The form and origin of orbital ordering in the electronic nematic phase of iron-based superconductors

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Abstract

We investigated the form of orbital ordering in the electronic nematic phase of iron-based superconductors by applying a group theoretical analysis on a realistic five-band model. We find the orbital order can be either of the inter-orbital s-wave form or intra-orbital d-wave form. From the comparison with existing ARPES measurements of band splitting, we find the orbital ordering in the 122 system is dominated by an intra-orbital d-wave component, while that of the 111 system is dominated by an inter-orbital s-wave component. We find both forms of orbital order are strongly entangled with the nematicity in the spin correlation of the system. The condensation energy of the magnetic ordered phase is found to be significantly improved (by more than 20%) when the degeneracy between the \((\pi, 0)\) and \((0, \pi)\) ordering pattern is lifted by the orbital order. We argue there should be a large difference in both the scattering rate and the size of the possible pseudogap on the electron pocket around the \(X = (\pi, 0)\) and \(Y = (0, \pi)\) point in the electronic nematic phase. We propose this as a possible origin for the observed nematicity in resistivity measurements.

Keywords: orbital ordering, electronic nematicity, iron superconductor

The most exciting new feature of iron-based superconductors is their multi-orbital nature. Many novel properties of iron-based superconductors, especially those referred to as electronic nematicity [1–7], have been argued to be related to orbital physics in these systems [8–15]. The ARPES observation of the rather large splitting between the \(3d_{xz}\) and \(3d_{yz}\)-dominated bands [4] in the magnetic ordered phase further implies that the orbital degree of freedom is deeply involved in the magnetic ordering phase transition. More recent measurements find that the breaking of tetragonal symmetry in the electronic structure can happen even without static magnetic ordering [20, 21]. At the same time, the multi-orbital character is also the key to understanding the complex manifestation of electron correlation effect and the structure of superconducting pairs in these systems [16, 17].

However, a comprehensive understanding of the role of orbital degree of freedom in these systems is still in its infancy. In particular, it is still a mystery how the observed electronic nematicity is related to the orbital physics of the system. It is also unclear what is the order parameter for orbital ordering in the electronic nematic phase of iron-based superconductors and how it is entangled with the magnetic, structural and superconducting properties of these systems.

The purpose of this paper is to determine the form of the order parameter for orbital ordering in the electronic nematic phase of iron-based superconductors and explore its physical origin. By applying group theoretical analysis to a realistic five-band model derived from band structure calculations, we are able to determine the form of the order parameter for orbital ordering in iron-based superconductors. We find the orbital order can take either an inter-orbital s-wave form or an intra-orbital d-wave form in the space spanned by the degenerate \(d_{xz}\) and \(d_{yz}\) orbitals. From comparison with ARPES measurements we find orbital ordering in different families of iron-based
superconductors takes different forms. More specifically, while the orbital order in the 122 system is dominated by an intra-orbital d-wave component, the 111 system choose to order mainly in the intra-orbital s-wave channel. We find both types of orbital ordering are strongly entangled with the nematicity of spin correlation in the system and can emerge spontaneously by lifting the degeneracy between the magnetic nematicity of spin correlation in the system and can emerge both types of orbital ordering are strongly entangled with the directions and are rotated by 45 degrees from the x- and y-axis of the Fe–Fe square lattice.

In the tetragonal phase, the point group around the Fe site is $D_{4h}$, whose generators are $\sigma_x$, $\sigma_y$ and $R_\pi$. Among the five MLWFs, $|XZ\rangle$ belongs to the identity representation, $|XY\rangle$ and $|X^2 - Y^2\rangle$ belong to the one-dimensional $B_1$ and $B_2$ representation, $|XZ\rangle$ and $|YZ\rangle$ belong to the 2D representation of the $D_{4h}$ group. If we denote the transformation of five MLWFs under the generators $R_m = R_\pi$, $\sigma_x$, $\sigma_y$ as $R_m|\mu\rangle = \sum_{\nu} D_{\mu,\nu}(R_m)|\nu\rangle$, then the hopping integrals in the tetragonal phase should satisfy the following equation

$$t_{\mu,\nu}^{\mu',\nu'} = \sum_{\mu',\nu'} D_{\mu',\mu}(R_m) D_{\nu',\nu}(R_m)t_{\mu,\nu}^{\mu',\nu'}, \quad (1)$$

in which $i' = R_{\pi}^{-1}i$.

