/2)\sin(k_y/2)$. $p_{\mu k\sigma}$ and $d_{k\sigma}$ are Fourier transforms of $p_{i+\mu/2,\sigma}$ 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]:

$$V_{kk'} = \frac{1}{N} \sum_{p\alpha\beta} \frac{f^{\alpha}_{k+k'+p} - f^{\beta}_{p}}{\varepsilon_\beta(p) - \varepsilon_\alpha(k+k'+p)} \left| \sum_{i=d,p_x,p_y} U_i z^\alpha_i(p) z^\beta_i(k+k'+p) z^0_i(k) z^0_i(k') \right|^2, \tag{3}$$

where $\varepsilon_\alpha(k)$ is the dispersion relation of the α-th band ($\alpha = 0, 1, 2$) and f_k^α 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 $U_p = U_{px} = U_{py}$. $z^\alpha \equiv \left(z_d^\alpha, z_{px}^\alpha, z_{py}^\alpha\right)$ indicates the eigenvector of the non-interacting Hamiltonian matrix shown above. Our gap equation is

$$\Delta_k = -\frac{1}{N}\sum_{k'} V_{kk'} \frac{\Delta_{k'}}{2E_{k'}}, \tag{4}$$

where Δ_k is the gap function and $E_k = \sqrt{\xi_k^2 + \Delta_k^2}$ for $\xi_k = \varepsilon_k^0 - \mu$.

3. Results and Discussion

The magnitude of the gap function is obtained as $\Delta = \exp\left(-2t_{dp}^2 / xU_d^2\right)$ 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 $\Delta_{dp} \equiv \varepsilon_p - \varepsilon_d$, the exponent x, namely T_c, increases quickly as seen in Fig.1 where x is shown as a function of Δ_{dp} using $t_{pp} = 0$ and $U_p = 0$ at the hole carrier density $n_h = 0.13$.

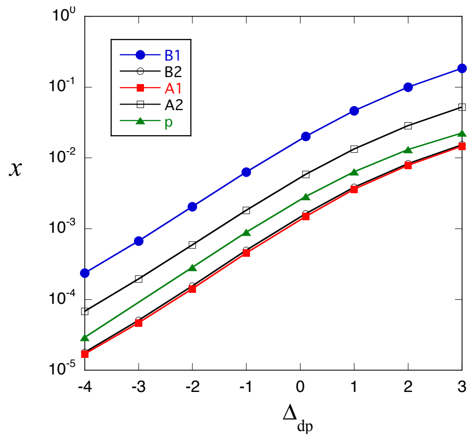


Fig.1. x as a function of Δ_{dp} with $t_{pp} = 0$ and $U_p = 0$.

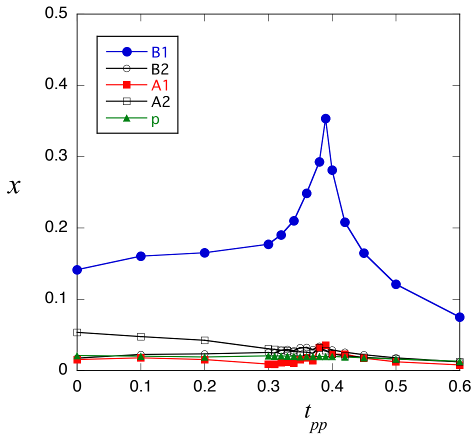
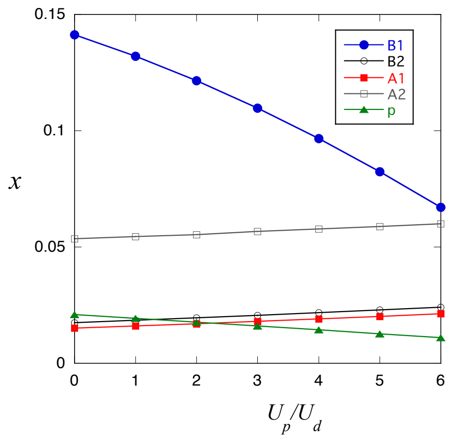


Fig.2. x as a function of t_{pp} with $\Delta_{dp} = 3$ and $U_p = 0$.

