Two-orbital view on the origin of the material dependence of T_c in the single-layer cuprates

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Abstract. Using the $d_{x^2-y^2}+d_{z^2}$ two orbital model of the high T_c cuprates obtained from the first-principle calculation, we show that the material dependence of the Fermi surface shape can be understood by the degree of the mixture between the $d_{x^2-y^2}$ and the d_{z^2} orbitals. We explain, through investigating the tightbinding hopping integrals, why some cuprates have square shaped Fermi surface, while others have more rounded ones. From this viewpoint, we explain the experimentally observed correlation between the curvature of the Fermi surface and T_c.

1. Introduction

In the high T_c cuprates, the 'main band' having strong Cu3$d_{x^2-y^2}$ orbital character constructs the Fermi surface, and the single band model that considers only the main band has often been adopted in the theoretical studies. Such single band or related models have provided us many understandings, but there still remain unresolved problems. One of the issues often discussed with controversy is the relationship between the curvature of the Fermi surface and the critical temperature (T_c). It is well known that even within the single-layered cuprates, there is significant difference of T_c, for example, the La compound with $T_c \simeq 40$K and the Hg compound with $T_c \simeq 90$K. From the band structure point of view, the La cuprate has relatively square shaped (diamond-like) Fermi surface, while the Hg material has a more round one. In fact, it has been recognized that low T_c materials have square shaped Fermi surface, while high T_c ones tend to have round Fermi surface[1, 2]. Although some phenomenological[3] or $t-J$ model[4, 5] studies describe such tendency, a number of Hubbard-type-model studies with realistic values of the on-site U have not succeeded in reproducing such a tendency[6]. For example, the dynamical cluster approximation studies that adopt a single band model [7], or a more realistic three band model[8] that considers p_σ orbitals show the opposite tendency.

To give insight into this long standing problem, we have constructed a $d_{x^2-y^2}+d_{z^2}$ two orbital model that considers all the orbitals that have e_g symmetry[9]. In this proceedings, we focus on the relationship between the conventional single orbital model and the two-orbital model, and explain the difference of the parameters that gives the material dependence.

2. $d_{x^2-y^2} + d_{z^2}$ two-orbital model

In Fig.1, we show the band dispersion of the two-orbital model constructed by exploiting maximally localized Wannier orbitals,[10] which are obtained from the first-principles calculation results[11]. The thickness of the lines represents the strength of the respective orbital character. In the La compound, a significant amount of d_{z^2} character is present in the main band around the wave vector $k = (\pi, 0)(0, \pi)$(denoted as N in La and M in Hg), while in the Hg compound such a mixture of the d_{z^2} component is absent[12, 13, 14, 15].
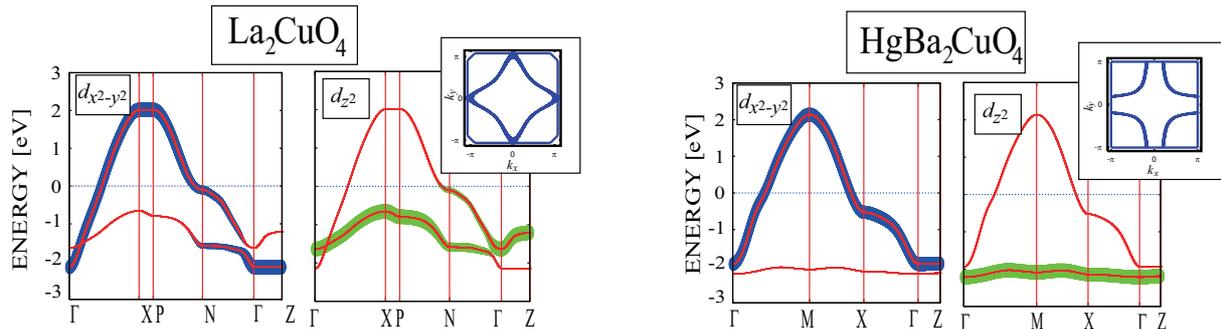
Figure 1. The band structure of the two orbital model for La_2CuO_4 (left) and $HgBa_2CuO_4$(right). The insets depict the Fermi surfaces (for the total band filling $n = 2.85$). The thickness of the lines represents the strength of the respective orbital character.

3. Comparison from the viewpoint of the hopping integrals

Let us now look into the hopping integrals of the models. In table I, the hopping integrals within the $d_{x^2-y^2}$ orbitals of the two orbital model are displayed for the La and Hg compounds. For comparison, we also show the values of the single band model obtained by the same method. Conventionally, the difference of the Fermi surface curvature is represented by the value of the second nearest neighbor hopping t_2 and the third nearest hopping t_3, where large $|t_2|$ and $|t_3|$ gives more rounded Fermi surface. This tendency is in fact seen in the table.

Table 1. Hopping integrals within the $d_{x^2-y^2}$ orbital for the single and two-orbital models, and $\Delta E \equiv E_{x^2-y^2} - E_{z^2}$.

