Material-dependent screening of Coulomb interaction in single-layer cuprates

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To explore material dependence of cuprate superconductors, we evaluate effective Coulomb interactions for Hg1201 and Tl1201, where Tl1201 having a nearly half value of \( T_c \) of Hg1201 even at the optimal oxygen concentration. Although structures are similar for these superconductors, there is an apparent difference in the occupied levels below \( E_F \). The characteristic difference in the band structure is correlated with oxygen contents in the buffer layer. By using constrained Random Phase Approximation, effective screened Coulomb interactions are estimated for HgBa\(_2\)CuO\(_4\) and TlBa\(_2\)CuO\(_4\). The results show that the value of screened on-site Coulomb interaction in Hg1201 is nearly twice bigger than that in Tl1201. In addition, The eigenvalues of the linearized Eliashberg equation of single-band Hubbard model within FLEX can show apparent difference in \( T_c \). When we assume that the twice big screened on-site Coulomb for Hg, the material dependent \( T_c \) might be explained.

1. Introduction

After the first discovery of a cuprate superconductor in 1986,\(^1\) the first discovery of cuprate superconductors has been reported.\(^2-5\) Especially Hg-based cuprates are well known because of their high transition temperatures. For the high-temperature superconductivity (high-\( T_c \)), in Hg-based cuprate crystal, the number \( n \) of CuO\(_2\) planes should be three in a basic stacked-layered structure,\( i.e. \) in the unit cell. The critical temperature \( T_c \) for superconductivity rises up to 135K even at ambient pressure when a triple-layered Hg-based cuprate \((n = 3)\) is chosen and when it is optimized with respect to its material parameters, e.g. the oxygen content.\(^4,5\) Although several other compounds have similar superconducting properties, \( T_c \) becomes maximum by a choice of the material and by the adjustment of its internal material parameters.

To explore a basic mechanism of high-\( T_c \), we consider several common features and detailed difference among cuprates, which should be explained by a unique theory. One of the special characters of high-\( T_c \) is material dependence of the superconducting properties. There are several known classification of cuprate superconductors in series,\( e.g. \) Hg-compounds, TI-compounds, and Bi-compounds, which essentially differ in the atomic structure of the buffer layer. When we see some specific materials, and if we compare \( T_c \) of some compounds in different series, we can actually find several hints to understand the relevant superconducting mechanism.

We see global similarity in doping dependence of the CuO\(_2\) planes. The optimal doping is often found at around a hole concentration of 0.16 per a CuO\(_2\) plane. To adjust the concentration, one often needs to modify the buffer layers in its oxygen contents. When a high-\( T_c \) material is optimized with respect to the hole concentration, at the optimal doping, the layer-number dependence of the transition temperature \( T_c \) in several series of cuprates may be derived. Comparison among materials categorized in these series was made in experiment.\(^6\) Triple-layer compounds provide the highest \( T_c \) among multi-layered compounds in various series. In addition, some special features of series dependence were concluded,\( e.g. \) existence of a large \( n \) regime. When the layer number \( n \) becomes more than around 7, \( T_c \) reaches at a saturated value for each series. Actually, experimental findings of material dependence in nature always extend our understanding of the high-\( T_c \) superconductivity.

Theoretically, there are many successful explanations on tendency of the material dependence. An example was the Fermi surface shape dependence of several cuprate series.\(^7,8\) In this direction, Sakakibara, \emph{et al.} have explored that the single-layer Hg-based cuprate is in a good condition for the orbital distillation effect\(^9,11\) while the 214 phase of La compounds may be a mixed multi-\( d \)-band system. They proposed that a purified 3d\(_{\pi-\gamma}\) band for Hg-compounds should provides better high-\( T_c \), while hybridization of 3d\(_{\pi-\gamma}\) and 3d\(_{\pi-\gamma}\) components around the Fermi level may causes reduction in \( T_c \). Even with this understanding, however, there remains unresolved material dependence.

Here an important hint can be found in the \( T_c \) difference between the Hg-series and the TI-series. A known experimental fact is that \( T_c \) of Hg1201 is \( T_c \approx 100\)K and that of TI1201 is \( T_c \approx 50\)K at the optimal doping.\(^6\) Indeed, \( T_c \) of TI1201 is only a half of the value of Hg1201. As we will show, the band structure calculation and the tight-binding fitting by the Wannierization technique\(^12,13\) tell that relevant 3d\(_{\pi-\gamma}\) bands of these compounds resemble each other.

