Orbital mixture effect on the Fermi surface-\(T_c\) correlation in the cuprate superconductors — bilayer vs single layer

Hirofumi Sakakibara\(^1\), Katsuhiro Suzuki\(^1\), Hidetomo Usui\(^2\), Satoaki Miyao\(^3\), Isao Maruyama\(^4\), Koichi Kusakabe\(^5\), Ryotaro Arita\(^6\,7\), Hideo Aoki\(^6\), and Kazuhiko Kuroki\(^2\)

\(^{1}\)Department of Engineering Science, The University of Electro-Communications, Chofu, Tokyo 182-8585, Japan
\(^{2}\)Department of Physics, Osaka University, Machikaneyama-Cho, Toyonaka, Osaka 560-0043, Japan
\(^{3}\)Department of Materials Engineering Science, Osaka University, Machikaneyama-Cho, Toyonaka, Osaka 560-8531, Japan
\(^{4}\)Department of Information and Systems Engineering, Fukuoka Institute of Technology, Wajiro-higashi, Higashi-ku, Fukuoka 811-0295, Japan
\(^{5}\)Department of Applied Physics, The University of Tokyo, Hongo, Tokyo 113-8656, Japan
\(^{6}\)Department of Physics, The University of Tokyo, Hongo, Tokyo 113-0033, Japan and JST, PRESTO, Kawaguchi, Saitama 332-0012, Japan

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By constructing \(d_{x^2-y^2} - d_{z^2}\) two-orbital models from first principles, we have obtained a systematic correlation between the Fermi surface warping and theoretically evaluated \(T_c\) for various bilayer as well as single-layer cuprates. This reveals that a smaller mixture of the \(d_{z^2}\) orbital component on the Fermi surface leads simultaneously to larger Fermi-surface warping and higher \(T_c\). The theoretical correlation strikingly resembles a systematic plot for the experimentally observed \(T_c\) against the Fermi surface warping due to Pavarini et al. [Phys. Rev. Lett. 87, 047003 (2001)], and the present result unambiguously indicates that the \(d_{z^2}\) mixture is one key factor that determines \(T_c\) in the cuprates.

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I. INTRODUCTION

In a family of superconductors in which the transition temperature \(T_c\) varies sensitively according to the lattice structure and/or the constituent elements, it is imperative to extract parameters that are systematically correlated with \(T_c\). For the high-\(T_c\) cuprates in particular, Pavarini et al. have shown that there is a striking correlation between the experimentally observed \(T_c\) and the Fermi-surface warping [see Fig.1(b)]\(^{1}\). Namely, they have obtained single-orbital tight-binding models for various cuprates to estimate the ratio \(r\) between the nearest and second-nearest-neighbor hoppings, which is a measure of the warping of the Fermi surface. Plotting the experimental \(T_c\) against the theoretically evaluated \(r\), they noticed that \(T_c\) empirically increases with the Fermi surface warping.

The trend for higher \(T_c\) for more degraded nesting is rather puzzling, since, while there have been some approaches for explaining the trend\(^{2}\), fluctuation exchange (FLEX)\(^{2}\) as well as dynamical cluster approximation studies\(^{2}\) have shown that the Fermi surface warping and \(T_c\) should theoretically be anti-correlated when the Cu-\(d_{x^2-y^2}\) orbital (plus the hybridized oxygen 2p orbitals) alone is taken into account in the models. In order to resolve this puzzle, some of the present authors have previously introduced a two-orbital model that explicitly considers the \(d_{z^2}\) Wannier orbital on top of the \(d_{x^2-y^2}\)\(^{9}\,10\). In fact, there has been a long history of the study on possible importance of the \(d_{z^2}\) orbital and/or the apical oxygen\(^{11}\,12\). In refs.\(^{9}\) and \(^{10}\), we showed that \(\Delta E\), the level offset between \(d_{x^2-y^2}\) and \(d_{z^2}\) Wannier orbitals, dominates both of the warping of the Fermi surface and \(T_c\). It was shown, focusing on the single-layer cuprates, that La\(_2\)CuO\(_4\) has, despite a better-nested Fermi surface, a lower \(T_c\) than those in HgBa\(_2\)CuO\(_4\), Tl\(_2\)Ba\(_2\)CuO\(_6\), and Bi\(_2\)Sr\(_2\)CuO\(_4\) due to a strong \(d_{z^2}\) orbital mixture on the Fermi surface that degrades \(T_c\). However, among the above mentioned four single-layer cuprates, only La\(_2\)CuO\(_4\) has a small \(\Delta E\) (i.e., a strong \(d_{z^2}\) mixture), so that we are still in need of a convincing study to clarify whether \(\Delta E\) indeed controls \(T_c\) systematically in a wider range of cuprates that include the multilayer ones as analyzed in Pavarini’s plot\(^{1}\).

