Pressure effects and orbital characters in cuprate and carbon-based superconductors

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Abstract Pressure effect is overviewed for the cuprates and carbon-based superconductors, with an emphasis on how their orbital characters are modified by pressure. For the high-Tc cuprates, we start from an observation for ambient pressure that, on top of the main orbital $(dx^2−y^2)$, a hybridization with the second $(dz^2)$ orbital around the Fermi energy significantly affects $T_c$ in the spin-fluctuation mediated pairing, where the hybridization is dominated by material parameters. We can then show that applying pressures along a, b axes enhances $T_c$ while a c axis pressure suppresses $T_c$, where not only the $dz^2$ hybridization but also Cu(4s) hybridization exert an effect. For the multi-layer cuprates, inter-layer pair hopping is suggested to be important, which may contribute to pressure effect. Pressure effect is also interesting in a recently discovered aromatic family of superconductors (picene, etc). There, we have again multi-band systems, which in this case derive from different molecular orbitals. The Fermi surface is an intriguing composite of different pockets/sheets having different dimensionalities arising from anisotropic transfers between the molecular orbitals, and pressure effects should be an important probe of these.

Keywords Cuprate · carbon-based superconductors · pressure effect

1 Introduction

Pressure effect is one of the most interesting and direct probes and ways to control of the relation between electronic structure and superconductivity. One starting point can be an observation that, in the high-Tc cuprates at ambient pressure, there exists significant material dependence of $T_c$, which remained an important puzzle even within the single-layer family. A recent work by the present author and coworkers [1,2,3] has demonstrated, with a two-orbital model, that, while the usual wisdom is to consider the cuprate as a one-band $(dx^2−y^2)$ system, a hybridization with the second $(dz^2)$ band around the Fermi energy significantly affects $T_c$ in the spin-fluctuation mediated pairing. There, the larger the energy offset ($\Delta E$) between the two orbitals (i.e., smaller the band mixing), the higher the $T_c$. We can then follow this line of approach to show that applying pressures can significantly affect $T_c$, through the pressure dependence of the $dz^2$ hybridization. If we turn to the multi-layer cuprates, inter-layer pair hopping is suggested to be important [4], which may have an interesting effect on pressure dependence.

Pressure effect is also interesting for carbon-based superconductors, typically fullerene systems, where both of the electron-electron and electron-phonon interactions are strong. We can then discuss the $T_c$ dome against the interactions [5]. In a recently discovered aromatic family of superconductors (picene, etc) [6], we have again multi-band systems [1], which in these class of materials derive from multiple molecular orbitals. As a result the Fermi surface is an intriguing composite of different pockets/sheets having different dimensionalities arising from anisotropic transfers between the molecular orbitals, and pressure effects should be an important probe of these.
Fig. 1. Left top: The main components for each of the two Wannier orbitals in the cuprate. Left bottom: Level offsets $\Delta E$ of the two Wannier orbitals as derived from the d-level offset $\Delta E_d$ and the p-level offset $\Delta E_p$. Right: $\Delta E$ plotted against $\Delta E_d$ and $\Delta E_p$ for various single-layered cuprates. An oblique plane indicates a rough correlation between $\Delta E$ and $(\Delta E_p, \Delta E_d)$. After [2].

2 Cuprates

In the physics of high-\(T_c\) cuprates, optimizing their \(T_c\) remains a fundamental yet still open problem. Empirically, important parameters that control \(T_c\) have been identified to be chemical composition, structural parameters, the number of layers, etc, besides the doping concentration. Specifically, several key structural parameters have been suggested: the bond length between copper and in-plane oxygen [7,8], and the Cu-apical oxygen distance \((h_O)\) [9,10,11,12,13,14,2].