On this problem, there had been several discussions on the \( T_c \) value and its dependence on materials parameters. The largeness of Madelung potential at the apical oxygen site,\(^14\) the orbital energy difference between 3d\(_{\pi-\gamma}\) and 3d\(_{\pi-\gamma}\),\(^9-11\) the largeness of interlayer tunneling effect,\(^15\) the lower amount of disorder on the CuO\(_2\) plane were considered. As for the former three factors, however, the band structure calculation had captured the material characteristics as far as the single-particle transfer terms are concerned. The third effect should be reconsidered with careful consideration of two-particle parts relevant for the interlayer pair-hopping processes described by an effective Hamiltonian.\(^16\) The last point would be experimental. However, we should note stiff nature of the cuprate high-temperature superconductivity against po-

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Here, we propose another factor of the material dependence. We focus on on-site Coulomb interaction and its screening effects. In many cases, Coulomb interaction is treated as material-independent values. However, we propose that on-site Coulomb interaction can strongly depend on oxygen contents in the buffer layer.

In this paper, we analyze the band structures given by the generalized-gradient approximation of DFT. By comparing the energy bands of Hg-based and Tl-based compounds, and then we apply constrained Random Phase approximation (constrained-RPA) method to evaluate Coulomb interactions. Then, to discuss the different strength of superconductivity in Hg-based and Tl-based compounds, we apply Fluctuation Exchange Approximation (FLEX) to single-band Hubbard model and solve the linearized Eliashberg equation.

2. Methods

2.1 constrained-RPA

In this section, we introduce constrained-RPA methods which is recently-developed calculation method. In this method, we divide polarization \( P \) into two contributions. One is by transition among target bands \( P_d \) and the other is by rest of transitions \( P_r \). The screened interaction \( W \) on the RPA level is given by

\[
W = [1 - vP]^{-1} v = [1 - vP_r - vP_d]^{-1} v
\]

(1)

\[
= [(1 - vP_r)(1 - vP_r)^{-1}vP_d]^{-1} v
\]

(2)

\[
= [1 - (1 - vP_r)^{-1}vP_d]^{-1}v
\]

(3)

\[
= [1 - W, P_d]^{-1} W_r
\]

(4)

where we have defined a screened interaction \( W_r \) that does not include the polarization from the 3d-3d transitions:

\[
W_r = [1 - vP_r]^{-1} v
\]

(5)

Screened Coulomb interactions at one time in the Wannier basis is expressed as

\[
V_{ij} = \int dr \int dr' \phi_i^*(r) \phi_j(r) W_{r}(r,r') \phi_i^*(r') \phi_j(r')
\]

(6)

Here \( i \) and \( j \) are the indices of the Wannier orbitals. \( W_{r}(r,r') \) is a screened Coulomb interaction.

\[
W_r(r,r') = \frac{4\pi}{\Omega} \sum_{qG'G} \frac{e^{i(q+G)r} e^{-i(q+G')r}}{|q + G|} e^{\epsilon_{GG'}(q)} e^{-i(q+G')r'}/|q + G|
\]

(7)

where \( \Omega \) is the crystal volume, \( e_{GG'}(q) \) is the inverse dielectric matrix, \( q \) is a wave vector in the first Brillouin zone, and \( G \) is a reciprocal lattice vector. The dielectric matrix is expressed as

\[
e_{GG'}(q) = \delta_{GG'} - v(q + G)x_{GG'}(q).
\]

(8)

Where \( v(q) = 4\pi/|q|^2 \) is the bare Coulomb interaction. The polarization matrix in constrained-RPA method is expressed as

\[
\chi_{GG'}(q) = \sum_k \sum_{\alpha\beta} \langle \phi_\alpha k + q | e^{-i(q+G)\cdot r} | \phi_\beta k \rangle \\
\times \langle \phi_\beta k | e^{-i(q+G')\cdot r} | \phi_\alpha k + q \rangle \frac{f_{\alpha k} + q - f_{\beta k}}{E_{\alpha k} + q - E_{\beta k}}
\]

(9)

Here \( \psi_{\alpha k} \) is the Bloch state, \( E_{\alpha k} \) is the energy of the state, and \( f_{\alpha k} \) is the occupancy. \( \alpha, \beta \) stand for the bands which do not include 3d-3d band transitions.