In the electronic nematic phase, the local symmetry around each Fe site is reduced to $D_2$. In principle, such a symmetry breaking may originate from either the electronic (for example, the charge, spin or orbital degree of freedom) or the lattice degree of freedom [25]. Here we will focus on the symmetry breaking pattern in the orbital space. As a result of this symmetry breaking, additional terms that are forbidden by equation (1) can appear in $t_{\mu,\nu}^{\mu',\nu'}$. These symmetry breaking terms can be interpreted as the order parameter of orbital order in the electronic nematic phase and can be detected from the band splitting in ARPES measurements. The general form of such symmetry breaking perturbations can be largely determined by group theoretical analysis. Here we will illustrate such a procedure for the on-site symmetry breaking term for clarity.

The basic idea is to find out all the bilinear terms in the orbital space that are allowed by the symmetry group of the orthorhombic phase ($D_2$), but are forbidden by the symmetry group of the tetragonal phase ($D_{4h}$). This can be done by operating the projection operators of the identity representation for the $D_{4h}$ and $D_2$ groups on an arbitrary initial bilinear Hamiltonian. The $D_2$ group has four one dimensional irreducible representations. Among the five MLWFs, $|X^2 - Y^2\rangle$ and $|XY\rangle$ both belong to the identity representation, $|X^2 - Y^2\rangle$ belongs to the B1 representation, the linear combinations $|XZ\rangle \pm |YZ\rangle$ belong to the B2 and B3 representations and have $d_{xz}$ and $d_{yz}$ character. Thus the symmetry allowed on-site Fermion bilinear terms in the orthorhombic phase have the general form of

$$H_2 = \sum_{i,\sigma} \left( \beta_1 c_{i,1,\sigma}^\dagger c_{i,1,\sigma} + \beta_2 c_{i,5,\sigma}^\dagger c_{i,5,\sigma} + \beta_3 c_{i,4,\sigma}^\dagger c_{i,4,\sigma} \right)$$

$$+ \beta_4 \sum_{i,\sigma} \left( c_{i,1,\sigma}^\dagger c_{i,5,\sigma} + c_{i,5,\sigma}^\dagger c_{i,1,\sigma} \right)$$

$$+ \beta_5 \sum_{i,\sigma} \left( c_{i,1,\sigma}^\dagger c_{i,3,\sigma} + c_{i,3,\sigma}^\dagger c_{i,1,\sigma} \right) + \beta_6 \sum_{i,\sigma} \left( c_{i,1,\sigma}^\dagger c_{i,3,\sigma} - c_{i,3,\sigma}^\dagger c_{i,1,\sigma} \right). \quad (2)$$

However, it can be shown that the bilinear forms $c_{i,1,\sigma}^\dagger c_{i,1,\sigma}$, $c_{i,4,\sigma}^\dagger c_{i,4,\sigma}$, $c_{i,5,\sigma}^\dagger c_{i,5,\sigma}$, and $c_{i,2,\sigma}^\dagger c_{i,2,\sigma} + c_{i,3,\sigma}^\dagger c_{i,3,\sigma}$ all belong to the identity representation of the $D_{4h}$ group. When these symmetric perturbations are removed from equation (2), we get the symmetry breaking perturbations in the orthorhombic phase, which now takes the simple form of

$$\Delta H = \lambda_1 \sum_{i,\sigma} \left( c_{i,2,\sigma}^\dagger c_{i,3,\sigma} + c_{i,3,\sigma}^\dagger c_{i,2,\sigma} \right) + \lambda_2 \sum_{i,\sigma} \left( c_{i,1,\sigma}^\dagger c_{i,5,\sigma} + c_{i,5,\sigma}^\dagger c_{i,1,\sigma} \right). \quad (3)$$