As mentioned in Introduction, Refs. [2] conclude that larger the level offset $\Delta E$ between the \(dx^2-y^2\) and \(dz^2\) Wannier orbitals, higher the \(T_c\). The key material parameters in the cuprates are: the apical oxygen height \((h_O)\) above the CuO\(_{2}\) plane and the separation \((d)\) between the CuO\(_{2}\) planes determine the level offset $\Delta E$ between the Cu(\(dx^2-y^2\)) and Cu(\(dz^2\)) Wannier orbitals through $\Delta E_p$ (offset between O(\(p_x\)) and O(\(p_y\)) and $\Delta E_d$ (offset between atomic Cu(\(dx^2-y^2\)) and Cu(\(dz^2\))). This captures the material dependence of $T_c$, covering a broad range of single-layer cuprates (La, Hg, Bi, and Tl). These are depicted in Fig. 1.

Pressure effect then is an ideal in situ way to probe the structure-dependence of $T_c$. So far we know for the cuprates that: (i) $T_c$ tends to be enhanced under hydrostatic pressure for pressure < 30 GPa [16,17], while (ii) uniaxial pressures produce anisotropic responses of $T_c$, namely, an \(a\)-axis compression generally raises $T_c$ while \(c\)-axis compression has an opposite effect [18,19,20]. Moreover, the magnitude of the pressure coefficient tends to be smaller for materials having higher $T_c$’s [18].

Basicall, the effects of uniaxial pressures come from the pressure-dependence of $\Delta E$ affected by the crystal field, as schematically shown in Fig. 2(a), where \(a\)-axis compression, which enhances the apex O height, raises $T_c$. More precisely, however, while the variation of $T_c$ under pressure is indeed affected by $\Delta E$, especially in the relatively low-$T_c$ cuprates, the higher-$T_c$ cuprates such as HgBa\(_2\)CuO\(_4\) (Hg1201) with large $\Delta E$ has a smaller $T_c$ variation against pressure. We can also show that one factor contributing the pressure effect is, on top of the $dx^2-y^2$ and $dz^2$ orbitals, Cu(\(4s\)) orbital can be relevant, whose level is raised with pressure, resulting in a better nested Fermi surface. This is shown in a model comprising all of the $dx^2-y^2$, $dz^2$, and $4s$ orbitals explicitly. This, along with the increase in the band width, is shown to cause a higher $T_c$ under pressure.

So we display the theoretical result, for La and Hg cuprates, for the dependence of the eigenvalue of the Eliashberg equation (a measure of $T_c$) on uniaxial pressures in Fig. 2(b) or on the hydrostatic pressure in Fig. 2(c). There we have decomposed the pressure effects into three contributions from the change of $\Delta E$ due to pressure, change of $W$, and change of the ratio, $r_{x^2-y^2} \equiv |t_2| + |t_4|/|t_1|$ of the further neighbour hoppings to the nearest neighbour one that determines the warping of the Fermi surface. For details see Ref. [3].
As for the contribution from $W$ a hydrostatic pressure increases $W$. However, in Fig. 2(c) we can notice that the increase in $W$ results in an enhancement of $\lambda$ in Hg, while the opposite occurs for La. If we vary $U$ with a fixed band width $W$, the absolute value of the renormalized Green’s function squared $|G|^2$ at $(k, \omega) = (\pi, 0, i\pi k_B T)$ monotonically decreases with $U$ as in Fig. 2 (for the Hg compound in this figure) due to an increased self-energy. On the other hand, the pairing interaction $V^\text{pair}$ increases with $U$ because the spin fluctuations develop monotonically. Consequently, $V^\text{pair}|G|^2$, a rough measure of the eigenvalue of the Eliashberg equation for $d$-wave superconductivity, exhibits a peak. If we repeat the calculation for the La cuprate, we can show that the Hg cuprate is located on the right of the peak, while the La cuprate on the left. This explains the opposite contributions for the $W$ effect.