To perform the calculation and derive effective interactions, we use RESPACK-code.

3. Results

3.1 Hg- and Tl-based cuprate compounds

For comparison, we consider Hg-compounds and Tl-compounds. When a cuprate crystal is prepared at an optimal doping, the structure often becomes an alloy or a mixed phase. To adopt reliable DFT codes, we included in our simulation, however, we need to consider a perfect periodic crystal with a unit cell. Therefore, the simulation becomes possible by limiting the filling factor at some special value allowing construction of a super cell. Owing to this reason, we treat a crystal phase fixing concentration of dopant and an oxygen composition ratio. In some cases, we look at a filling factor corresponding to the half-filling of the CuO plane.

HgBa\(_2\)CuO\(_4\) (Hg1201) lacks oxygen atoms at each HgO plane. (Fig. 1 (a)) We have a local OHgO structure along the c axis. Oxygen atoms in this OHgO structure may be interpreted as apical oxygen atoms of CuO\(_2\) plane. In this figure, O(1) is oxygen in copper-oxygen layer, O(2) is apical oxygen and O(3) is oxygen in the buffer layer.
stress tensor being less than 0.5 [kbar]. The internal atomic structures are optimized with a criterion that the summation of the absolute values of force vector elements becomes smaller than $1.0 \times 10^{-3}$ [Ry/a.u.].

We show the hopping parameters for the $3d_{x^2−y^2}$ band in Hg1201,Tl1201 in Table I. Here, a little larger value of $t$ for the Tl-compound comes from its shrunk lattice constant. When we use the lattice constant of Tl1201 for Hg1201, the value of $t$ becomes close to -0.57. We can see that the general form of the band structures are almost same. However, Tl1201 has more dense bands below the Fermi energy than Hg1201 has.

Here we also show the total density of states and partial density of states onto orbitals and atoms. According to the results in Fig. 3, p orbitals of oxygen in the buffer layer have a large contribution to density of states in the occupied levels slightly below $E_F$ in Tl1201.

Table I. The hopping parameters for the $3d_{x^2−y^2}$ band in Hg1201,Tl1201.

|           | Hg1201 | Tl1201 |
|-----------|--------|--------|
| $t$ [eV]  | -0.450 | -0.574 |
| $r'$ [eV] | 0.102  | 0.0919 |
| $r''$ [eV]| -0.095 | -0.0764|

3.2 constrained-RPA and model calculation

We show the calculation results of on-site Coulomb interaction in Table II. In the course of calculation, the wave function and the charge density are (100, 400) [Ry] and cutoff energy for polarization functions are 10 [Ry]. We use 8x8x8 k-point mesh in the 1st Brillouin zone and take 100 bands into account in all calculations. According to Table II, the amplitudes of screened on-site Coulomb interaction($U_{\text{screened}}$) are drastically smaller than bare on-site Coulomb interaction($U_{\text{bare}}$) in both cuprates. The values of $U_{\text{bare}}$ are not so different between the two cuprates. On the other hand, the value of $U_{\text{screened}}$ in Hg1201 is nearly twice bigger than that in Tl1201. We also calculate on-site Coulomb repulsion in CaCuO$_2$ which is mother compounds of infinite-layer cuprates and do not have the buffer layer. We found that $U_{\text{screened}}$ in CaCuO$_2$ is also much larger than that in Tl1201, which indicate that the buffer layer has an important role of deciding the reduction of $U_{\text{screened}}$.

Table II. The parameters of effective Coulomb interactions for the $3d_{x^2−y^2}$ band in Hg1201,Tl1201 and CaCuO$_2$.

|           | Hg1201 | Tl1201 | CaCuO$_2$ |
|-----------|--------|--------|-----------|
| $U_{\text{bare}}$ [eV] | 12.2783 | 13.7685 | 13.7885 |
| $U_{\text{screened}}$ [eV] | 2.9462  | 1.7088  | 3.0397   |

To discuss the strength of superconductivity, we introduce the effective single-band Hubbard model. The single-band Hubbard Hamiltonians is

$$H = \sum_{ij\sigma}[t_{ij}c^\dagger_{i\sigma}c_{j\sigma} + H.c.] + U \sum_{i}n_{i\uparrow}n_{i\downarrow}, \quad (10)$$

Here $c^\dagger_{i\sigma}$ ($c_{i\sigma}$) stands for creation (annihilation) operator for electrons of site $i$ and spin $\sigma$. $n$ represent particle number operators for site $i$ and spin $\sigma$. To discuss the strength of superconductivity, we perform the so-called Fluctuation Exchange Approximation (FLEX)$^{29,30}$ with different amplitude of $U$. 