	Single-orbital		Two-orbital	
	La	Hg	La	Hg
t_1[eV]	-0.444	-0.453	-0.471	-0.456
t_2[eV]	0.0284	0.0874	0.0932	0.0993
t_3[eV]	-0.0357	-0.0825	-0.0734	-0.0897
$(|t_2|+|t_3|)/|t_1|$	0.14	0.37	0.35	0.41
ΔE[eV]	-	-	0.91	2.19

If we turn to the hopping integrals of the two orbital model, the values shown in Table I is surprising in that the $d_{x^2-y^2}$ orbital has large $|t_2|$ and $|t_3|$ even for the La compound, just as in the Hg compound. Namely, the curvature of Fermi surface is not governed by the $d_{x^2-y^2}$ distant hoppings in the two orbital model that considers the d_{z^2} orbital explicitly, and another parameter plays an important role. In fact, the parameter is the on-site energy difference $\Delta E \equiv E_{x^2-y^2} - E_{z^2}$. In other words, ΔE in the two-orbital model determines the $(|t_2|+|t_3|)/|t_1|$ ratio in the effective single-orbital model. This can be understood as follows.
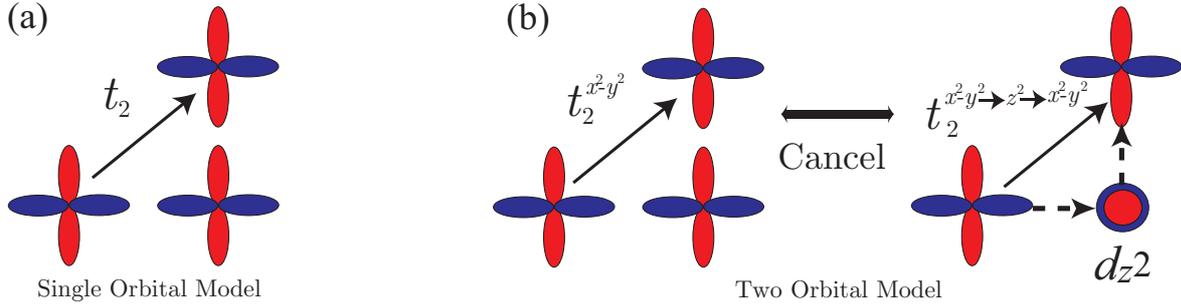
Figure 2. A schematic image of the $d_{x^2-y^2}$ -$d_{x^2-y^2}$ diagonal hopping within the single (a) and two-orbital(b) models. The left side of (b) shows the direct path, while the right side is the indirect path via the d_{z^2} orbital.

An electron can hop from a $d_{x^2-y^2}$ orbital to its second nearest neighbor mainly via the direct diagonal $d_{x^2-y^2}$-$d_{x^2-y^2}$ path or the indirect $d_{x^2-y^2} \to d_{z^2} \to d_{x^2-y^2}$ path. The latter can be considered as a second order perturbation process when the d_{z^2} orbital degrees of freedom is integrated out to obtain the effective single band model. As shown in table I, the value of the direct hopping is nearly equal between the La and the Hg compound, so that the material dependence comes from the indirect term.

The amplitude of the indirect term is generally large for smaller ΔE. In the La compound, the relatively small ΔE mainly enhances the indirect path $d_{x^2-y^2} \to d_{z^2} \to d_{x^2-y^2}$. From the first-principles result, the direct hopping and the indirect term are found to have the opposite sign, so the cancellation is strong when the amplitude of the indirect path is strong. As a result, the small ΔE for the La compound gives the small effective t_2 and t_3.

The above analysis shows that the curvature of the Fermi surface in the La cuprate is suppressed due to the large mixture between $d_{x^2-y^2}$ and d_{z^2} orbitals. Therefore, the strong d_{z^2} mixture in the Fermi surface around the wave vectors $(\pi, 0)/(0, \pi)$ is the origin of the weak curvature.

4. The relationship between Fermi surface and T_c

Now, we finally discuss how ΔE affects the many body properties, especially d-wave superconductivity. We consider a many body Hamiltonian that considers the on-site multiorbital interactions with realistic values. In Fig.3, we plot the d-wave eigenvalue of the linearized Eliashberg equation, where the Green's functions are obtained within the fluctuation exchange approximation[16, 17]. The eigenvalue reaches unity when $T = T_c$, so λ at a fixed temperature (here $T = 0.01$[eV]) can be used as a qualitative measure for T_c. In the figure, the points indicated by the arrows are the results of the model constructed from the experimentally determined lattice parameters[18, 19]. This shows that the Hg compound has higher T_c than the La compounds, so the result is consistent with the experiments. We also plot λ when ΔE is varied hypothetically in the La system. Note that $t_2^{d_{x^2-y^2}}$ and $t_3^{d_{x^2-y^2}}$ are fixed because in the first principles calculation they are not so much material dependent, as mentioned above. From Fig.3, it can be seen that λ increases monotonically with ΔE, and comes close to the value of the Hg result. From this result, we can say that ΔE governs both the shape of the Fermi surface (via the effective t_2 and t_3) and T_c.

5. Conclusion

In conclusion, we have shown that the degree of the orbital mixture controls the shape of the Fermi surface, and this gives the correlation between the Fermi surface shape and T_c. In this picture, the parameter that largely contributes to the material dependence is ΔE, the on-site level offset between the $d_{x^2-y^2}$ and d_{z^2} Wannier orbitals. This picture also explains the conventionally adopted material dependence of the second and third nearest neighbor hoppings in the single band model.
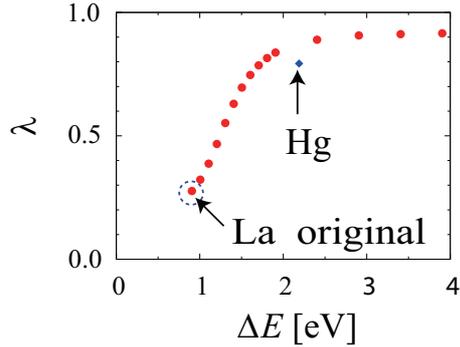
Figure 3. The eigenvalue λ of the Eliashberg equation for d-wave superconductivity plotted against $\Delta E \equiv E_{x^2-y^2} - E_{z^2}$. The points with arrows are the results obtained using the original lattice structure (determined experimentally). Circles are the results obtained by hypothetically varying ΔE in the La system.

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