Thus the purpose of the present paper is to examine the systematics, where we extend the analysis to bilayer cuprates as well as those single-layer ones that have relatively lower \(T_c\). This has enabled us to study the correlation between the theoretically estimated \(T_c\) and the Fermi-surface warping for a much wider class of existing materials (Fig.1(a)). The systematics have turned out to reproduce the experimental trend in \(T_c\), and we shall unambiguously conclude that the \(d_{z^2}\) orbital mixture is indeed a key factor that strongly governs the \(T_c\) in the cuprates.

II. ORIGIN OF THE MATERIAL DEPENDENCE OF FERMI-SURFACE WARPING

A. Construction of the two-orbital model

Let us start with the construction of the two-orbital model. First-principles electronic structures of the mate-
rations are obtained with the VASP package\textsuperscript{22}, where experimentally determined lattice parameters are adopted. We have used the PBE exchange-correlation functional. We then employ the $d_{z^2}$ and $d_{x^2-y^2}$ Wannier orbitals as projection functions\textsuperscript{22} to model the band structure around the Fermi energy. The main band around the Fermi energy contains considerable contributions from the oxygen 2$p$ orbitals, so that they are effectively included in the Wannier functions. Similarly, the $p_z$ orbital in the apical oxygens is implicitly included in the $d_{z^2}$ Wannier orbital. Namely, we consider two kinds of anti-bonding state between the $d$ orbitals of copper and $p$ orbitals of oxygen in this model. In the bilayer systems, the total number of Wannier orbitals is four. Let us mention in passing that the $p_z$ orbital compo-
the Fermi energy. The main band around the Fermi en-
terpretation energy observed experimentally in, e.g., the RIXS experiments measure the energy that includes full electron correlation effects.

Figure 2 compares the band dispersion of the two-orbital model for eight cuprates\textsuperscript{22}, single-layer (a) La$_2$CuO$_4$, (b) Pb$_2$Sr$_2$Cu$_3$O$_6$, and bilayer (c) La$_2$CaCu$_2$O$_6$, (d) Pb$_2$Sr$_2$YC$_{u}Cu$_3$O$_8$, (e) EuSr$_2$NbCu$_2$O$_8$, (f) YBa$_2$Cu$_3$O$_{7-\delta}$ (YBCO), (g) HgBa$_2$CaCu$_2$O$_8$ (HBCO) and (h) Tl$_2$Ba$_2$CaCu$_2$O$_8$. The crystal structures are given in refs.\textsuperscript{33–40}, respectively. Experimentally, the first five materials are known to have relatively lower $T_c$ (< 70 K), while the last three have higher $T_c$ (> 90 K)\textsuperscript{41}. In Fig.2 we display the weight of the $d_{z^2}$ Wannier orbital with the thickness of the lines, which shows that there exist significantly strong $d_{z^2}$ mixtures around the flat portions of the bands near the Fermi energy in (a)-(e). By contrast, compounds (f)-(h) have the $d_{z^2}$ orbital components mostly on the bands well below the Fermi energy. In bilayer systems the main band is split into two, where the $d_{z^2}$ component, if any, is seen to primarily reside on the upper band. The band splitting is known to be caused by the interlayer hoppings, which are mediated by orbitals spreading along the $c$–axis such as the $4s$ and $d_{x^2-y^2}$ orbitals. In Fig.2 we also display the Fermi surfaces at $k_z = 0$, where we can see that in (a)-(e) the (outer) Fermi surfaces are basically concave against the $\Gamma$ point ($\langle k_x, k_y \rangle = (0, 0)$), while the inner Fermi surfaces (arising from the upper band) that have larger $d_{z^2}$ weights are convex for bilayer systems in (e)-(h).
B. Suppression of the Fermi surface warping by the $d_{z^2}$ orbital mixing