The above arguments can be easily generalized to determine the form of the symmetry breaking perturbations on longer distances. The necessity for such nonlocal terms can be seen clearly from the strong momentum dependence of the band splitting observed in ARPES measurements on 122 systems [4]. Following the same procedures, we find there are a total of 9 independent symmetry breaking perturbations on nearest-neighboring Fe–Fe bonds, which can be classified into the extended s-wave, p-wave and d-wave channels,

$$\Delta H = \Delta H_s + \Delta H_p + \Delta H_d.$$

In the subspace spanned by the $d_{xz}$ and $d_{yz}$ orbitals, only an inter-orbital extended s-wave term and an intra-orbital d-wave term are allowed. Combining these terms with the on-site term found above, we find that the symmetry breaking perturbation
in the orthorhombic phase is given by

\[
\Delta H = \eta_1 \sum_{i,\sigma} \left( c_{i,2,\sigma}^\dagger c_{i,3,\sigma} + c_{i,3,\sigma}^\dagger c_{i,2,\sigma} \right) \\
+ \eta_2 \sum_{i,\ell,\sigma} \left( c_{i,2,\sigma}^\dagger c_{i+\ell,3,\sigma} + c_{i+\ell,3,\sigma}^\dagger c_{i,2,\sigma} \right) \\
+ \eta_3 \sum_{i,\ell,\sigma} \delta_3 \left( c_{i,2,\sigma}^\dagger c_{i+\ell,2,\sigma} + c_{i,3,\sigma}^\dagger c_{i+\ell,3,\sigma} \right).
\]

Here \( \delta \) denotes the vectors connecting nearest-neighboring Fe sites and \( \delta_3 \) is the d-wave form factor. In principle, symmetry breaking terms on longer bonds can also be determined in the same manner. However, from comparison with the ARPES measurements, we find it suffices to keep only the on-site and nearest-neighboring terms. A list of all independent symmetry breaking terms up to the next-nearest-neighboring bonds is given in the appendix for reference.

The three parameters \( \eta_{1,2,3} \) in equation (4) can be determined from fitting the momentum dependence of the band splitting found in ARPES measurements. In particular, they can be extracted from band splitting at the high symmetry momentum of \( \Gamma = (0,0,0) \), \( \chi = (\pi,0,0) \), \( \chi = (0,0,\pi) \), and \( \mathbf{M} = (\pi,\pi,\pi) \). From the group theoretical point of view, the electronic state at these high symmetry momentums should form basis functions of an irreducible representation of the \( D_2 \) group, which is also the wave vector point group at these momentums in the electronic nematic phase. Thus, the electronic state in the \( 3d_{xz} \) and \( 3d_{yz} \)-dominated bands should have pure \( d_{xz} \) and \( d_{yz} \) character at these momenta. The band splitting at these momenta are given by

\[
\Delta E_{d_{xz}} (\Gamma) = \eta_1 + 4\eta_2, \quad \Delta E_{d_{yz}} (\Gamma) = -\eta_1 - 4\eta_2 \\
\Delta E_{d_{xz}} (X) = \eta_1 - 4\eta_3, \quad \Delta E_{d_{yz}} (X) = -\eta_1 - 4\eta_3 \\
\Delta E_{d_{xz}} (Y) = \eta_1 + 4\eta_3, \quad \Delta E_{d_{yz}} (Y) = -\eta_1 + 4\eta_3 \\
\Delta E_{d_{xz}} (M) = \eta_1 - 4\eta_2, \quad \Delta E_{d_{yz}} (M) = -\eta_1 + 4\eta_2
\]

Since the \( 3d_{xz} \) and \( 3d_{yz} \)-dominated bands are far away from the Fermi level around the \( \mathbf{M} \) point, we will focus on the band splitting along the \( \Gamma-X \) and \( \Gamma-Y \) directions in the following.

