S4 Symmetric Microscopic Model for Iron-Based Superconductors

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Although iron-based superconductors are multi-orbital systems with complicated band structures, we demonstrate that the low energy physics which is responsible for high-Tc superconductivity is essentially governed by one effective Hamiltonian with two almost decoupled orbitals near half filling. This underlying electronic structure is protected by the S4 symmetry. With repulsive or strong next nearest neighbor antiferromagnetic exchange interactions, each single-orbital effective Hamiltonian results in a robust A1g s-wave pairing which can be exactly mapped to the d-wave pairing observed in cuprates. The classification of the superconducting (SC) states according to the S4 symmetry leads to a natural prediction of the existence of two different phases named A and B phases. In the B phase, the superconducting order has an overall sign change along c-axis between the top and bottom As (Se) planes in a single Fe-(As)Se trilayer structure, which is an analogy of the sign change under the 90° degree rotation in the d-wave SC state of cuprates. Our derivation provides a unified understanding of iron-pnictides and iron-chalcogenides, and suggests that cuprates and iron-based superconductors share identical high-Tc superconducting mechanism.

I. INTRODUCTION

Since the discovery of iron-based superconductors1–4, there has been considerable controversy over the choice of the appropriate microscopic Hamiltonian5–6. The major reason behind such a controversy is the complicated multi-d-orbital electronic structure of the materials. Although the electronic structure has been modeled by using different numbers of orbitals, ranging from minimum two orbitals4, three orbitals5, to all five d orbitals8,10, a general perception has been that any microscopic model composed of less than all five d-orbitals and ten bands is insufficient8,10. Such a perception has blocked the path to understand the superconducting mechanism because of the difficulty in identifying the key physics responsible for high Tc. Realistically, in a model with five orbitals, it is very difficult for any theoretical calculation to make meaningful predictions in a controllable manner.

Iron-based superconductors include two families, iron-pnictides1–3 and iron-chalcogenides4. They share many intriguing common properties. They both have the highest Tc’s around 50K9,11,12. The superconducting gaps are close to isotropic around Fermi surfaces14–19 and the ratio between the gap and Tc, 2Δ/Tc, are much larger than the BCS ratio, 3.52, in both families. However, the electronic structures in the two families, in particular, the Fermi surface topologies, are quite different in the materials reaching high Tc. The hole pockets are absent in iron-chalcogenides but present in iron-pnictides14,15. The presence of the hole pockets has been a necessity for superconductivity in the majority of studies and models which deeply depend on the properties of Fermi surfaces. Therefore, the absence of the hole pockets in iron-chalcogenides causes a strong debate over whether both families belong to the same category that shares a common superconducting mechanism. Without a clear microscopic picture of the underlying electronic structure, such a debate can not be settled.

Observed by angle-resolved photoemission microscopy (ARPES), a very intriguing property in the SC states of iron-pnictides is that the SC gaps on different Fermi surfaces are nearly proportional to a simple form factor cosk_x cosk_y in reciprocal space. This form factor has been observed in both 12217,20–22 and 11123,24 families of iron-pnictides. Just like the d-wave form factor cosk_x – cosk_y in cuprates, such a form factor indicates that the pairing between two next nearest neighbour iron sites in real space dominates. In a multi orbital model, many theoretical calculations based on weak coupling approaches have shown that the gap functions are very sensitive to detailed band structures and vary significantly when the doping changes6,25–29. The robustness of the form factor has been argued to favor strong coupling approaches which emphasize electron-electron correlation or the effective next nearest neighbour (NNN) antiferromagnetic (AF) exchange coupling J′29,30 as a primary source of the pairing force. However, realistically, it is very difficult to imagine such a local exchange interaction remains identical between all d-orbital electrons if a multi d-orbital model is considered.

In this paper, we demonstrate that the underlying electronic structure in iron-based superconductors, which is responsible for superconductivity at low energy, is essentially governed by a two orbital model obeying the S4 symmetry. The two orbital model includes two nearly decoupled single-orbital parts that can be mapped to each other under the S4 transformation. This electronic structure stems from the fact that the dynamics of dxz and dyz orbitals are divided into two weakly coupled groups that are separately coupled to the top and bottom As (Se) planes in a in a single Fe–(As)Se trilayer structure. The two groups can thus be treated as a S4 iso-spin.

The underlying electronic structure becomes transparent after performing a gauge mapping in the five orbital model30. The gauge mapping also reveals the equivalence between the A1g s-wave pairing and the d-wave pairing.
After the gauge mapping, the band structure for each $S_4$ iso-spin component is characterized by Fermi surfaces located around the anti $d$-wave nodal points in Brillouin zone, corresponding to the sublattice periodicity of the bipartite iron square lattice as shown in Fig.1(a). In the presence of an AF exchange coupling $J_2$ or an effective on-site Hubbard interaction, the $d$-wave pairing defined in the sublattices can be argued to be favored, just like the case in cuprates. The $d$-wave pairing symmetry maps reversely to a $A_{1g}$ $s$-wave pairing in the original gauge setting. These results provide a unified microscopic understanding of iron-pnictides and iron-chalcogenides and explain why an $s$-wave SC state without the sign change on Fermi surfaces in iron chalcogenides driven by repulsive interaction can be so robust. More intriguingly, since the different gauge settings do not alter any physical measurements, the results suggest that in the $A_{1g}$ $s$-wave state, for each $S_4$ iso-spin component, there is a hidden sign change between the top As(Se) and the bottom As(Se) planes along c-axis.