Since the important units in the cuprates come in two flavours, CuO octahedron and CuO pyramid, the difference in the effect of the apex oxygen height between them is intriguing. Figure 3 shows the relationship between the apical oxygen height $h_O$ and $\Delta E_d$ (the energy difference between the $dx^2-y^2$ and the $dz^2$ atomic orbitals). We can see that, while $\Delta E_d$ is positively correlated with the apical oxygen height in both octahedral and pyramidal systems. More precisely, while the value of $\Delta E_d$ is significantly greater for pyramids, dependence on $h_O$ is smaller for pyramids with only one apical O per unit. This may be 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.[27]

The orbital effects can be unified into a picture in which higher $T_c$ can be achieved by the “distillation”[3] of the main (i.e., $dx^2-y^2$) band, namely, the higher the one-band character the better. This may also possibly help materials-design for higher $T_c$.

In the cuprate family, the record holder of the highest $T_c$ is still the multilayered cuprates that have $n$ CuO$_2$ planes in a unit cell, typically the Hg-based HgBa$_2$Ca$_{n-1}$Cu$_n$O$_{2n+2+\delta}$ (Hg-12$(n-1)n$), where $T_c$ increases for $n = 1 - 3$ and decreases for $n \geq 4$.[21] While there have been several theoretical studies for multilayered cuprates, Nishiguchi et al have recently examined various microscopic processes.[3] The interlayer one-electron hopping has little effects on the band structure, and

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Fig. 2 (a) A schematic effect of uniaxial compression along c or a axis. (b) For uniaxial compressions for La(Hg) cuprates, the eigenvalue $\lambda$ of the Eliashberg equation is plotted against $c/c_0$ (left panel) or $a/a_0$ (right). Triangles (circles) indicate the result for the La (Hg) cuprates. Arrows depict the contributions to the pressure effect from $\Delta E$, $W$, and $r_{x^2-y^2} \equiv (|t_2|+|t_3|)/|t_1|$, respectively. (c) For hydrostatic compression, $\lambda$ is plotted against the volume $V/V_0$. Arrows indicate various contributions as in (b). After[9].

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Fig. 3 $U$ dependence of the absolute value of the renormalized Green’s function squared $|G|^2$ at $(k, \omega) = (\pi, 0, i\pi k_B T)$, the effective pairing interaction $V^\text{pair}$ at $(q, \omega) = (\pi, \pi, 0)$ and the product $V^\text{pair}|G|^2$.[3].
3 Fullerene superconductor

There is a class of superconductors in which the electron-electron Coulomb repulsion and the electron-phonon coupling are strong at the same time. This most typically applies to alkali-doped fullerides. Although the pairing is an \( s \)-wave, \( T_c \) has recently been found to be dome-shaped and sits next to an antiferromagnetic phase in the temperature-pressure phase diagram\[22, 23-24\]. Thus an interplay of the electron-electron and electron-phonon interactions becomes an interesting problem. This may also apply to the aromatic superconductors in the next section.

We can tackle this problem with the Holstein-Hubbard model, which is a simple model that incorporates both electron-electron and electron-phonon interactions. The model is characterized by the energy \( \omega_0 \) of dispersionless (Einstein) phonons, the on-site Hubbard interaction \( U \) and the electron-phonon coupling \( g \). There is a body of works which investigates the competition between the two interactions in this model. The study of the one-dimensional case based on the density matrix renormalization group (DMRG) technique or quantum Monte Carlo analysis has revealed some general features\[25,26,27\] In the opposite limit of infinite spatial dimensions, \( D = \infty \), where the dynamical mean-field theory (DMFT) becomes exact, the effect of the competition between the two kinds of interactions have been studied \[31,32,33,34,28,29,30,35\]. Two-dimensional system is also studied\[36\].