The momentum dependence of the band splitting induced by the three types of orbital orders are plotted in figure 1. To see the band splitting more clearly, we overlay the dispersion along the \( \Gamma-Y \) direction on that along the \( \Gamma-X \) direction. In the tetragonal phase, the dispersion of the \( 3d_{yz} \)-dominated band along the \( \Gamma-Y \) direction should be identical to that of the \( 3d_{xz} \)-dominated band along the \( \Gamma-Y \) direction, which are plotted as thin lines in figure 1 for reference. The band splitting caused by the on-site orbital order is nonzero in the whole Brillouin zone and is only weakly momentum dependent. For the extended s-wave orbital order, band splitting reaches its maximum (denoted as \( \Delta_{\text{max}} \)) at the \( \Gamma \) point and is exactly zero at the \( X \) and \( Y \) points. For the d-wave orbital order, the band splitting vanishes at the \( \Gamma \) point and \( \Delta_{\text{max}} \) is reached at the \( X \) and \( Y \) points.

We now compare the theoretical predictions with the ARPES measurements. In the Co-doped Ba122 system, the observed band splitting in the \( \Gamma-X \) and \( \Gamma-Y \) direction exhibits strong momentum dependence and is very similar to the d-wave presented above. In particular, the band splitting is negligible around the \( \Gamma \) point but is most evident at the \( X \) and \( Y \) points [4]. On the other hand, in both the Na111 system or Li111 system, the observed band splitting is clearly nonzero at the \( \Gamma \) point and momentum dependence along the \( \Gamma-X \) and \( \Gamma-Y \) direction is much less pronounced than that in the Co-doped Ba122 system [18, 19, 21]. Thus, the order parameter
for orbital ordering in the 111 system is more likely of the on-site form. In principle, an extended s-wave component is also possible in the 111 system. However, as we will show below, the appearance of the extended-s-wave component is very unlikely from energetic considerations. Thus, the form of orbital ordering in iron-based superconductors depends on the family of the material studied. It would be interesting to know if there is any generic reason that the Co-doped Ba122 system and the Na111 system or Li111 system choose different orbital ordering patterns.

Now we discuss the possible origin of the orbital ordering in iron-based superconductors. From the point of view of symmetry, the orbital ordering in the electronic nematic phase can be just a secondary effect caused by the breaking of tetragonal symmetry in other channels such as the spin, charge or lattice degree of freedom and has little contribution to the condensation energy of the ordered phase. Here we will adopt a more exotic point of view and assume that the orbital ordering can contribute significantly to the condensation energy of the electronic nematic phase and thus emerge spontaneously. This is a reasonable assumption since the size of the observed band splitting in the electronic nematic phase is already comparable to or even larger than energy scales of other major ordering tendencies in the system such as SDW order and superconductivity. However, RPA calculations on the five-band model indicates that iron-based superconductors are far from a pure orbital ordering instability. To resolve this problem, we assume that orbital ordering is strongly entangled with the nematicity of spin correlation in iron-based superconductors, which is dominated by two degenerate channels with wave vector $\mathbf{Q}_x = (\pi, 0)$ and $\mathbf{Q}_y = (0, \pi)$. As we will show below, the orbital order can lift such a degeneracy and help the system to gain significantly more condensation energy by selecting the favored ordering wave vector in a way similar to the conventional Jahn–Teller effect.

