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To cite this article: Hirofumi Sakakibara *et al* 2013 *J. Phys.: Conf. Ser.* **454** 012021

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First-principles band structure and FLEX approach to the pressure effect on T_c of the cuprate superconductors

Hirofumi Sakakibara¹, Katsuhiko Suzuki¹, Hidetomo Usui¹, Kazuhiko Kuroki¹, Ryotaro Arita^{2,5}, Douglas J Scalapino³ and Hideo Aoki⁴

¹Department of Engineering Science, The University of Electro-Communications, Chofu, Tokyo 182-8585, Japan

²Department of Applied Physics, The University of Tokyo, Hongo, Tokyo 113-8656, Japan

³Physics Department, University of California, Santa Barbara, California 93106-9530, USA

⁴Department of Physics, The University of Tokyo, Hongo, Tokyo 113-0033, Japan

⁵JST, PRESTO, Kawaguchi, Saitama 332-0012, Japan

E-mail: hiro_rebirth@vivace.e-one.uec.ac.jp

Abstract. High-temperature cuprate superconductors have been known to exhibit significant pressure effects. In order to fathom the origin of why and how T_c is affected by pressure, we have recently studied the pressure effects on T_c adopting a model that contains two copper d -orbitals derived from first-principles band calculations, where the d_{z^2} orbital is considered on top of the usually considered $d_{x^2-y^2}$ orbital. In that paper, we have identified two origins for the T_c enhancement under hydrostatic pressure: (i) while at ambient pressure the smaller the hybridization of other orbital components the higher the T_c , an application of pressure acts to reduce the multiorbital mixing on the Fermi surface, which we call the orbital distillation effect, and (ii) the increase of the band width with pressure also contributes to the enhancement. In the present paper, we further elaborate the two points. As for point (i), while the reduction of the apical oxygen height under pressure tends to increase the d_{z^2} mixture, hence to lower T_c , here we show that this effect is strongly reduced in *bi-layer* materials due to the pyramidal coordination of oxygen atoms. As for point (ii), we show that the enhancement of T_c due to the increase in the band width is caused by the effect that the many-body renormalization arising from the self-energy is reduced.

1. Introduction

Although many kinds of superconductors have been discovered, the superconducting transition temperature T_c of the cuprate superconductors still remains to be the highest, and the possibility of further enhancing T_c still attracts much attention. To achieve higher T_c , it is important to understand the key parameters that control T_c , and from this viewpoint, there have been studies that have focused on the correlation between T_c and the lattice parameters such as the in-plane bond length(l)[1, 2] or the apical oxygen height(h_O) [3, 4, 5, 6, 7, 8, 9, 10, 11] measured from the CuO₂ planes. Theoretically, we have studied the material dependence of T_c in [10, 11], and introduced a two-orbital model that takes into account the $d_{x^2-y^2}$ and d_{z^2} Wannier orbitals. In most of the theories of the cuprates, only the $d_{x^2-y^2}$ (and the hybridized oxygen p) orbital is considered, but actually it has been noticed from the early days that in (La,Sr)₂CuO₄, which



has small h_O and relatively low T_c , there is a strong mixture of the d_{z^2} orbital component near the Fermi level[12, 13, 14]. In fact, nowadays there have been more studies that focus on the d_{z^2} orbital or the related apical oxygen [7, 8, 15, 16, 17, 18]. In [10, 11], we have shown that this mixture of the d_{z^2} orbital component near the Fermi level works destructively against d -wave superconductivity, and hence this is the main reason of the material dependence of T_c .

Studying the pressure effect on T_c is an *in situ* way of attacking the problem of the correlation between T_c and the lattice structure. It is well known that in most of the cuprates, application of pressure enhances T_c [19, 20]. On the other hand, it has been revealed that the pressure effect exhibits strong anisotropy[21, 22, 23]. In our recent theoretical study on the pressure effect in the cuprates, it has been revealed that in addition to the d_{z^2} effect, the roundness of the Fermi surface, which is controlled by Cu-4s- $d_{x^2-y^2}$ hybridization, and also the band width are important parameters that governs T_c under pressure[24].