However, an important question remains as follows: a usual wisdom in capturing the system is to regard it as having an effective interaction \( U_{\text{eff}} \equiv U - \lambda \), where \( \lambda \) is the static effective electron-electron interaction mediated by phonons. However, this is only valid in the antiadiabatic limit for \( \omega_0 \to \infty \) where the phonon-mediated interaction becomes non-retarded, so that the real question is to what extent this approximation remains valid when we vary \( U \) and/or \( \omega_0 \). In other words how can we go beyond Migdal theorem\[37,38\] or the MacMillan equation\[39\]. In the fullerene superconductor, \( U, \lambda, \) and \( \omega_0 \) are all comparable to the electronic bandwidth \( W \), so the question becomes real.

We have studied the Holstein-Hubbard model, at half-filling, with the dynamical mean-field theory (DMFT), with a continuous-time quantum Monte Carlo impurity solver, which enables us to work in the regime where \( U, \lambda, \) and \( \omega_0 \) are comparable to the bandwidth\[5\]. We show in Fig.\[6\] that the phonon-induced retardation or the Coulomb repulsion have the effect of significantly decreasing and shifting the \( T_c \) dome against \( U_{\text{eff}} \). In order to understand and interpret the observed behavior we can introduce an effective static model derived...
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from a Lang-Firsov transformation. As for the pressure effects, the quantities \( \omega_0 \), \( U \) and \( \lambda \) should be affected by pressure, which is an interesting future problem to elaborate. In real fullerides there is also a complication coming from the Jahn-Teller degree of freedom \[23\].

\[ \omega_0 = -\left( U - \frac{2g^2}{\omega_0} \right) \]

\[ = \frac{2g^2}{\omega_0} \]

Fig. 6 \( T_C \) against \( -U_{\text{eff}} \) for various values of the phonon energy \( \omega_0 \) with the Hubbard \( U = 0 \) (top panel), and for various values of \( U \) with \( \omega_0 = 6.0 \) (bottom), with the hopping integral \( t \) as the unit of energy. The lines connecting symbols are guides for the eye, while the black curve in each panel indicates \( T_c \) in the attractive Hubbard model. After \[4\].

4 Aromatic superconductor

Let us move on to the pressure effects on the aromatic hydrocarbon superconductors, especially picene superconductors \[6\]. Potassium (K) doped picene has been attracting much attention after the experimental report of superconductivity with transition temperature \( T_c=18 \) K, which is very high as an organic material. Furthermore, there is a very recent report for a striking pressure effect, where \( T_c \) is raised to about 30 K by applying pressure \( \sim 1 \) GPa \[40\]. At present, neither the pressure effect nor is even the superconducting mechanism itself well understood theoretically. If the picene superconductor obeys conventional BCS theory, the density of states (DOS) at the Fermi energy will be an important factor determining \( T_c \). The positive pressure dependence of \( T_c \) seems to contradict with a conventional mechanism, since applying a pressure is likely to decrease DOS. Specifically, we have to carefully examine how the pressure affects the electronic structure, since the theoretical band structure of picene superconductors, being multi-orbital systems, is rather complex \[41\]. This is important, since, if an unconventional mechanism, such as the electron-electron correlation, is at work, \( T_c \) will be sensitive to the Fermi surface structure. Thus, in the following, we show some results on the electronic structure under pressure.