The $S_4$ symmetry adds a new symmetry classification to the SC states. For example, even in the $A_{1g}$ $s$-wave pairing state, there are two different phases called $A$ and $B$ phases, with respect to the $S_4$ symmetry. In the $A$ phase, the relative SC phase between the two $S_4$ iso-spin components is zero while in the $B$ phase, it is $\pi$. Therefore, there is an overall $\pi$ phase shift between the top As(Se) and the bottom As(Se) planes in the $B$ phase along the c-axis. Such a sign change should be detectable experimentally. This property makes iron-based superconductors useful in many SC device applications. An experimental setup, similar to those for determining superconductors in a different gauge setting, is proposed to detect the $\pi$ phase shift. The detection of the sign change will strongly support that cuprates and iron-based superconductors share identical microscopic superconducting mechanism.

The paper is organized in the following way. In Section II, we perform a gauge mapping and discuss the emergence of the underlying electronic structure. In Section III, we show that the underlying electronic structure can be constructed by a two orbital model obeying the $S_4$ symmetry and discuss many general properties in the model. In Section IV, we discuss the classification of the SC states under the $S_4$ symmetry and propose a measurement to detect the $\pi$ phase shift along c-axis between the top and bottom As(se) planes. In Section V, we discuss the analogy between iron-based superconductors and cuprates.

II. GAUGE MAPPING AND THE EQUIVALENCE OF S-WAVE AND D-WAVE PAIRING

Gauge Mapping: We start to ask whether there is an unidentified important electronic structure in iron-based superconductors in a different gauge setting. Giving a translational invariant Hamiltonian that describes the electronic band structure of a Fe square lattice,

$$\hat{H}_0 = \sum_{ij,\alpha\beta,\sigma} t_{ij,\alpha\beta} \hat{f}_{i\alpha,\sigma} \hat{f}_{j\beta,\sigma}^\dagger,$$  \hspace{1cm} (1)

where $i,j$ label Fe sites, $\alpha,\beta$ label orbitals and $\sigma$ labels spin. We consider the following gauge transformation. As shown in Fig.1(a,b), we group four neighbouring iron sites to form a super site and mark half super sites by red color. The gauge transformation, $\hat{U}$, adds a minus sign to all Fermionic operators $\hat{f}_{i\alpha,\sigma}$ at every site $i$ marked by red color. After the transformation, the Hamiltonian becomes

$$\hat{H}'_0 = \hat{U}^+ \hat{H}_0 \hat{U}.$$  \hspace{1cm} (2)

The gauge mapping operator $\hat{U}$ is an unitary operator so that the eigenvalues of $\hat{H}_0$ are not changed after the gauge transformation. It is also important to notice that the mapping does not change standard interaction terms, such as conventional electron-electron interactions and spin-spin exchange couplings. Namely, for a general Hamiltonian including interaction terms $\hat{H}_I$, under the mapping,

$$\hat{H} = \hat{H}_0 + \hat{H}_I \rightarrow \hat{H}' = \hat{U}^+ \hat{H} \hat{U} = \hat{H}_0' + \hat{H}_I,'$$  \hspace{1cm} (3)

It is also easy to see that every unit cell of the lattice in the new gauge setting has four iron sites. The original translational invariance of a Fe-As(Se) layer has two Fe sites per unit cell. As we will show in the following section, the doubling of the unit cell matches the
true hidden unit cell in the electronic structure when the orbital degree of freedom is considered. This is the fundamental reason that the new gauge happens to reveal the underlying electronic structure.

**Equivalence of s-wave and d-wave pairing:** The gauge mapping has another important property. As shown in Fig. 1(c,d), this transformation maps the $A_{1g}$ s-wave $\cos(k_x)\cos(k_y)$ pairing symmetry in the original Fe lattice to a familiar d-wave $\cos k'_x - \cos k'_y$ pairing symmetry defined in the two sublattices, where $(k_x, k_y)$ and $(k'_x, k'_y)$ label momentum in Brillouin zones of the origin lattice and sublattice respectively. A similar mapping has been discussed in the study of a two-orbital iron ladder model\textsuperscript{34} to address the equivalence of s-wave and d-wave pairing symmetry in one dimension.

In an earlier paper\textsuperscript{12}, one of us and his collaborator suggested a phenomenological necessity for achieving high $T_c$ and selecting pairing symmetries: when the pairing is driven by a local AF exchange coupling, the pairing form factor has to match the Fermi surface topology in reciprocal space. If this rule is valid and the iron-based superconductors are in the $A_{1g}$ s-wave state, we expect that the Fermi surfaces after the gauge mapping should be located in the d-wave anti-nodal points in the sublattice Brillouin zone.