In the present paper, after briefly reviewing the main results obtained in [24], we study more closely the effect of the band width by applying the fluctuation exchange approximation(FLEX)[25, 26, 27] to the two-orbital model. Secondly, we will explain the difference of the d_{z^2} orbital effect between the multi-layer and single-layer systems under hydrostatic pressure.

2. Calculation Method

2.1. Determination of the Crystal Structure Under Pressure

We first obtain the crystal structure of the single-layer cuprates La_2CuO_4 and $\text{Hg}_2\text{BaCuO}_4$ under ambient pressure. Namely, we calculate the total energy by first principles calculation[28] varying the lattice constants, and fit the result by the standard Burch-Marnaghan formula[29] to obtain the structure at the most stable point. From such calculation, we can obtain the crystal structure within one percent discrepancy from the lattice constants determined experimentally[30, 31]. To obtain the lattice structure under hydrostatic pressure, we optimize the Poisson's ratio and atomic position by first principles reducing the cell volume to 95% or 90% of the lattice structure under ambient pressure. Since the compressibility in the cuprates is known to be about $\sim 0.01 \text{ GPa}^{-1}$ [32], $V = 0.9V_0$ corresponds to a pressure of about 10 GPa.

2.2. Construction of the two-orbital model and FLEX approximation

Using the obtained crystal structure under ambient or hydrostatic pressure, we construct maximally localized Wannier orbitals[33, 34] to extract the hopping parameters of the $d_{x^2-y^2}$ - d_{z^2} two-orbital model[10]. As for the electron-electron interactions, we consider the on-site intraorbital Coulomb repulsion U , interorbital repulsion U' , the Hund's coupling J and the pair-hopping J' . Here we also keep the orbital SU(2) requirement, $U - U' = 2J$. We set $U = 3.0 \text{ eV}$, $U' = 2.4 \text{ eV}$ and $J = J' = 0.3 \text{ eV}$ unless mentioned otherwise. Estimates of U for the cuprates is $7 - 10t$, $t \simeq 0.45\text{eV}$ (namely, U is about $3 \simeq 4.5 \text{ eV}$), and $J(J') \simeq 0.1U$, so the values adopted here are within the widely accepted range.

We apply FLEX to this model to obtain the Green's function renormalized by the many-body self-energy correction. In FLEX, we define the spin and charge susceptibilities as follows;

$$\hat{\chi}_s(q) = \frac{\hat{\chi}^0(q)}{1 - \hat{S}\hat{\chi}^0(q)}, \quad (1)$$

$$\hat{\chi}_c(q) = \frac{\hat{\chi}^0(q)}{1 + \hat{C}\hat{\chi}^0(q)}, \quad (2)$$

where $q \equiv (\vec{q}, i\omega_n)$, the irreducible susceptibility is

$$\chi_{l_1, l_2, l_3, l_4}^0(q) = \sum_q G_{l_1 l_3}(k+q)G_{l_4 l_2}(k) \quad (3)$$

with the interaction matrices

$$S_{l_1 l_2, l_3 l_4} = \begin{cases} U, & l_1 = l_2 = l_3 = l_4 \\ U', & l_1 = l_3 \neq l_2 = l_4 \\ J, & l_1 = l_2 \neq l_3 = l_4 \\ J', & l_1 = l_4 \neq l_2 = l_3, \end{cases} \quad (4)$$

$$C_{l_1 l_2, l_3 l_4} = \begin{cases} U & l_1 = l_2 = l_3 = l_4 \\ -U' + J & l_1 = l_3 \neq l_2 = l_4 \\ 2U' - J, & l_1 = l_2 \neq l_3 = l_4 \\ J' & l_1 = l_4 \neq l_2 = l_3, \end{cases} \quad (5)$$

here, l_1, l_2 are orbital indices. Considering the self-energy correction originating from these susceptibilities, we solve the Dyson equation in a self-consistent manner. Then the renormalized Green's function is substituted to the linearized Eliashberg equation for superconductivity,

$$\lambda \Delta_{ll'}(k) = -\frac{T}{N} \sum_q \sum_{l_1 l_2 l_3 l_4} V_{ll_1 l_2 l'}(q) G_{l_1 l_3}(k-q) \Delta_{l_3 l_4}(k-q) G_{l_2 l_4}(q-k). \quad (6)$$

