Effective five band analysis on $T_c$ vs. lattice structure correlation in iron pnictides

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Abstract. In the present study, we investigate the effect of the lattice structure in the iron pnictides within the spin fluctuation pairing theory based on the effective five band models of several hypothetical lattice structures of LaFeAsO. We show that the presence and absence of Fermi surface pockets is sensitive to the Fe-As-Fe bond angle due to the multiorbital nature of the system, which is reflected to the nodeless/nodal form of the superconducting gap and $T_c$. Superconductivity is maximized within the maximum hole Fermi surface multiplicity regime where the arsenic atoms form a regular tetrahedron. Superconductivity has an overall tendency of increasing upon increasing Fe-As bond length. We provide a guideline of higher $T_c$ from the lattice structure point of view.

1. Introduction

One of the striking features of the iron-based superconductors is its lattice structure dependence of the superconductivity. For instance, Lee et al. have shown that $T_c$ systematically varies with the Fe-Pn-Fe (Pn=pnictogen) bond angle, and takes its maximum around 109 degrees, at which the pnictogen atoms form a regular tetrahedron (“Lee’s plot”)[1]. Also, although many of the experiments on the arsenides gives evidence for fully open superconducting gap, some experiments for the phosphides indicates presence of nodes in the gap[2]. Theoretically, we have previously explained this lattice structure effect within a spin fluctuation mediated pairing theory on a five orbital model, and pointed out that superconductivity is strongly affected by the Fermi surface (FS) around the wave vector $(\pi, \pi)$ in the unfolded Brillouin zone [3] which exists at high pnictogen height $h_{Pn}$ measured from the iron plane. However, it is becoming clearer that materials having very large $h_{Pn}$ ($\geq 1.5$ Å) do not have high $T_c$[4]. In this context, it is interesting to focus on a $T_c = 28.3$K[5] superconductor $\text{Ca}_4\text{Al}_2\text{O}_6\text{Fe}_2\text{As}_2$, which is a variation of the materials having perovskite block layers (21311 systems)[6]. This material has very large $h_{Pn}$ ($\geq 1.5$ Å) and consequently a very small bond angle ($\sim 102$ degrees). Such a high pnictogen position should give strong spin fluctuations, and it seems difficult to understand the low $T_c$. In this context, a recent band structure calculation of $\text{Ca}_4\text{Al}_2\text{O}_6\text{Fe}_2\text{As}_2$ has found an interesting feature; one of the hole FSs around $(0,0)$ is missing, resulting in two hole FSs[7]. This is found to be due to the very small bond angle.

Given this background, we have studied the condition for optimizing superconductivity in the iron pnictides, varying hypothetically the lattice structure of LaFeAsO varying the bond angle...
Figure 1. The band structure of hypothetical lattice structures of LaFeAsO with (a) varying the Fe-As-Fe bond angle while fixing the Fe-As bond length. (b) The bond angle range where three hole FSs coexist is shown for LaFeAsO and Ca$_4$Al$_2$O$_6$Fe$_2$As$_2$.

$\alpha$ from 95 deg. to 120 deg[8]. Here we focus not only on $T_c$, but also on the lattice structure dependence of the superconducting gap.

2. Band structure and FS against bond angle/length

We first obtain the band structure of hypothetical lattice structures of LaFeAsO using the Quantum-ESPRESSO package[9], and construct five band models from maximally localized Wannier functions[10]. We fix the bond length at its original length[11] and hypothetically vary the bond angle $\alpha$(Fig.1(a)) as has been done for Ca$_4$Al$_2$O$_6$Fe$_2$As$_2$ by Miyake et al[7]. The FS is obtained for the band filling (=number of electrons per site) of $n=6.1$. When the bond angle is large, two hole FSs, $\alpha_1$ and $\alpha_2$ are present around the wave vector (0,0). As $\alpha$ decreases, the $\gamma$ FS appears around (\pi,\pi), and we now have three hole FSs. This is what has been noticed as an effect of increasing the pnictogen height [3, 12, 13]. As we decrease $\alpha$ even further, the $\alpha_1$ FS disappears, and again there are only two hole FSs but in this case one around (0,0) and another around (\pi,\pi). So the tendency found in Ca$_4$Al$_2$O$_6$Fe$_2$As$_2$ holds also for LaFeAsO. However, the range of the bond angle in which there are three hole FSs (three hole FS zone in Fig.1(c)) turns out to be much larger for LaFeAsO than for Ca$_4$Al$_2$O$_6$Fe$_2$As$_2$. We find that the three hole FS zone tends to be small for materials with large c-axis length. Another point that should be mentioned is that the total band width is almost unchanged as the bond angle is varied.

In the above, we varied the bond angle while fixing the bond length, so we can also do the opposite, namely, fix the angle and vary the length. We calculate the band structure where we fix $\alpha = 108$ and vary the Fe-As bond length (not shown). The band width is reduced upon increasing the bond length as expected, but interestingly, the FS is barely affected. In fact, we find that multiplying the bands for each bond length by certain overall factors gives nearly the identical band structures, indicating only the band width, but not the shape, is affected by the bond length, thereby barely affecting the FSs.