In the following, we will illustrate the coupling between the orbital order and nematicity in spin correlation at the mean field level for the SDW ordered state. For this purpose, we introduce the standard Kanamori–Hubbard Hamiltonian for on-site interactions on the Fe site. We then solve the mean filed equations for the SDW order parameters in the presence of orbital order. The SDW order is assumed to be collinear and has a wave vector of either $\mathbf{Q}_x = (\pi, 0)$ or $\mathbf{Q}_y = (0, \pi)$. More specifically, the SDW order parameter is assumed to be of the form $\langle \sum_{\sigma} c_{\mathbf{i},\mu,\sigma}^\dagger c_{\mathbf{i},\nu,\sigma} \rangle = e^{i \mathbf{Q}_x \cdot \mathbf{R}_i} S_{\mu,\nu}$, in which $S_{\mu,\nu}$ is a $5 \times 5$ matrix describing the distribution of the magnetic moment in the orbital space. In the following, we will adopt $\text{Tr} S = \sum_{\mu} S_{\mu,\mu}$ as a measure of the magnitude of the ordered moment. In the calculation, we set the interaction strength as $U = 1.5$ eV, $U' = 1.0$ eV and $J_H = 0.25$ eV, which is large enough to induce a moderate-sized ordered moment. The electron density is fixed at $n = 6.0$ in the calculation.

The solution to the mean field self-consistent equation is shown in figure 2. We find all three types of orbital ordering can couple to the nematicity in spin correlation. However, the strength of the coupling is quite different for the three types of orbital ordering. In particular, the coupling of extended s-wave orbital order to the nematicity of spin correlation is much weaker than that of the on-site and the d-wave orbital order. For both the on-site and the d-wave orbital order, the disfavored ordering pattern is totally suppressed when the maximal band splitting $\Delta_{\text{max}}$ exceeds 160 meV, while in the case of the extended s-wave orbital order, the change in size of the ordered moment is less than 20% even for $\Delta_{\text{max}} = 200$ meV. To see if the orbital order can emerge spontaneously from such a coupling, we calculate the condensation energy of the system as a function of the orbital order, which is also shown in figure 2. We find both the on-site and d-wave orbital order can improve the condensation energy significantly (more than 20%) and a sizeable orbital order can be stabilized in both

![Figure 2. Selection of SDW ordering pattern by orbital ordering. Left: the ordered moment in the presence of on-site (a), extended s-wave (c) and d-wave (e) orbital order. Right: the condensation energy per unit cell in the presence of on-site (b), extended s-wave (d) and d-wave (f) orbital order.](image-url)
channels. On the other hand, the improvement in condensation energy from the extended s-wave orbital order is rather small and the induced orbital order is also much smaller than in the other two channels.

Such a difference in the coupling strength can be understood intuitively in the weak coupling picture from the nesting property of the Fermi surface, which is important for the spin correlation. More specifically, the band splitting between the X and Y points will enhance the nesting of the electron pocket (with the hole pocket around the Γ point) around one of these two momentum and suppress the nesting of the electron pocket around the other momentum. However, in the extended s-wave channel, the band splitting is suppressed around the X and Y points. This explains its weak entanglement with the nematicity in the spin correlation. Since orbital order can make such a significant contribution to the condensation energy of the ordered phase, it is more reasonable to think of orbital order as a component of a composite order parameter involving both the spin and orbital degree of freedom, rather than a secondary effect of magnetic ordering. Recently, evidence for reentrant tetragonal phase with magnetic ordering at both \( Q_x = (\pi, 0) \) or \( Q_y = (0, \pi) \) has been reported [24]. It is interesting to see if the band splitting also vanishes in this phase.

We note the entanglement between the orbital order and the nematicity in spin correlation is not limited in the magnetic ordered phase. In the paramagnetic phase, such a coupling can be realized through the so called Aslamazov–Larkin type vertex correction [23]. In particular, when the spin correlation breaks the tetragonal symmetry, it can be shown that a nonzero orbital order will be induced through a second order perturbation calculation [26]. At the same time, a recent ARPES study of BaFe\(_2\)(As\(_2\))\(_2\) has found simultaneously evidence of pseudogap opening on the Fermi surface, which is most likely due to strong scattering from spin fluctuation, and band splitting between the X and Y points in the electronic nematic phase of the system [20]. Following our line of reasoning, we should expect a rather different scattering rate and different size of the pseudogap on the electron pocket around the X and Y points in the electronic nematic phase of iron-based superconductors. We propose this as a possible origin for the observed nematicity in resistivity measurements in the electronic nematic phase.