The maximum eigenvalue λ in the above equation reaches unity at the superconducting transition temperature $T = T_c$, so that λ calculated at a fixed temperature can be used as a measure for T_c . Here, we calculate λ at $T = 0.01$ eV for La and $T = 0.03$ eV for Hg. The reason for this is because $T_c \sim 100$ K of Hg is about three times larger than for La with $T_c \sim 40$ K[35].

3. Results and Discussions: effect of band width

3.1. Orbital Distillation

In figure 3.1, λ is depicted as a function of the unit cell volume. λ increases in La and in Hg cuprates with hydrostatic pressure, and this agrees with the well-known experimental result that T_c goes up monotonically under pressure in the cuprates[19, 20]. To understand this result, we have introduced three important parameters, the level offset ΔE , the roundness of Fermi surface ($r_{x^2-y^2}$ defined below) and the band width W [24]. To decompose the pressure effect into the contribution from the variation of these parameters, we vary each parameter ‘‘by hand’’ from the original value at $V = V_0$ to the value at $V = 0.9V_0$ separately, and calculate the variation in λ . This result is also depicted in figure 3.1 as the length of arrows. ΔE is the on-site energy difference between $d_{x^2-y^2}$ and d_{z^2} Wannier orbitals in the two-orbital model, so this is a measure of the d_{z^2} orbital effect, which has been found to work destructively against d -wave superconductivity in our previous study[10]. The effect of ΔE is dominant in La compound because La originally has small ΔE thereby suppressing T_c , so its increase under pressure is effective for the T_c enhancement. Note that in La system, ΔE increases under pressure because the absolute magnitude of the crystal field increases in spite of the reduction of h_O/l . On the other hand, in the Hg compound the pressure effect through ΔE is negligible because ΔE is intrinsically large. Instead, the other two parameters are effective. $r_{x^2-y^2}$ is defined as $r_{x^2-y^2} \equiv (|t_2| + |t_3|)/|t_1|$, where t_i is the i -th neighbor hopping within the $d_{x^2-y^2}$ orbital. The roundness of Fermi surface is enhanced by the increase of this value, and t_2 and t_3 are mostly mediated by the Cu-4s orbital (which is effectively included in the two Wannier orbitals in the present model) with the path of $d_{x^2-y^2} \rightarrow 4s \rightarrow d_{x^2-y^2}$ [4]. It is known that the roundness of the Fermi surface works against the spin-fluctuation-mediated superconductivity[36], so the reduction of the 4s effect enhances T_c . The 4s orbital effect is reduced by hydrostatic pressure because the energy level offset between the $d_{x^2-y^2}$ and the 4s orbital is enhanced when the oxygen ligands approach Cu. The effect of d_{z^2} and 4s orbitals put together, we can say that T_c increases when the main band has more pure $d_{x^2-y^2}$ component, namely, when the ‘‘orbital distillation’’ takes place.

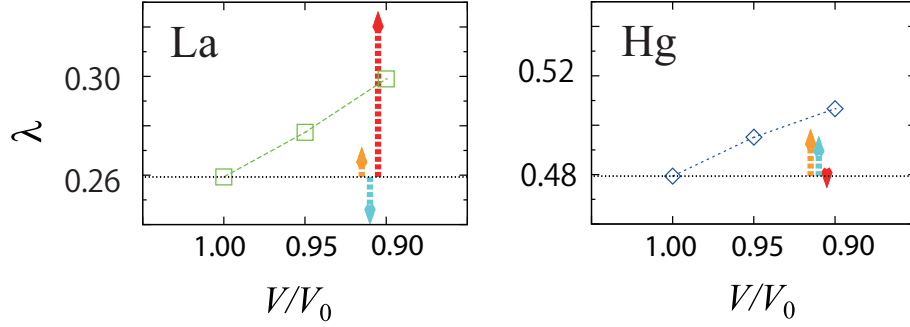


Figure 1. Eigenvalue λ of the Eliashberg equation plotted against the volume compression V/V_0 . Arrows indicate the contribution to the λ variance from the parameters $r_{x^2-y^2}$ (leftmost), W (center) and ΔE (rightmost)(see text).