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 $d_{x2\text{-}y2}$ symmetry is in B_1 and d_{xy} symmetry is in B_2. The Fig.1 implies that $d_{x2\text{-}y2}$ pairing symmetry is realized for all the Δ_{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 $\Delta_{dp} = \varepsilon_p - \varepsilon_d = 3$ 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 $U_p = U_d$, $d_{x2\text{-}y2}$ pairing state changes into d_{xy} state as Δ_{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 $\varepsilon_p - \varepsilon_d < 0$. 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.



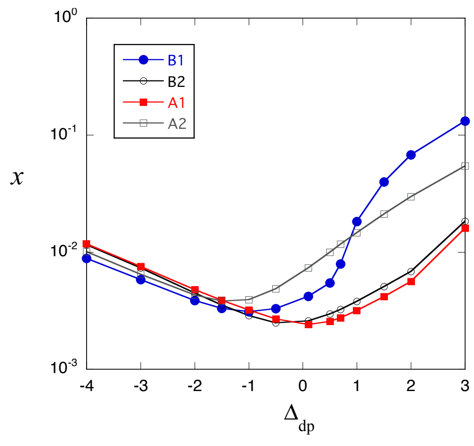


Fig.3. x as a function of U_p/ U_d for $\Delta_{dp} = 3$ and $t_{pp} = 0$. Fig.4. x as a function of Δ_{dp} for $U_p = U_d$ and $t_{pp} = 0$.

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 $U_p = 0$, (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_{x2-y2} pairing while U_p induces d_{xy} pairing, (6) T_c has a peak as a function of t_{pp}.

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References

[1] The Physics of Superconductors Vol.I and Vol. II edited by Bennemann KH, Ketterson JB. Springer-Verlag, Berlin (2003).
[2] Hirsch JE, Loh D, Scalapino DJ, Tang S. Phys. Rev. B39 243 (1989).
[3] Scalettar RT, Scalapino DJ, Sugar RL, White SR. Phys. Rev. B39 243 (1989).
[4] Weber C, Lauchi A, Mila F, Giamarchi T. Phys. Rev. Lett. 102 017005 (2009).
[5] Lau B, Berciu M, Sawatzky GA. Phys. Rev. Lett. 106 036401 (2011).
[6] Yanagisawa T, Koike S, Yamaji K, J. Phys. Soc. Jpn. 67 3867 (1998).
[7] Yanagisawa T, Koike S, Yamaji K. Phys. Rev. B64 184509 (2001).
[8] Yanagisawa T, Koike S, Yamaji K, Phys. Rev. B67 132408 (2003).
[9] Koike S, Yamaji K, Yanagisawa T, J. Phys. Soc. Jpn. 68 1657 (1999).
[10] Yanagisawa T, Miyazaki M, Yamaji K. J. Phys. Soc. Jpn. 78 013706 (2009).
[11] Miyazaki M, Yanagisawa T, Yamaji K. J. Phys. Soc. Jpn. 73 1643 (2004).
[12] Miyazaki M, Yamaji K, Yanagisawa T, Kadono R. J. Phys. Soc. Jpn. 78 043706 (2009).
[13] Yanagisawa T, Miyazaki M, Yamaji K. J. Mod. Phys. 4 No.6A 33 (2013).
[14] Yamaji K, Yanagisawa T, Koike S. Physica B284-288 415 (2000).
[15] Yamaji K, Yanagisawa T, Miyazaki M, Kadono R. J. Phys. Soc. Jpn. 80 083702 (2011).
[16] Zheng G-q, Kitaoka Y, Ishida K, Asayama K. J. Phys. Soc. Jpn. 64 2524 (1995).
[17] Koikegami S, Yamada K. J. Phys. Soc. Jpn. 69 768 (2000).
[18] Koikegami S, Yanagisawa T. J. Phys. Soc. Jpn. 70 3499 (2001); 71 671 (2001) (E).
[19] Koikegami S, Yanagisawa T. Phys. Rev. B67 134517 (2003).
[20] Yanagisawa T. New J. Phys. 10 023014 (2008).
[21] Yamaji K, Yanagisawa T. Physica C497 93 (2013).
[22] Kondo J. J. Phys. Soc. Jpn. 70 808 (2001).
[23] Kondo J. Bull. Electrotech. Lab. 64 67 (2001).