**Band structures after gauge mapping:** There have been various tight binding models to represent the band structure of $\hat{H}_0$. In Fig. 2 we plot the band structure of $\hat{H}_0$ and the corresponding $\hat{H}'_0$ for two different models: a maximum five-orbital model for iron-pnictides\textsuperscript{34}, and a three-orbital model constructed for electron-overdoped iron-chalcogenides\textsuperscript{31}.

As shown in Fig. 2, although there are subtle differences among the band structures of $\hat{H}'_0$, striking common features are revealed for both models. First, exactly as expected, all Fermi surfaces after the gauge mapping are relocated around $X'$, the anti-nodal points in a standard d-wave superconducting state in the sublattice Brillouin zone. This is remarkable because a robust d-wave superconducting state can be argued to be favored in such a Fermi surface topology in the presence of repulsive interaction or nearest neighbour (NN) AF coupling in the sublattice. If we reverse the original gauge, the Hamiltonian must have a robust s-wave pairing symmetry. Therefore, an equivalence between the $A_{1g}$ s-wave and the d-wave pairing is clearly established by the gauge mapping.

Second, the bands previously located at the different places on the Fermi surface are magically linked in the new gauge setting. In particular, the two bands that contribute to electron pockets are nearly degenerate and in the five orbital model, the bands that contribute to hole pockets are remarkably connected to them. Considering the fact that the unit cell has four iron sites in the new gauge setting, this unexpected connections lead us to believe that in the original gauge, there should be just two orbitals which form bands that make connections from lower energy bands to higher energy ones and determine Fermi surfaces. Moreover, the two orbitals should form two groups which provide two nearly degenerate band structures. Finally, since the mapping does not change electron density, Fig. 2 reveals the doping level in each structure should be close to half filling.

In summary, the gauge mapping reveals that the low energy physics is controlled by a two orbital model that produces two nearly degenerated bands.

**III. THE CONSTRUCTION OF A TWO-ORBITAL MODEL WITH THE $S_4$ SYMMETRY**

With above observations, we move to construct an effective two orbital model to capture the underlying electronic structure revealed by the gauge mapping.

**Physical picture:** Our construction is guided by the following several facts. First, the d-orbitals that form the bands near the Fermi surfaces are strongly hybridized with the p-orbitals of As(Se). Since the $d_{x^2-y^2}$ and $d_{y'z}$ have the largest overlap with the $p_x$ and $p_y'$ orbitals, it is natural for us to use $d_{x^2-y^2}$ and $d_{y'z}$ to construct the model. Second, in the previous construction of a two-orbital model, the $C_{4v}$ symmetry was used. The $C_{4v}$ symmetry is not a correct symmetry if the hopping parameters are generated through the p-orbitals of As(Se). Considering the As(Se) environment, a correct symmetry for the d-orbitals at the iron-sites is the $S_4$ symmetry group. Third, there are two As(Se) planes which are separated in space along c-axis. Since there is little coupling between the p orbitals of the two planes and the hopings through the p-orbitals are expected to dominate over the direct exchange hopings between the d-orbitals themselves, the two orbital model essentially could be decoupled into two weakly coupled one orbital models. Finally, the model should have a translational invariance with respect to the As(Se) plane.
FIG. 3. A sketch of the $d_{x^2-y^2}$ and $d_{y^2}$ orbitals, their orientations and their coupling into the two As(Se) layers. The hopping parameters are indicated: the nearest neighbor hopping is marked by $t_{1s,1y}$, the next nearest neighbor hoppings are $t_2$ and $t'_2$ due to the broken symmetry along two different diagonal directions, the third NN hopping is marked by $t_{3x,3y}$. The coupling between two layers is marked by the nearest neighbor hopping $t_c$.

With above guidelines, it is very natural for us to divide the two $d$-orbitals into two groups as shown in Fig. 3. One group includes the $d_{x^2-y^2}$ in the A sublattice and the $d_{y^2}$ in the B sublattice, and the other includes the $d_{x^2-y^2}$ in the B sublattice and the $d_{y^2}$ in the A sublattice, where A and B label the two sublattices of the iron square lattice as shown in Fig. 2(a). The first group strongly couples to the p-orbitals in the up As(Se) layer and the second group couples to those in the bottom As(Se) layer. We denote $\hat{c}_{i\sigma}$ and $\hat{d}_{i\sigma}$ as Fermionic operators for the two groups respectively at each iron site.

$S_4$ symmetry and the two-orbital model: Without turning on couplings between the two groups, we seek a general tight binding model to describe the band structure based on the $S_4$ symmetry. The $S_4$ transformation maps $\hat{c}_{i\sigma}$ to $\hat{d}_{i\sigma}$. If we define the corresponding operators in momentum space as $\hat{c}_{k\sigma}$ and $\hat{d}_{k\sigma}$, the $S_4$ transformation takes

$$
\begin{pmatrix}
\hat{c}_{k\sigma} \\
\hat{d}_{k\sigma}
\end{pmatrix} \rightarrow 
\begin{pmatrix}
-\hat{d}_{k'+Q\sigma} \\
\hat{c}_{k'+Q\sigma}
\end{pmatrix},
$$  

where $k'=(k_y,-k_x)$ and $Q=(\pi,\pi)$ for given $k=(k_x,k_y)$.