3.2. The Effect of Band Width W

Now, we turn to the first main topic of this paper, i.e., the effect of the band width W . The band width W is defined as the energy range between the top and the bottom of the main band. It is evident that the band width is controlled by the in-plane bond length l , so that hydrostatic pressure enhances W . In figure 3.1, we can see that the increase in W results in an enhancement of λ in Hg, while the opposite occurs for La. The reason for this can be understood as follows. Let us first start with the U dependence of T_c for a fixed band width. In the top of figure 3.2, we show the absolute value of the renormalized Green's function squared $|G|^2$ in the Hg compound at $(\vec{k}, i\omega) = (\pi, 0, i\pi k_B T)$ for several values of $2 < U < 5$ eV. The value of $|G|^2$ monotonically decreases with larger U because the self-energy, which increases with U , suppresses $|G|^2$. On the other hand, the pairing interaction shown in the middle increases with U because the spin fluctuations develop monotonically. Consequently, $V|G|^2$ shown on the right exhibits a maximum at a certain U . Since $V|G|^2$ can be considered as a rough measure of the eigenvalue of the Eliashberg equation for d -wave superconductivity, λ (and thus T_c) is expected to be *maximized* around a certain U_{optim} .

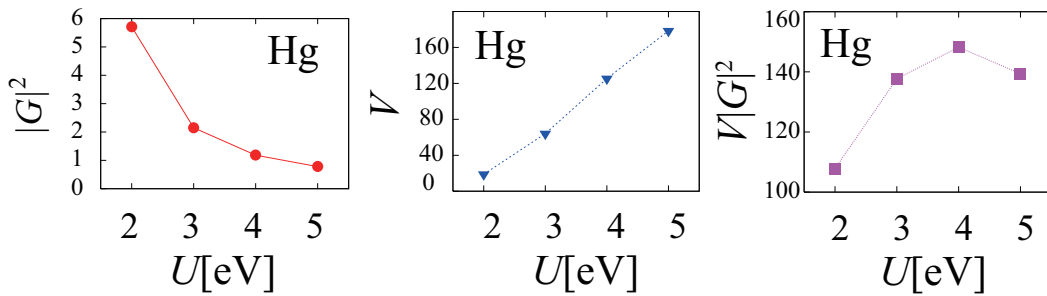


Figure 2. U dependence of the FLEX calculation result for the Hg compound. (left) the absolute value of the renormalized Green's function squared $|G|^2$ at $(\vec{k}, i\omega) = (\pi, 0, i\pi k_B T)$, (middle) the effective pairing interaction V at $(\vec{q}, i\omega) = (\pi, \pi, 0)$ and (right) the product $V|G|^2$.

In the left panels of figure 3.2, we show the U dependence of λ for $3 < U < 5$ eV for the two compounds with $V = V_0$ and $0.9V_0$. We can see that $U < 5$ eV lies on the left side of U_{optim} for La, while $3 \text{ eV} < U$ is on the right side of U_{optim} in Hg. This means that larger values of

U is necessary for La to be in the “strongly correlated regime”. This is because electrons can avoid the strong intraorbital repulsion within $d_{x^2-y^2}$ orbitals by using the d_{z^2} orbital degrees of freedom in materials with small ΔE .

In the right panel of figure 3.2, we show the U dependence of the increment $\Delta\lambda$ of the eigenvalue λ induced by the increase of W under pressure. In this calculation, W is increased “by hand” up to its value at $V = 0.9V_0$, while the other two parameters are fixed at their original values. From this figure, we can see that the increase in W always enhances T_c in the Hg cuprate within the realistic U range. For the La cuprate on the other hand, $\Delta\lambda$ is negative for small values of U , and this is the reason why W affects superconductivity in opposite ways between La and Hg in figure 3.1. For larger values of U , however, $\Delta\lambda$ becomes positive even for La.