![Fig. 2. Band structures of HgBa$_2$CuO$_4$ (left) and TlBa$_2$CuO$_5$ (right). Wannier interpolated bands are plotted with red line. Here the Fermi level is set to 0.](image)

![Fig. 3. Density of states of HgBa$_2$CuO$_4$ (upper) and TlBa$_2$CuO$_5$ (lower). Here the Fermi level is set to 0. In Hg1201, we show partial density of states onto d orbitals of copper (Cu:d), p orbitals of oxygen in copper-oxygen plane and apical site (O(1):p+O(2):p). In addition to it, we show partial density of states onto p orbitals of oxygen in the buffer layer (O(3):p) in Tl1201.](image)
4. Discussion

In TI-compounds, it is not so easy to access the optimal doping by the reduction of oxygen in the buffer layer. In a real TI superconductor, La substitution was used to adjust the filling of CuO$_2$. In the real material of TlBa$_{1-x}$La$_x$CuO$_5$, it is known that $T_c$ does not reach the value over 50K even by adjusting the hole concentration.$^{31,32}$ Thus, we may propose to consider a careful control of oxygen in Tl1210 without La doping. If we can adjust the Fermi energy by the reduction of oxygen in the buffer layer, screening effect might be reduced and it will lead to make Coulomb interactions stronger. Therefore, this procedure might make an enhancement of $T_c$. Actually, this way of approach is consistent with some reported facts.$^{33}$

In this paper, we mention that metal oxygen in the buffer layers plays an important role to determine the strength of electron-electron interactions, consequently strength of superconductivity. We formed a tendency of material dependence in the screening. When we need to have a strong screened $U$, it is better to make a choice of a divalent metal atom as an element of the buffer layer. This consideration request us to keep essential material structure, i.e. the crystal symmetry. In this respect Cd or Cn in the place of Hg are candidates. Actually there are several reports on similarity in Cd compounds,$^{34,35}$ we might be able to say that if additional characters not appear, other divalent metal atoms in oxides without spin moments, e.g. Hf and W may work. As for as we know, there was no good report on these atoms for replacement. This may come from a reason that there are many atomic sites in cuprates. For example Ca and Ba are often needed. It may not so easy to maintain a crystal symmetry when replacement is done preferably only at Hg site in real materials.

To estimate the screened interaction, we utilized the constrained-RPA method. This method is formulated within RPA for the screened interaction $W$, where the function form of $W_r$ is justified in this approximation. With respect to this limitation, there might be a criticism on the use of $W_r$ for the effective interaction $U$ of the correlated electron model, i.e. the Hubbard Hamiltonian. Here, we open another route to approach this formulation. Introduction of correlation effects in a generalization of the density functional theory (DFT) as the multi-reference DFT (MR-DFT)$^{36}$ is possible by usage of a projection operator $P_A$. This operation projects a full correlated state $|\Psi\rangle$ in multi-Slater determinants onto a reference state $P_A|\Psi\rangle$ with quantum entanglement only in a correlated $d$ band formally without any approximation. With this step, we can derive a series of correlated electron models, e.g. a multi-band extended Hubbard model. When we introduce a projection $P_A$ on $d$ bands, and $P_B = 1 - P_A$, for example, we have the direct interaction in the $d$ band $P_AV_P^A = v_{dd}$ and the higher order contributions. As a result, we have the next expression for the full effective screened interaction.

\[
v_{eff,dd}(\omega) = v_{dd} + v(P_{A,dd}(\omega) + P_{dd,v}v_P^A)W_r(\omega) = W_r(\omega). \tag{13}
\]

The approximation leads us to reach an expression similar to constrained-RPA. Lets suppose that resulted $W_r(\omega)$ is used for a $d$-band model, so that we can omit subscripts in $v_{dd}$.

\[
W_r(\omega) = \left[1 - v(P_{A,dd}(\omega) + P_{dd,v}(\omega))\right]^{-1}v. \tag{14}
\]

In this expression, a partial polarization function is given by an effective screened on-site interaction. The term comes from a quantum fluctuation contribution prohibiting fluctuation in
the occupation number of the $d$ band.