In conclusion, by applying group theoretical analysis to a realistic five-band model, we have determined the form of orbital ordering in the electronic nematic phase of iron-based superconductors. We find orbital ordering in these systems can be either of the inter-orbital s-wave form or the intra-orbital d-wave form. From comparison with ARPES observations, we find the orbital ordering in the 122 systems is dominated by the intra-orbital d-wave component, while that in the 111 system is better described with an on-site intra-orbital form. From a mean field calculation, we find both types of orbital ordering are strongly entangled with the nematicity of the spin correlation and can emerge spontaneously in the model we have studied. We find that orbital order can contribute significantly to the condensation energy of the magnetic ordered phase and it is thus more reasonable to think of orbital order as a component of a composite order parameter involving both the spin and orbital degree of freedom, rather than a secondary effect of magnetic ordering. We predict that both the scattering rate and size of the pseudogap should be quite different on the electron pocket around the X and Y points in the electronic nematic phase of iron-based superconductors. We propose this as a possible origin for the observed nematicity in resistivity measurements in the electronic nematic phase.

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### Appendix

In this appendix, we present all possible symmetry breaking terms in the electronic nematic phase in the full five-dimensional orbital space up to the next-nearest-neighbor bonds. Here we will assume that both the translational and time reversal symmetry is respected in the electronic nematic phase. Following the procedure as outlined in the main text, we find there are a total of 9 independent symmetry breaking perturbations on nearest-neighbor Fe–Fe bonds and 6 independent symmetry breaking perturbations on the next-nearest-neighbor bonds. The form of the symmetry breaking terms on the nearest-neighboring bonds is given by

\[
\Delta H = \Delta H_s + \Delta H_p + \Delta H_d,
\]

in which

\[
\Delta H_s = \kappa_1 \sum_{i,\delta,\sigma} (c_{i,2,\sigma}^\dagger c_{i+\delta,3,\sigma} + c_{i,3,\sigma}^\dagger c_{i+\delta,2,\sigma}) + \kappa_2 \sum_{i,\delta,\sigma} (c_{i,1,\sigma}^\dagger c_{i+\delta,5,\sigma} + c_{i,5,\sigma}^\dagger c_{i+\delta,1,\sigma})
\]

\[
\Delta H_p = \kappa_3 \sum_{i,\delta,\sigma} (p_{i,1,\sigma}^\dagger c_{i+\delta,2,\sigma} + p_{i,2,\sigma}^\dagger c_{i+\delta,1,\sigma}) + \kappa_4 \sum_{i,\delta,\sigma} (p_{i,3,\sigma}^\dagger c_{i+\delta,5,\sigma} + p_{i,5,\sigma}^\dagger c_{i+\delta,3,\sigma}) + \kappa_5 \sum_{i,\delta,\sigma} (p_{i,4,\sigma}^\dagger c_{i+\delta,4,\sigma} - p_{i,4,\sigma} c_{i+\delta,4,\sigma}) + \kappa_6 \sum_{i,\delta,\sigma} (p_{i,4,\sigma}^\dagger c_{i+\delta,5,\sigma} - p_{i,5,\sigma}^\dagger c_{i+\delta,4,\sigma})
\]

\[
\Delta H_d = \kappa_7 \sum_{i,\delta,\sigma} (c_{i,2,\sigma} c_{i+\delta,3,\sigma} - c_{i,3,\sigma} c_{i+\delta,2,\sigma}) + \kappa_8 \sum_{i,\delta,\sigma} (c_{i,1,\sigma} c_{i+\delta,5,\sigma} + c_{i,5,\sigma} c_{i+\delta,1,\sigma}) + \kappa_9 \sum_{i,\delta,\sigma} (p_{i,1,\sigma} c_{i+\delta,2,\sigma} + p_{i,2,\sigma} c_{i+\delta,1,\sigma}) + \kappa_{10} \sum_{i,\delta,\sigma} (p_{i,3,\sigma} c_{i+\delta,5,\sigma} + p_{i,5,\sigma} c_{i+\delta,3,\sigma})
\]