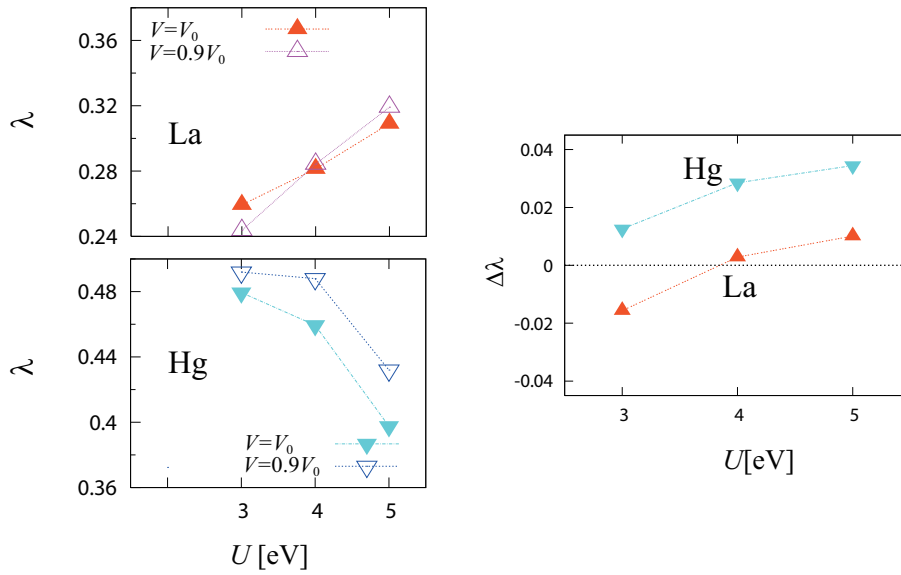


Figure 3. (Left) λ against U for La (top) and Hg (bottom). Filled (opened) symbols displays the result for $V = V_0$ ($V = 0.9V_0$). (Right) $\Delta\lambda$ (increment in λ when W is increased up to its value at $V = 0.9V_0$) against U .

To see the effect of the band width more clearly, we provide in figure 3.2 a schematic band width dependence of the U vs T_c plot. Namely, T_c should depend on U and W essentially in the form $Wf(U/W)$, where f is a certain function that gives the overall dependence of T_c against the electron correlation strength. Therefore, as the pressure is applied, W increases so that U_{optim} (peak position of the curve) also increases accordingly keeping U_{optim}/W constant. At the same time, the absolute value of the maximized T_c is enhanced by the application of the pressure because the entire energy scale increases (i.e., both U_{optim} and W are enhanced).

4. The d_{z^2} Orbital Effect: Multi-layer vs Single-layer Systems

So far, we have concentrated on single-layer systems. In this section, we will discuss the difference of the pressure effect through ΔE between single and multi-layer systems. Here, we focus on the comparison between single- and bi-layer La, Hg, Tl, Bi, and Y cuprates. We consider ΔE_d , the energy difference between the $d_{x^2-y^2}$ and the d_{z^2} orbital in the d - p model which considers all of the Cu $3d$ and O $2p$ orbitals explicitly. In the d - p model, the basis functions for the hopping part are close to the atomic orbitals, so ΔE_d can be considered as the energy difference between the $d_{x^2-y^2}$ and the d_{z^2} atomic orbitals. ΔE is the energy difference between the $d_{x^2-y^2}$ and the

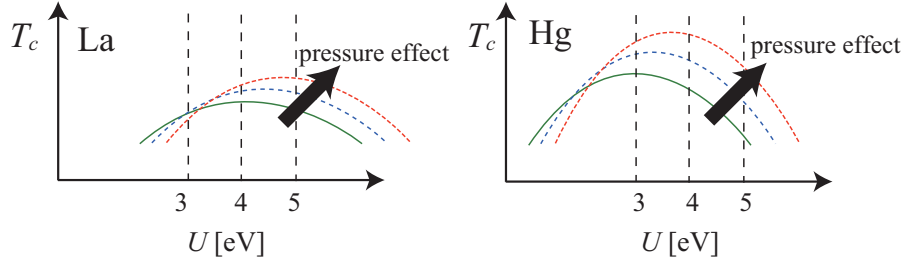


Figure 4. Schematic figure of T_c variation induced by applied pressure. Each line is a U vs. T_c plot for fixed W , and W is larger for solid green \rightarrow dashed blue \rightarrow dotted red.

d_{z^2} Wannier orbitals which effectively take the $O2p$ orbitals into account, so ΔE_d and ΔE are positively correlated[11].