From the above result, we can see that the warping of the inner Fermi surface decreases as the $d_{z^2}$ mixture becomes stronger. In the figure the band filling is fixed at $n = 2.85$, but we have checked that this tendency persists when the band filling is varied. Although this trend has been noticed in our previous studies, we can now describe this more systematically and quantitatively for various materials. For this purpose we have first to quantify the degree of warping of the Fermi surface. This is accomplished by constructing a single-orbital model so that the main bands intersecting the Fermi level are reproduced with a single Wannier orbital per site. This Wannier orbital mainly consists of the $d_{x^2-y^2}$ orbital, but also has tails with a $d_{z^2}$ orbital character. We can then define the parameter, $r = (|t_2| + |t_3|)/|t_1|$ in terms of the second ($t_2$) and third ($t_3$) neighbor hoppings of the single-orbital model, which is a direct measure of the Fermi surface warping. For bilayer materials, $r$ can be defined with hoppings within each layer. Bilayers have two sites per unit cell with outer and inner Fermi surfaces, so that we can also obtain the respective measures of the warping of the outer and inner Fermi surfaces as $r_{outer,inner} = (|t_2 \pm t_3|)/|t_1|$, where $t_i \pm$ is the interlayer hopping to the sites vertically above (or below) the $i$-th neighbor. We stress that $r$ in the single-orbital model includes the effects of both the hoppings within the $d_{x^2-y^2}$ Wannier orbitals and those between the $d_{x^2-y^2}$ and $d_{z^2}$ Wannier orbitals in the two-orbital model.

In Fig(3a), we plot $r$ against $\Delta E$ for all the bilayer cuprates considered. The result shows that $r$ tends to increase with $\Delta E$, which can be understood as follows. In the two-orbital model that explicitly considers the $d_{z^2}$ orbital, the second (and also the third) neighbor hopping takes place via two paths, i.e., (i) directly between $d_{x^2-y^2}$ Wannier orbitals and (ii) indirectly via the $d_{z^2}$ orbital. As $\Delta E$ becomes smaller, path (ii) becomes more effective. In the single-orbital model, the two paths both contribute to $t_2$ and $t_3$, but they have opposite signs, so that $t_2(t_3)$ and hence $r$ are smaller when the contribution from path (ii) is larger. To be precise, $\gamma t_{HBCO}$ is larger than $r_{HBCO}$ despite $\Delta E_{YBCO}$ being smaller than $\Delta E_{HBCO}$. By analyzing the two-orbital model, we find that the ratio $(|t_2| + |t_3|)/|t_1|$ within the $d_{x^2-y^2}$ Wannier orbitals, i.e., path (i), which we refer to as $r_{x^2-y^2}$ (Ref.12), is significantly larger in YBCO, and we are coming back to this point below.