$$P_{c(d)}(r, r'; \omega) = 2 \sum_{\mathbf{k} \in \text{occupied}} \sum_{\mathbf{\lambda}, \mathbf{\lambda}'} \phi_i^\ast(r) \phi_j(r) \phi_i^\ast(r') \phi_j(r') \times \frac{1}{\omega - E_j - U_{\text{eff}} + E_i + i\delta} - \frac{1}{\omega + E_j + U_{\text{eff}} - E_i - i\delta}$$

(15)

$$P_{d(s)}(r, r'; \omega) = 2 \sum_{\mathbf{k} \in \text{valence}} \sum_{\mathbf{\lambda}, \mathbf{\lambda}'} \phi_i^\ast(r) \phi_j(r) \phi_i^\ast(r') \phi_j(r') \times \frac{1}{\omega - E_j - U_{\text{eff}} + E_i + i\delta} - \frac{1}{\omega + E_j + U_{\text{eff}} - E_i - i\delta}$$

(16)

Here, notations $c$ and $v$ represent unoccupied conduction bands and fully filled valence bands. Therefore, in Eq. (15), $E_j + U_{\text{eff}} > E_i$, where $U_{\text{eff}}$-contribution is owing to reduction in the number of electrons in $d$ bands. Namely, fluctuation is prohibited by $U_{\text{eff}}$ so that $E_j > E_i + U_{\text{eff}}$. While in Eq. (16), we have $E_j + U_{\text{eff}} > E_i$. In this process, the $d$ band is partially doubly occupied. The energy denominator is determined by the condition $E_j - E_i + U_{\text{eff}} > 0$. Appearance of $U$ in the denominator of each expression of $P_{c(d)}$ and $P_{d(s)}$ represents the final-state correlation effect. In the expression of the super process, we have the two-particle Green function for the expression of the polarization function. Since we have change in the $d$ occupation in each high-energy process, the energy denominator is affected by the quantum fluctuation. In a correlated $d$ band, the consistency in the above expression is certified by

$$U_{\text{eff}} = \int dr \int dr' \phi_i^\ast(r) \phi_j(r) W_{ij}(r, r'; \omega = 0^+) \phi_i^\ast(r') \phi_j(r').$$

(17)

This is an ansatz in our proposed procedure. When we replace $P_{c(d)} + P_{d(s)}$ with $P_s$ as an approximation, if we apply $U_{\text{eff}} \sim 0$ in the denominators of Eqs. (15) and (16), we arrive at the expression Eq. (5) by constrained-RPA.

5. Summary and conclusions

By applying the constrained-RPA method, we evaluated an effective Coulomb interaction for Hg and Tl compounds. As a result, we have an indication of stronger screening in the on-site correlation in a $T$ compound relative to Hg compound. Analyzing the nature of the electronic band structures of these compounds, we found that there is apparent difference in the occupied levels below $E_F$. These differences reflect the varying crystal structures. Especially, we paid attention to different electronic structures originated from oxygen contents in buffer layer. From analyzing partial density of states and evaluating on-site Coulomb interaction in CaCuO$_2$, we deduce that oxygen contents in the buffer layer have a large effects on screening of Coulomb interactions. However, quantitative evaluation of orbital-decomposed screening effects is future problem.

The eigenvalue of the linearized Eliashberg equation within FLEX showed that the estimated difference in $U_{\text{screened}}$ for Hg and Tl can show apparent difference in $T_c$. When we assume that the twice big $U_{\text{screened}}$ for Hg, the material dependent $T_c$ might be explained.

We also comment on an another effect from the buffer layers. We paid attention to different electronic structure above the Fermi energy. By using MR-DFT method, we evaluated an effective exchange scattering amplitude for some Hg and Tl compounds. Analyzing the nature of the electronic band structures of these compounds, we found that the high energy levels originated from the Hg-O buffer layer contributes well creating enhancement of exchange interaction, which should lead the increase in $T_c$ via the spin fluctuation mechanism. In Tl compounds, however, the enhancement is not so apparent. This is because of the absence of the Tl-O branch around $E_F$, which also may explain strange difference between $T_c$s of Hg- and Tl-compounds.\(^\text{37}\)

The calculations were done in the computer centers of Kyushu University and ISSP, University of Tokyo. The work is supported by joint-project for “Study of a simulation program for the correlated electron systems” with Advancsoft co. J1611101009, and JSPS KAKENHI Grant Numbers JP26400357.

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