Now, we consider a tight binding model for the first group. Here we limit the hopping parameters up to the third NN (TNN). As illustrated in Fig. 3 the tight binding model can be approximated by including NN hoppings, $t_{1s}$, $t_{1y}$, NNN hoppings, $t_2$, $t'_2$, and TNN hoppings, $t_{3x}$ and $t_{3y}$. The longer range hoppings can be included if needed. For convenience, we can define $t_{1s}=(t_{1s}+t_{1y})/2$, $t_{1d}=(t_{1s}-t_{1y})/2$, $t_{2s}=(t_2+t'_2)/2$ and $t_{2d}=(t_2-t'_2)/2$, $t_{3s}=(t_{3s}+t_{3y})/2$ and $t_{3d}=(t_{3s}-t_{3y})/2$, where the labels, s and d, indicate s-wave (hopping parameter is symmetric under the 90° degree rotation) and d-wave (hopping parameter changes sign under the 90° degree rotation) type hoppings respectively. A general tight binding model can be written as

$$
\hat{H}_{0,\text{one}} = \sum_{k,\sigma} \left[ 2t_{1s}(\cos k_x + \cos k_y) - \frac{\mu}{2} + t_{1d}(\cos k_x - \cos k_y) \right] \hat{c}_{k\sigma}^+ \hat{c}_{k\sigma} + 4[t_{2s}\cos k_x \cos k_y \hat{c}_{k\sigma}^+ \hat{c}_{k\sigma} + t_{2d}\sin k_x \sin k_y \hat{c}_{k\sigma}^+ \hat{c}_{k\sigma} + \cdots]
$$

$$
\hat{H}_{0,\text{two}} = \sum_{k,\sigma} \left[ 4t_{2s}\cos k_x \cos k_y - \mu \right] \left[ \hat{c}_{k\sigma}^+ \hat{c}_{k\sigma} + \hat{d}_{k\sigma}^+ \hat{d}_{k\sigma} \right] + 2t_{1s}(\cos k_x + \cos k_y) \left( \hat{c}_{k\sigma}^+ \hat{c}_{k\sigma} - \hat{d}_{k\sigma}^+ \hat{d}_{k\sigma} \right)
$$

We can apply the $S_4$ transformation on $\hat{H}_0$ to obtain the tight binding model for the second group. It is straightforward to see that the transformation invariance requires $t_{1s}$, $t_{2d}$ and $t_{3d}$ to change signs. Therefore, the two-orbital model is described by

$$
\hat{H}_{0,\text{two}} = \sum_{k,\sigma} \left[ 2t_{1d}(\cos k_x - \cos k_y) \right] \left( \hat{c}_{k\sigma}^+ \hat{c}_{k\sigma} + \hat{d}_{k\sigma}^+ \hat{d}_{k\sigma} \right) + 2t_{2d}\sin k_x \sin k_y \left( \hat{c}_{k\sigma}^+ \hat{c}_{k\sigma} - \hat{d}_{k\sigma}^+ \hat{d}_{k\sigma} \right) + \cdots
$$

$H_{0,\text{two}}$ provides the following energy dispersions for the two orbitals,

$$
E_{c\pm} = \epsilon_k \pm 2t_{3d}(\cos 2k_x - \cos 2k_y) + 4\sqrt{\frac{t_{2d}^2\sin^2 x \sin^2 y + \frac{t_{1s}(\cos k_x + \cos k_y) \pm t_{1d}(\cos k_x - \cos k_y)}{2}}{2}},
$$

$$
E_{h\pm} = \epsilon_k \pm 2t_{3d}(\cos 2k_x - \cos 2k_y) - 4\sqrt{\frac{t_{2d}^2\sin^2 x \sin^2 y + \frac{t_{1s}(\cos k_x + \cos k_y) \pm t_{1d}(\cos k_x - \cos k_y)}{2}}{2}}.
$$
where $\epsilon_k = 4t_2\cos k_x \cos k_y + 2t_3(\cos 2k_x + \cos 2k_y) - \mu$. $E_{\pm}$ captures the electron pockets at M points and $E_{\pm}$ captures the hole pockets at $\Gamma$ points. Based on the previous physical picture, $t_{1s}$, $t_{2s}$, and $t_{2d}$ should be the largest parameters because they are generated through the p-orbitals. In Fig. 4, we show that by just keeping these three parameters, the model is already good enough to capture the main characters of the bands contributing to Fermi surfaces in the five-orbital model. After performing the same gauge mapping, this Hamiltonian, as expected, provides pockets located at $X'$ as shown in Fig. 4.