III. MANY-BODY ANALYSIS

We now move on to superconductivity. As shown in our previous studies, it is imperative to adopt the two-orbital model that explicitly considers the $d_{z^2}$ orbital to have a reliable estimate of $T_c$. In the two-orbital model we consider intra- and inter-orbital electron-electron interactions. The intra-orbital $U$ is considered to be in the range of 7-10t (where $t \approx 0.45$ eV is the nearest-neighbor hopping) for the cuprates, so we take the intra-orbital $U = 3.0$ eV. The Hund’s coupling $J$ and the pair-hopping $J'$ are typically $\sim 0.1U$, so we take $J = J' = 0.3$ eV. Here we observe the orbital rotational symmetry which gives the inter-orbital $U' = U - 2J = 2.4$ eV. We apply FLEX to this multi-orbital Hubbard model, and solve the linearized Eliashberg equation. In multiorbital FLEX, the Green’s function and spin and charge susceptibilities are given as matrices. The eigenvalue of the Eliashberg equation $\lambda$ increases upon lowering the temperature, and reaches unity at $T = T_c$. Therefore $\lambda$ at a fixed temperature can be used as a qualitative measure for $T_c$. The temperature is fixed at $k_B T = 0.01 eV$ in the present calculation. The total band filling (number of electrons /site) is fixed at $n = 2.85$, for which the filling of the main band amounts to 0.85 (15 % hole doping). We take a $32 \times 32 \times 4$ k-point mesh for the three-dimensional lattice with 1024 Matsubara frequencies. FLEX takes account of the self-energy correction self-consistently and amends the overestimated tendency toward magnetism in the random-phase approximation. On the other hand, FLEX cannot reproduce the Mott transition that should be present at half-filling nor the $T_c$ suppression in the underdoped regime. Therefore, we stick to the optimal doping regime in the present study.

IV. CORRELATION AMONG $T_c$, FERMI SURFACE, AND LATTICE STRUCTURE

A. Correlation between $T_c$ and the Fermi surface

In Fig(3b) we plot $\lambda$ against $\Delta E$ calculated for the five bilayer cuprates. We can see a very well-defined correlation between $\Delta E$ and $\lambda$. If we combine Figs(3a)(b), we can look at the relation between $\lambda$ (obtained for the two-orbital model) against the measure of the Fermi surface warping $r$ (defined in terms of the single-orbital model), which is precisely Fig(1a). Since $\lambda$ is a measure of $T_c$, we can immediately notice that the figure strikingly resembles Pavarini’s plot1 for the experimentally observed $T_c$ against $r$ in Fig(1b). This is the key result in the present work.

For comparison, we show in the inset of Fig(1a) the eigenvalue of the Eliashberg equation within the single-orbital model, $\lambda^{\text{single}}$, for the same materials. Here we take the same value of on-site $U$ as in the two-orbital model, but raise the temperature to $T = 0.02$ eV, since FLEX convergence in the single-orbital model is degraded for small $r$ at lower temperatures. The result for $\lambda^{\text{single}}$ exhibits an opposite tendency of decreasing with $r$, which firmly endorses that the $d_{z^2}$ orbital mixture is indeed a key factor that determines $T_c$ of the cuprates.

Besides the overall trend, we can also note the following two features. First, in our $\lambda-r$ plot $\lambda$ is larger for bilayer
systems than in single-layer ones, which reflects the difference in $\Delta E$. There may be some interlayer many-body interactions (such as the pair hopping\cite{50}) that can further enhance $T_c$ in the bilayer systems, which is not taken into account here. Another point to note is the comparison between YBCO and HBCO. Despite $r_{YBCO} > r_{HBCO}$, $\lambda$ obtained here is larger for HBCO, which agrees with the experimental results for $T_c$. As mentioned above, $r_{x^2-y^2}$ is very large for YBCO, which is the main reason why the single-orbital $r$ is large in this material. Namely, a smaller $\lambda$ in YBCO is caused by a large $r_{x^2-y^2}$ rather than by a small $\Delta E$, which we have actually checked by varying these quantities in a range covering these materials.