In figure 4, we show the relationship between the apical oxygen height h_O and ΔE_d . We can see that, while ΔE_d is positively correlated with the apical oxygen height in both single- and bi-layer systems as expected, ΔE_d is overall significantly greater in the bi-layer systems than in the single-layer systems. This is because bi-layer cuprates take pyramidal coordination of the oxygen ligands, while the single-layer cuprates take an octahedral one. Hence the effect of the apical oxygen should be weaker in the bi-layer systems, so that the “effective h_O ” is larger. As we have seen in the previous section, ΔE (and hence the d_{z^2} orbital) plays minor role in the T_c enhancement under pressure in materials with large ΔE , so the effect of ΔE should become less relevant as the number of the layers increases. This can be considered as one reason why T_c increases in spite of somewhat larger reduction in h_O in bi-layer system than in single-layer system under hydrostatic pressure[1].

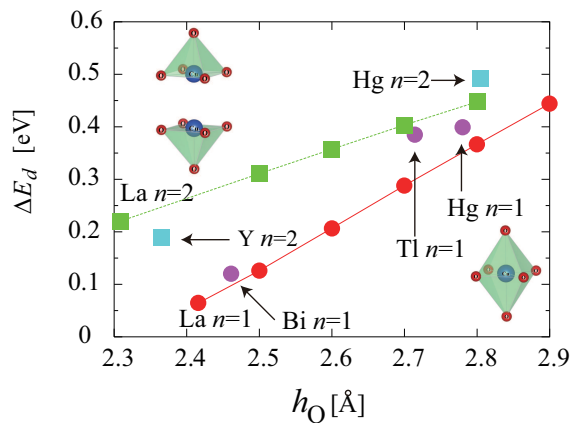


Figure 5. Relationship between the apical oxygen height h_O [Å] and the level difference ΔE_d [eV]. The squares(circles) show the value of ΔE_d in each bi-layer(single-layer) system(the materials are indicated by arrows). The dashed(solid) line presents the calculation result when h_O is varied hypothetically in bi-layer (single-layer) La system by hand.

5. Conclusion

In conclusion, we have performed first-principle calculation+FLEX study to analyze the pressure effect on T_c of the cuprates. To explain the T_c enhancement induced by hydrostatic pressure, we introduce three important parameters, level offset ΔE , roundness of the Fermi surface $r_{x^2-y^2}$ and the band width W . ΔE and $r_{x^2-y^2}$ are the measure of "orbital purity" in the main band, and T_c is enhanced by "orbital distillation". We have shown that hydrostatic pressure enhances the distillation, thereby enhancing T_c . We have also analyzed the effect of the band width W in detail. It has been shown that λ (and hence T_c) is maximized around a certain U , which depends on the band width as well as ΔE . For materials with large ΔE such as the Hg compound, the increase of W under pressure leads to an enhancement of λ for realistic values of U .

We also discuss the difference between bi- or single-layer systems from the view point of ΔE . Even when h_O is suppressed under pressure in bi-layer systems, the effect on T_c should be small because of the pyramidal coordination of the oxygen ligands.

6. Acknowledgments

The numerical calculations were performed at the Supercomputer Center, ISSP, University of Tokyo. This study has been supported by Grants-in-Aid for Scientific Research from JSPS (Grants No. 23340095, RA; No. 23009446, HS; No. 21008306, HU; and No. 22340093, KK and HA). RA acknowledges financial support from JST-PRESTO. DJS acknowledges support from the Center for Nanophase Material Science at Oak Ridge National Laboratory.

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