Now we can turn on the couplings between the two groups. It is straightforward to show that the leading order of the couplings that satisfies the $S_4$ symmetry is given by

$$\hat{H}_{0,c} = \sum_k 2t_c(\cos k_x + \cos k_y)(\hat{c}_{k,\sigma}^\dagger \hat{d}_{k,\sigma} + h.c.).$$  \hspace{1cm} (9)$$

This term can be generated through the NN hopping between two orbitals with the same orbital characters. Due to the form factor $(\cos k_x + \cos k_y)$, the coupling has little effect on the electron pockets while has visible effect on the hole pockets. Without this coupling, the two hole pockets are not only degenerate at $\Gamma$ but also have four degenerate points along the two $\Gamma - X$ directions. The coupling can lift the later degeneracy on the hole pockets.

Combining the $\hat{H}_{0,two}$ and $\hat{H}_{0,c}$, we obtain an effective $S_4$ symmetric two orbital model whose band structure is described by

$$\hat{H}_{0,eff} = \hat{H}_{0,two} + \hat{H}_{0,c}.$$ \hspace{1cm} (10)

The $\hat{c}$ and $\hat{d}$ Fermionic operators can be viewed as two iso-spin components of the $S_4$ symmetry.

**General properties of the model:** The above model is good enough to quantitatively describe the experimental results measured by ARPES. Although the hopping parameters are dominated by $t_{1s}$, $t_{2d}$ and $t_{2s}$, other parameters can not be ignored. For example, at the same $M$ points, there is energy splitting between two components, which indicates the existence of a sizable $t_{3s}$. To match the detailed dispersion of the bands, the TNN hoppings have to be included. The existence of the TNN hoppings may also provide a microscopic justification for the presence of the significant TNN AFM exchange coupling $J_3$ measured by neutron scattering in iron-chalcogenides.$^{33, 50, 51}$

While the detailed quantitative results for different families of iron-based superconductors will be present elsewhere, we plot a typical case for iron-pnictides with parameters $t_{1s} = 0.4$, $t_{1d} = -0.03$, $t_{2s} = 0.3$, $t_{2d} = 0.6$, $t_{3s} = 0.05$, $t_{3d} = -0.05$ and $\mu = -0.3$ in figs. 4a-d. In Fig. 4a, the coupling $t_c = 0$. In Fig. 4c, $t_c = 0.02$. It is clear that the degeneracy at the hole pockets along $\Gamma - X$ direction is lifted by $t_c$. The Fermi surfaces in Fig. 5 are very close to those in the five orbital model. This result really suggests the coupling between two orbitals is rather small.

There are several interesting properties in the model. First, it is interesting to point out that we can make an exact analogy between the $S_4$ transformation on its two iso-spin components and the time reversal symmetry transformation on a real 1/2-spin because $S_4^2 = -1$. This analogy suggests in this $S_4$ symmetric model, the degeneracy at high symmetric points in Brillouin zone is the type of the Kramers degeneracy.

Second, in this model, if the orbital degree of freedom is included, the true unit cell for each iso-spin component includes four irons. The gauge mapping in the previous section exactly takes a unit cell with four iron sites. Such a match is the essential reason why the low energy physics becomes transparent after the gauge mapping.

Third, the model unifies the iron-pnictides and iron-chalcogenides. When other parameters are fixed, reducing $t_{2s}$ or increasing $t_{1s}$ can flatten the dispersion along $\Gamma - M$ direction of $E_{\pm}$ and cause the hole pocket completely vanishes. Therefore, the model can describe both iron-pnictides and electron-overdoped iron-chalcogenides by varying $t_{2s}$ or $t_{1s}$.

Finally, carefully examining the hopping parameters, we also find that the NNN hopping for each $S_4$ iso-spin essentially has a $d$-wave symmetry, namely $|t_{2d}| > t_{2s}$. Since the hole pockets can be suppressed by reducing $t_{2s}$ value, this $d$-wave hopping symmetry is expected to be stronger in iron chalcogenides than in iron-pnictides.

**The two-orbital model with interactions:** By projecting all interactions into these two effective orbital model, a general effective model that describes iron-based superconductors obeying the $S_4$ symmetry can be written as

$$H_{eff} = H_{0,eff} + U \sum_{i,\alpha=1,2} \hat{n}_{i,\alpha\uparrow} \hat{n}_{i,\alpha\downarrow} + U' \sum_i \hat{n}_{i,1} \hat{n}_{i,2} + J_H \sum_i \hat{S}_{i,1} \cdot \hat{S}_{i,2}$$  \hspace{1cm} (11)$$

where $\alpha = 1, 2$ labels the $S_4$ iso-spin, $U$ describes the effective Hubbard repulsion interaction within each com-
ponent, $U'$ describes the one between them and $J'_H$ describes the effective Hunds coupling. Since the two components couple weakly, we expect $U$ dominates over $U'$ and $J'_H$. In the first order approximation, the model becomes a single band-Hubbard model near half filling. A similar t-J model can also be discussed within the same context as cuprates. It is clear that the model naturally provides an explanation for the stable NNN AF exchange couplings $J_2$ observed by neutron scattering and its dominating role in both magnetism and superconductivity.