B. Origin of the material dependence of $\Delta E$

Finally, let us pinpoint the origin of the material dependence of $\Delta E$. For this purpose, we now construct a model that explicitly considers all of the Cu-3$d$ and O-2$p$ orbitals by introducing as many number of Wannier orbitals. Namely, the level offset $\Delta E_d$ between Cu-$d_{x^2-y^2}$ and Cu-$d_{z^2}$ and the level offset $\Delta E_p$ between in-plane O-$p_{\sigma}$ and apical-O-$p_z$, determine the final $\Delta E$ as shown in our previous study\cite{10}. The level offsets, $\Delta E_d = E(d_{x^2-y^2}) - E(d_{z^2})$ and $\Delta E_p = E(p_{\sigma}) - E(p_z)$, are defined as the differences in the on-site energies between the atomic-like orbitals. In Fig.3(c)(d), we plot $\Delta E$ against $\Delta E_d$ and $\Delta E_p$.

We are now in position to discuss how the two level-offsets are determined by the lattice structure. The apical oxygen height $h_0$ controls the crystal-field splitting, so that $h_0$ is correlated with $\Delta E_d$ (ref\cite{10}). In the bilayer materials, however, we can see that $\Delta E_d$ tends to be larger than in the single-layer ones despite the small $h_0$. We can identify this to be coming from the pyramidal coordination of the oxygen atoms with one apical oxygen per Cu in the bilayer cuprates, as opposed to the octahedral coordination with two apical oxygens in single-layer cuprates. Thus the effect of the apical oxygen is more or less halved in the bilayer systems, so that the effective $h_0$ becomes larger. This in turn makes $\Delta E_p$ play a more important role in the material dependence of $\Delta E$ and hence $T_c$. For example, La$_2$CaCu$_2$O$_6$ and YBCO have very small values of $h_0$ [in Fig.3(c)], and consequently they have similar values of $\Delta E_d$. However, YBCO has a much larger $\Delta E_p$ (smaller absolute value), which results in a larger $\Delta E$. $\Delta E_p$ playing a more important role than $\Delta E_d$ is also seen in terms of the Madelung energy differ-
en, $\Delta V_A$, between the apical and in-plane oxygens. $T_c$ is found to be correlated with $\Delta V_A$ rather than the apical oxygen height as in a previous study (Ref. [21]), where $\Delta V_A$ is in turn correlated with $\Delta E_{p10}$. One way to control $h_O$ is to apply a hydrostatic pressure to decrease it, but this has small effect on $T_c$ especially for multilayer cuprates because of the reason mentioned above.[21]

### V. CONCLUDING REMARKS

To summarize, we have revealed a systematic correlation between the Fermi surface warping and the theoretically evaluated $T_c$ by constructing two- and single-orbital models of various bilayer as well as single-layer cuprates. A striking agreement of the theoretical result with Pavarini's plot for experimental $T_c$'s[1] unambiguously indicates that the $d_{z^2}$ mixture is indeed a key factor that determines $T_c$ in the cuprates. The level offset $\Delta E$ between $d_{x^2-y^2}$ and $d_{z^2}$ Wannier orbitals mainly depends on two parameters, $\Delta E_d$ and $\Delta E_p$, but in multi-layer cuprates the latter plays a more important role than the former, so that the apical oxygen height is less important.

Let us recapitulate that the strongly warped Fermi surface is not the cause of the high $T_c$, but a consequence of the $r-T_c$ correlation where the $d_{z^2}$ orbital mixture (i.e.,
small \( \Delta E \) happens to suppress both of the warping (the single-orbital \( r \)) and \( T_c \) at the same time. Conversely, we can exploit this to note that higher-\( T_c \) materials can in principle be conceived if we can realize smaller \( r \) where \( r \) is reduced due to smaller \( r_{x^2-y^2} \) (the hopping ratio within the \( d_{x^2-y^2} \) Wannier orbitals) rather than due to smaller \( \Delta E \). The reason why we have to advance an universal \( r-T_c \) correlation in actual materials is traced back to \( r \) that increases with \( \Delta E \) (Fig 1a) because \( r_{x^2-y^2} \) does not vary widely within the known cuprates. From these observations, we here propose that designing materials with small \( d_{x^2} \) mixture and strongly reduced \( r_{x^2-y^2} \) (which would give a small \( r \)) may lead to higher \( T_c \) than the known cuprates, provided other conditions are essentially unchanged.  

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