where \( \kappa_i \) are the coupling constants.
and
\[ \Delta H_d = \kappa_6 \sum_{i,\delta,\sigma} d_i \left( c_{i,2,\sigma}^{\dagger} c_{i+\delta,2,\sigma}^{\dagger} + c_{i,3,\sigma}^{\dagger} c_{i+\delta,3,\sigma}^{\dagger} \right) \]

represent the extended s-wave, p-wave and d-wave components of the symmetry breaking perturbations. Here \( p_\delta, p'_\delta \) and \( d_\delta \) are p-wave form factors, \( d_\delta \) is the d-wave form factor. The value of these form factors is illustrated in figure 3.

In the subspace spanned by the \( d_{XZ} \) and \( d_{YZ} \) orbitals, there are only two possible terms on the nearest-neighboring bonds and are given by
\[ \Delta H = \eta_2 \sum_{i,\delta,\sigma} \left( c_{i,2,\sigma}^{\dagger} c_{i+\delta,3,\sigma}^{\dagger} + c_{i,3,\sigma}^{\dagger} c_{i+\delta,2,\sigma}^{\dagger} \right) \]

in which \( \eta_2 = \kappa_1 + \kappa_2 + \kappa_6 \).

The 6 allowed symmetry breaking perturbations on the next-nearest-neighboring bonds are given by
\[ \Delta H' = \Delta H_{d'} + \Delta H_{p'} + \Delta H_{d''}, \]

in which
\[ \Delta H_{d'} = \kappa_1 \sum_{i,\delta,\sigma} \left( c_{i,1,\sigma}^{\dagger} c_{i+\delta,5,\sigma}^{\dagger} + c_{i,5,\sigma}^{\dagger} c_{i+\delta,1,\sigma}^{\dagger} \right) \]
\[ \Delta H_{p'} = \kappa_2 \sum_{i,\delta,\sigma} \left( p_{i,\delta,\sigma}^{\dagger} c_{i+\delta,2,\sigma}^{\dagger} + p_{i,\delta,\sigma}^{\dagger} c_{i+\delta,1,\sigma}^{\dagger} \right) \]
\[ \Delta H_{d''} = \kappa_3 \sum_{i,\delta,\sigma} \left( p_{i,\delta,\sigma}^{\dagger} c_{i+\delta,5,\sigma}^{\dagger} + p_{i,\delta,\sigma}^{\dagger} c_{i+\delta,1,\sigma}^{\dagger} \right) \]

and
\[ \Delta H' = \kappa_6 \sum_{i,\delta,\sigma} d_i \left( c_{i,4,\sigma}^{\dagger} c_{i+\delta,5,\sigma}^{\dagger} + c_{i,5,\sigma}^{\dagger} c_{i+\delta,4,\sigma}^{\dagger} \right) \]

(7)

Here \( \delta' \) denotes the vectors connecting next-nearest-neighboring Fe sites and \( p_\delta, p'_\delta \) and \( d_\delta \) are the p-wave and the d-wave form factor on the next-nearest-neighboring bonds, which are illustrated in figure 4. In the subspace spanned by the \( d_{XZ} \) and \( d_{YZ} \) orbitals, there is only one allowable symmetry breaking perturbation on the next-nearest-neighboring bonds, which has the form of
\[ \Delta H = \eta_4 \sum_{i,\delta,\sigma} \left( c_{i,2,\sigma}^{\dagger} c_{i+\delta,3,\sigma}^{\dagger} + c_{i,3,\sigma}^{\dagger} c_{i+\delta,2,\sigma}^{\dagger} \right) \]

Here \( \eta_4 = \kappa_4' \).

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