**Couplings between $d_{xz, yz}$ and other $d$ orbitals:** Although the low energy physics is governed by $d_{xz, yz}$ orbitals, it is interesting to ask their couplings to other $d$ orbitals in particular, the $d_{xy}$ orbitals. Under the $S_4$ transformation, the $d_{xy}$ is in the B representation while $d_{xz}, d_{yz}$ are in the E representations of the $S_4$ group. Therefore, the coupling between them is only possible through other E representations. $(sink_x, sink_y)$ naturally forms two E representations. The leading coupling between $d_{xz, yz}$ and $d_{xy}$ is thus given by

$$H_{xy} = t_x \sum_{k,\sigma} \hat{a}^+_k \hat{a}_k^{\dagger} (sink_x \hat{c}_k^{\dagger} - sink_y \hat{d}_k^{\dagger})$$

$$+ t_y \sum_{k,\sigma} \hat{a}^+_k \hat{a}_k^{\dagger} (sink_y \hat{c}_k^{\dagger} + sink_x \hat{d}_k^{\dagger}) + h.c.,$$

(12)

where $\hat{a}_k^{\dagger}$ is the Fermionic operator for the $d_{xy}$ orbital. This form is uniquely determined by the time reversal symmetry and the $S_4$ symmetry. It is interesting to point out the coupling has been obtained where the authors tried to construct a three orbital model. This coupling can correctly account for the third hole pocket around $(\pi, \pi)$ observed in the 122 structure. Other $d$ orbitals can also be constructed similarly. In principle, the entire band structure can be constructed within the $S_4$ symmetry if necessary.

**Comparison between the $S_4$ and the $C_{4v}$ symmetry:** It is interesting to compare the $S_4$ to the $C_{4v}$ symmetry. If the $C_{4v}$ symmetry is forced, the $c_4$ operation imposes,

$$\begin{pmatrix} \hat{c}_k \sigma \\ \hat{d}_k \sigma \end{pmatrix} \rightarrow \begin{pmatrix} \hat{d}_{k' + Q} \sigma \\ -\hat{c}_{k' + Q} \sigma \end{pmatrix},$$

(13)

and the reflection operator $\sigma_v$ in the $C_{4v}$ group imposes additional requirements,

$$\begin{pmatrix} \hat{c}_k \sigma \\ \hat{d}_k \sigma \end{pmatrix} \rightarrow \begin{pmatrix} \hat{d}_{k' + Q} \sigma \\ \hat{c}_{k' + Q} \sigma \end{pmatrix},$$

(14)

where $k'' = (k_y, k_x)$. It is easy to see that if we force the $C_{4v}$ symmetry, the reflection $\sigma_v$ invariance requires $t_{1s} = 0$. However, without such a reflection invariance, this term is allowed, which is the case for the $S_4$ symmetry. The existence of $t_{1s}$ suggests that $\sigma_v$ symmetry must be broken in an effective model for $d$-orbitals. However, since $\sigma_v$ symmetry appears to be present in Fe-As(Se) structure, it is natural to ask what mechanism can break $\sigma_v$. While a detailed study of this symmetry breaking is in preparation, we give a brief analysis. If we include the $\sigma_v$ together with the $S_4$ group, the total group is enlarged to $D_{2d}$. Therefore, in general, one can write down a $D_{2d}$ symmetry model by including all $p$ orbitals of As(Se). When the model is reduced to an effective model based on the $d$-orbitals, because the $p$ orbitals are fully occupied, the $t_{1s}$ hopping between two NN $d_{xz}, d_{yz}$ orbitals can only be generated through the following virtual hopping processes: one electron first hops from the $p_x$ to the $d_{xz}$, then, an electron in the $p_y$ at the same As(Se) site can hop to the $p_x$, finally, an electron in the $d_{yz}$ orbital hops to the $p_y$. In such a process, the reflection symmetry is broken due to the existence of the hopping between the $p_x$ and $p_y$ orbitals at the same As(Se) site when the two orbitals host total 3 electrons.

**The coupling between two $S_4$ iso-spin and $S_4$ symmetry breaking:** The couplings between the two iso-spins can either keep the $S_4$ symmetry or break it. Without breaking the translational symmetry, the coupling between two orbitals can be written as

$$\hat{H}_c = \sum_{k,\sigma} f_\sigma(k) \hat{G}_\sigma(k) + \sum_{k,\bar{\sigma}} f_{\bar{\sigma}}(k) \hat{G}_{\bar{\sigma}}(k)$$