3. Superconductivity and spin fluctuations

Based on the obtained tightbinding model, we construct a many body Hamiltonian by considering the standard multiorbital interactions (intraorbital and interorbital repulsion, Hund’s coupling, and the pair hopping interaction). We apply fluctuation-exchange approximation(FLEX)[14], and obtain the spin susceptibility, which is plugged into the linearized Eliashberg equation. Since the three dimensionality is not strong in LaFeAsO, we take a two
Figure 2. (a) (Top) the Eliashberg equation eigenvalue for $s\pm$-wave pairing against the bond angle for temperatures $T = 0.005$ and $0.01\text{eV}$ (dashed). The interaction reduction factor is $f = 0.6$. (b) The eigenvalue of the Eliashberg equation against the bond length. $T = 0.005\text{eV}$ and $f = 0.5$. (c) A schematic $T_c$ diagram in the bond angle and length space.

Figure 3. The $s$-wave gap functions for forth band from top in the band representation for the five-band model of hypothetical structure of LaFeAsO with $n = 6.1$. Solid lines represent the Fermi surface, and dashed lines the nodes in the gap.

dimensional model where we neglect the out-of-plane hopping integrals, and take $32 \times 32$ $k$-point meshes and 4096 Matsubara frequencies. As for the electron-electron interaction values, we adopt the orbital-dependent interactions as obtained from first principles calculation in ref.\cite{15} for LaFeAsO, but multiply all of them by a constant reducing factor $f$. The reason for introducing this factor is the FLEX for models obtained from LDA calculations tend to overestimate the effect of the self-energy because LDA already partially takes into account the effect of the self-energy in the exchange-correlation functional as has been studied in refs.\cite{16, 17, 18}.

In Fig.2(a), we plot the eigenvalue of the Eliashberg equation $\lambda$ for the $s\pm$-wave superconductivity as functions of the bond angle while fixing the bond length at its original value. In the large angle regime, the eigenvalue of the Eliashberg equation remains relatively small. As the angle is decreased, the $\gamma$ FS around $(\pi, \pi)$ becomes effective and the eigenvalue becomes large. If we decrease the angle even further, superconductivity tends to be suppressed, although the variation of the eigenvalue is not monotonic. Thus, the superconductivity is optimized around 110 degrees, which is in agreement with the Lee’s plot\cite{1}. The fact that superconductivity is optimized for maximum FS multiplicity can be considered as natural since larger number of FSs gives rise to larger number of pair scattering channels. We note here that due to the quasi-two-dimensionality, the density of states is not affected by the size of the FS, so two small FSs is more favorable than one large FS regarding the number of pair scattering channels.

In Fig.3, we show the bond angle dependence of the superconducting gap. At $\alpha = 120$ degrees, there are nodes in the electron Fermi surface, which is expected from previous studies for systems with low pnictogen height \cite{3, 19, 20, 21}. This is because the $\gamma$ Fermi surface around $(\pi, \pi)$ in the unfolded Brillouin zone is absent. As the bond angle degrees, the nodes on the electron Fermi surface go away, and finally at $\alpha = 100$ degrees, where the $\gamma$ Fermi surface is...
robust, the gap is fully open on the Fermi surface. Therefore, we expect a completely open, nearly isotropic superconducting gap for Ca$_4$Al$_2$O$_6$Fe$_2$As$_2$, although $T_c$ is not so high because of the absence of the $\alpha_1$ Fermi surface.

Let us now turn to the bond length dependence. In Fig.2(b), we plot the eigenvalue of the Eliashberg equation as a function of the bond length. The eigenvalue monotonically increases with the increase of the bond length$^{[22]}$. Since the change in the FSs is small here, the enhancement of the superconductivity is mainly due to the increase of the density of states originating from the narrowing of the band width.

In Fig.2(c), we present a schematic $T_c$ diagram in the bond angle and bond length space. High $T_c$ is obtained when the bond angle is around 110 deg. (the regular tetrahedron angle) so that there are (nearly) three hole FSs and also when the bond length is large so that the band width is narrow.

4. Conclusion

To summarize, we have studied the condition for optimizing superconductivity in the iron pnictides from the lattice structure point of view. As found in Ca$_4$Al$_2$O$_6$Fe$_2$As$_2$$^{[7]}$, the band structure of the hypothetical lattice structure of LaFeAsO also exhibits a disappearance of one of the hole FSs in the small bond angle regime, and therefore, the hole FS multiplicity is maximized around the bond angle regime where the arsenic atoms form a regular tetrahedron. Superconductivity is optimized within this three hole FS regime, which is consistent with experimental observations. The present study provides a natural explanation as to why the regular tetrahedron bond angle has a significant meaning for superconductivity. Combining also the effect of varying the Fe-As bond length, we have provided a schematic $T_c$ diagram, which may give a guiding principle for obtaining higher $T_c$ materials. We acknowledge Takashi Miyake and Kiyoyuki Terakura for motivating us to start the present study. The numerical calculations were in part performed at the Supercomputer Center, ISSP, University of Tokyo. This work was supported by Grants-in-Aid from MEXT, Japan. H.U. acknowledges support from JSPS.

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[22] This monotonic enhancement of $\lambda$ is restricted to the regime of $f$ where the spin fluctuations develop at $(\pi, 0)$. When large $f$ is taken, the spin fluctuation wave vector changes from $(\pi, 0)$ to $(\pi, \pi)$ as the bond length is increased, and in that case $\lambda$ takes a maximum value at a certain bond length.