Here electronic and crystalline structures of K-doped picene crystals are investigated based on the density functional theory (DFT) with local density approximation (LDA) adopted for exchange-correlation functionals. The actual calculations are performed using Quantum Espresso package \[42\]. We concentrate on the case in which three K atoms are doped per a picene molecule, for which the superconductivity is reported. At ambient pressure, the lattice constants are fixed to the most updated experimental values \[40\] in the present study, and the internal coordinates are relaxed by minimizing calculated forces on each atom. For the pressure effect, the calculation is done for an “artificial” pressure introduced as decreased lattice parameters, as a first step towards understanding of pressure effects in picene superconductors. Thus the pressure effect is simulated by repeating the calculation with reduced lattice parameters. For simplicity, lattice constants in three directions are scaled by a common scaling factor, which means that the anisotropy in the bulk modulus is neglected. We carried out calculations with scaling factors 100% (experimental lattice constants at ambient pressure), down to 95%. Ideally, a fully theoretical method is desirable, where the lattice constants are relaxed within a theoretical structural optimization under pressure. However, precise prediction of the lattice constants within DFT is difficult for the present target material. There are several reasons for this. A theoretical factor is that we should have, especially for the undoped molecular crystals \[43\], calculation with the van der Waals interaction taken into account, but the method is still under improvements. Once the lattice constants are given, the difference between LDA and generalized-gradient approximation (GGA) is less significant for internal coordinates. A second, experimental factor here is that there is no definite experimental lattice constants, which is mainly because the superconducting fraction is very tiny (\( \sim 1 \) per cent), even at ambient pressure. These are why we have opted for the artificial treatment of
pressure effects, and leave more sophisticated works as future problems.

Even when the lattice constants are fixed and only internal coordinates are relaxed, calculation is still hard, since the organic system has many metastable structures. For example, there are several possible ways for putting the doped K atoms (three per molecule) into the molecular crystal. Here we focus on, following the previous theoretical work by Kosugi et al.\footnote{Kosugi et al.}, two kinds of K atom arrangements, which we call K₃Picene and K₂K₁Picene structures, as most probable candidates. In K₃Picene, all the K atoms are doped within the layer of picene molecules arranged in a herringbone pattern. On the other hand, K₂K₁Picene has one K atom resides in the interlayer region while the other two in the intralayer region. In practice, we start internal coordinate relaxation from the K₃- or K₂K₁-structure for each set of lattice constants.

Fig. 7(a) shows the calculated crystal structures along with the two Wannier functions (basically the LUMO and LUMO+1 of the picene molecule) for the conduction band (which comprises four bands) at ambient pressure. The ambient pressure result, with the experimentally updated lattice constants, shows that K₃- and K₂K₁ continue to be the (meta)stable structures. If we turn to Fig. 7(b), which displays the change of the structure when the lattice constants are reduced to 95%, we can see that the main features of K₃- and K₂K₁-structures are respectively retained even with the shrunk lattice. However, a closer examination reveals that there are significant differences in the dopant positions and the relative angle between two picene molecules.

The calculated band structures are plotted in Fig. 8. We first note that the obtained band structures are different from the previous theoretical work\footnote{Kosugi et al.} even at ambient pressure. This naturally comes from the adaptation in the present calculation of the updated experimental lattice constants\cite{Aoki2020}. Basically the c-axis is elongated in the update, so that the band structure becomes more two-dimensional and simpler compared with the previous calculation. If we turn to the pressure effect, a notable feature in Fig. 8 is that the band structure changes in a nonmonotonic manner against pressure, especially for K₃-structure. This comes from the dopant positions and relative angle between molecules that change nonmonotonically against pressure, where the band structure is sensitive to the change. Although a discussion of Tc would require a more sophisticated treatment of the pressure, a message here is that a decrease in the lattice constants can exert an effect beyond a simple expansion of band width.

This fact is highlighted in the Fermi surfaces in Fig. 9 which plots the change in the Fermi surface as...
the lattice constants are reduced down to 96%. With the updated experimental lattice constants the Fermi surface at ambient pressure is remarkably simpler. We have however the sensitivity to the dopant positions: Namely, K₃Picene has a composite of a two-dimensional cylinder and a pair of one-dimensional sheets, while K₂K₁Picene has two pairs of more or less one-dimensional sheets. For both K₃- and K₂K₁-structures, the pressure induces some complexity in the Fermi surface structures. Remarkably, we can see that the topology of the Fermi surface changes, i.e., a Lifshitz transition occurs as the lattice is shrunk, for both of K₃- and K₂K₁-structures. It is an interesting future issue to investigate the relation between Tc and the dopant arrangement, especially the Lifshitz transition.

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