(15)

where $\hat{G}_\sigma(k)$ and $\hat{G}_{\bar{\sigma}}(k)$ are operators constructed according to the $S_4$ one dimensional representations as follows,

$$G_1(k) = \sum_{\sigma} c_{k\sigma}^{\dagger} \hat{d}_{k\sigma} + c_{k+Q\sigma}^{\dagger} \hat{d}_{k+Q\sigma} + h.c. \quad (16)$$

$$G_2(k) = \sum_{\sigma} c_{k\sigma}^{\dagger} \hat{d}_{k\sigma} - c_{k+Q\sigma}^{\dagger} \hat{d}_{k+Q\sigma} + h.c. \quad (17)$$

$$G_3(k) = \sum_{\sigma} c_{k\sigma}^{\dagger} \hat{d}_{k+Q\sigma} + c_{k+Q\sigma}^{\dagger} \hat{d}_{k\sigma} + h.c. \quad (18)$$

where $k'' = (k_y, k_x)$. It is easy to see that if we force the $C_{4v}$ symmetry, the reflection $\sigma_v$ invariance requires $t_{1s} = 0$. However, without such a reflection invariance, this term is allowed, which is the case for the $S_4$ symmetry. The existence of $t_{1s}$ suggests that $\sigma_v$ symmetry must be broken in an effective model for $d$-orbitals. However, since $\sigma_v$ symmetry appears to be present in Fe-As(Se) structure, it is natural to ask what mechanism can break $\sigma_v$. While a detailed study of this symmetry breaking is in preparation, we give a brief analysis.
IV. THE CLASSIFICATION OF THE SUPERCONDUCTING ORDERS ACCORDING TO THE $S_4$ SYMMETRY

The presence of the $S_4$ symmetry brings a new symmetry classification of the superconducting phases. The $S_4$ point group has four one-dimensional representations, including $A, B$ and $2E$. In the $A$ state, the $S_4$ symmetry is maintained. In the $B$ state, the state changes sign under the $S_4$ transformation. In the $2E$ state, the state obtains a $\pm \pi/2$ phase under the $S_4$ transformation. Therefore, the $2E$ state breaks the $C_2$ rotational symmetry as well as the time reversal symmetry.

Since the $S_4$ transformation includes two parts, a 90° degree rotation and a reflection along c-axis, the $S_4$ symmetry classification leads to a natural correlation between the rotation in a-b plane and c-axis reflection symmetries in a SC state. In the A-phase, rotation and c-axis reflection can be both broken, while in the B-phase, one and only one of them can be broken. This correlation, in principle, may be observed by applying external symmetry breaking. For example, even in the A-phase and the rotation symmetry is not broken, we may force the c-axis phase-flip to obtain the phase change in the a-b plane.

As shown in this paper, the iron-based superconductors are rather unique with respect to the $S_4$ symmetry. It has two iso-spin components governed by the symmetry. This iso-spin degree of freedom and the interaction between them could lead to many novel phases. The future study can explore these possibilities.

Here we specifically discuss the $S_4$ symmetry aspects in the proposed $A_{1g}$ s-wave state, a most-likely phase if it is driven by the repulsive interaction or strong AF in iron-based superconductors as we have shown earlier. First, let’s clarify the terminology issues. The $A_{1g}$ s-wave pairing symmetry is classified according to $D_{4h}$ point group. This classification is not right in the view of the true lattice symmetry. However, for each iso-spin components, we can still use it. Here we treat it as a state that the superconducting order $\Delta \propto cosk_x cosk_y$. Since the $A_{1g}$ phase is equivalent to the $d$-wave in cuprates in a different gauge setting, the $d$-wave picture is more transparent regarding the sign change of the superconducting phase in the real space. As shown in Fig.4 the sign of the SC order alternates between neighboring squares in the iron lattice.

Based on the underlying electronic structure revealed here, with respect to the $S_4$ symmetry, the $A_{1g}$ state can have two different phases, A phase and B phase. In the A phase,

$$<\hat{c}_{k\uparrow}\hat{c}_{-k\downarrow}> = <\hat{d}_{k\uparrow}\hat{d}_{-k\downarrow}> = \Delta_0 \cos k_x \cos k_y$$

and in the B phase,

$$<\hat{c}_{k\uparrow}\hat{c}_{-k\downarrow}> = - <\hat{d}_{k\uparrow}\hat{d}_{-k\downarrow}> = \Delta_0 \cos k_x \cos k_y$$

Therefore, in the view of the $d$-wave picture, in both A and B phases, the superconducting phase for each component alternates between neighboring squares, which is...
corresponding to the sign change between the top and bottom planes in the view of the $S_4$ symmetry. However, in the A phase, since the $S_4$ symmetry is not violated, the relative phase between the two components are equal to $\pi$ in space, while in the B phase, the relative phase is zero. A picture of the phase distribution of the two iso-spin components in the A and B phases are illustrated in Fig.7(b,c).

The sign change of the order parameter or the phase shift of $\pi$ between the top and bottom planes along c-axis can be detected by standard magnetic flux modulation of dc SQUIDS measurement. If we consider a single Fe-As(Se) trilayer structure, which has been successfully grown by MBE recently, we can design a standard dc SQUIDS as shown in Fig.7(a) following the similar experimental setup to determine the $d$-wave pairing in cuprates.

For the B phase, there is no question that the design can repeat the previous results in cuprates. However, if the tunneling matrix elements to two components are not symmetric, even in the A phase, this design can obtain the signal of the $\pi$ phase shift since the two components are weakly coupled and each of them has a $\pi$ phase shift. For the B phase, the phase shift may be preserved even in bulk materials. However, for the A phase, it will be difficult to detect the phase shift in bulk materials. A cleverer design is needed. Measuring the phase shift between the upper and lower As planes will be a smoking-gun experiment to verify the model and determine iron-based superconductors and cuprates sharing identical superconducting mechanism.

![Figure 7](image)

**FIG. 7.** (a) An illustration of a single Fe-As(Se) layer and the setup for a dc SQUIDS measurement to measure the sign change of the SC phase between top and down As(Se) layers; (b) The phase distribution in the A phase of the $A_{1g}$ S-wave state in the view of a $d$-wave picture ( red for one iso-spin component and blue for the other); (c) The phase distribution in the B phase of the $A_{1g}$ S-wave state.

![Figure 8](image)

**FIG. 8.** A sketch of the correlation between the hopping and pairing symmetries for both iron-based superconductors and cuprates.

### V. DISCUSSION AND SUMMARY

We have shown that the $A_{1g}$ s-wave pairing in iron-based superconductors is a $d$-wave pairing in a view of a different gauge setting. This equivalence answers an essential question why a $A_{1g}$ s-wave pairing can be robust regardless of the presence or absence of the hole pockets. With repulsive interactions, a sign changed order parameter in a superconducting state is usually inevitable. This statement, however, is only true when the hopping parameters follow the same lattice symmetry. Gauge transformation can exchange the phases between superconducting order parameters and hopping parameters. In the case of cuprates, the $d$-wave order parameter can be transformed to a s-wave form by changing hopping parameters to obey $d$-wave symmetry. As we pointed out earlier, the NNN hopping in our model is close to a $d$-wave symmetry, rather than a s-wave symmetry. This is the essential reason why the superconducting order can have a s-wave form and be stable in iron-based superconductors. A simple picture of this discussion is illustrated in Fig.8. The vanishing of the hole pockets in electron-overdoped iron-chalcogenides indicates the hopping is even more $d$-wave like in these materials, a case supporting stronger s-wave pairing, which was indeed observed recently. The presence of the dominant form $\cos k_x \cos k_y$ is also straightly linked to the $d$-wave pairing form $\cos k_x' - \cos k_y'$ because of the stable AF $J_2$ coupling, similar to cuprates. Moreover, since the different gauge setting does not alter physical measurements, a phase sensitive measurement should reveal a $\pi$ phase shift in the real space along c-axis for each components in the $A_{1g}$ s-wave state, just like the phase shift along a and b direction in the $d$-wave pairing state of cuprates.

After obtaining the underlining electronic structure, we can ask how the physics in the cuprates and iron-based superconductors are related to each other. In Table I we list the close relations between two high $T_c$ superconductors. From the table, it is clear that by determining these physical properties of iron-based superconductors listed in the table can help to determine the high $T_c$ supercon-
The model completely changes the view of the origin of the generation of sign-changed s± pairing symmetry in iron-pnictides, which were argued in many theories that the origin is the scattering between electron pockets at M and hole pockets at Γ due to repulsive interactions.6,9 With the new underlining electronic structure revealed, the analysis of the sign-change should be examined after taking the gauge transformation so that the underlining hopping parameters become symmetric. In this case, the sign change is driven by scatterings between all pockets, including both hole and electron pockets, located at two d-wave anti-nodal X′ points. Therefore, the scattering between electron and electron pockets is also important.

While the model appears to be rotational invariant due to the $S_4$ symmetry, the dynamics of each iso-spin component is intrinsically nematic. A small $S_4$ symmetry breaking can easily lead to an overall electronic nematic state. The electronic nematic state has been observed by many experimental techniques22 and studied by different theoretical models.56–63 The underlining electronic structure in the model can provide a straightforward microscopic understanding between the interplay of all different degrees of freedoms based on the $S_4$ symmetry breaking.

In summary, we have shown the underlining electronic structure, which is responsible for superconductivity at low energy in iron-based superconductors, is essentially two weakly-coupled electronic structures governed by the $S_4$ symmetry. We demonstrate the s− wave pairing in iron-based superconductors is equivalent to the d-wave in cuprates. A similar conclusion has also been reached in the study of 2-layer Hubbard model.34 The $S_4$ symmetry reveals possible new superconducting states and suggests the phase shift in the SC state in real space is along c-axis. These results strongly support the microscopic superconducting mechanism for cuprates and iron-based superconductors are identical, including both iron-pnictides and iron-chalcogenides. Our model establishes a new foundation for understanding and exploring properties of iron based superconductors, a unique, elegant and beautiful class of superconductors.

**Acknowledgement:** JP thanks H. Ding, D.L. Feng, S. A, Kivelson, P. Coleman, X Dai, Y.P. Wang, EA Kim and F. Wang for useful discussion. JP specially thanks H. Ding, F. Wang, M. Fischer and W. Li for the discussion of the symmetry properties of the model. The work is supported by the Ministry of Science and Technology of China 973 program(2012CB821400) and NSFC-1190024.

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