Orbital-selective superconductivity, gap anisotropy, and spin resonance excitations in a multiorbital $t$-$J_1$-$J_2$ model for iron pnictides

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We study the orbital-selective superconducting pairing in a five-orbital $t$-$J_1$-$J_2$ model for iron pnictides. Depending on the orbital selectivity of electron correlations and the orbital characters along the Fermi surface, the superconducting gap in an $A_{1g}$ pairing state may exhibit anisotropy. This anisotropy varies with the degree of $J_1$-$J_2$ magnetic frustration. In the superconducting state, the frequency dependence of the dynamical spin susceptibility at the antiferromagnetic wave vector ($\pi, 0$) shows a resonance, whose width is enhanced by the orbital selectivity of the superconducting gap. When the degree of the orbital selectivity is sufficiently strong, the resonance peak may be split in two. We discuss the implications of our results on the recent angle-resolved photoemission and neutron-scattering measurements in several superconducting iron pnictides.

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I. INTRODUCTION

One of the central questions in the field of unconventional superconductivity is whether a single mechanism operates across a variety of superconducting (SC) materials, such as iron pnictides, cuprates, heavy fermions, and organic superconductors. In many cases, including for the iron-based superconductors [1–3], superconductivity arises at the border of antiferromagnetic order and electron correlations make the normal state a bad metal. As such, it is desirable to provide an affirmative answer to this question. At the same time, there are some important apparently distinct features in the different material classes. For example, for many heavy fermions, quantum criticality is clearly important, raising the question of whether it is also relevant for the other materials families. In the same vein, there is rapidly growing evidence that multiorbital physics plays an important role in the properties of the iron-based materials, raising the possibility that this physics in general, and orbital selectivity in particular, is not only important to the iron-based materials, but it also represents a mechanism that boosts the SC pairing in general.

Orbital selectivity in the normal state of the iron pnictides and chalcogenides has recently been studied extensively [4–9]. Nondegenerate Fe 3d orbitals, particularly the $xz/yz$ and $xy$ orbitals, yield different mass renormalization and, in the extreme case, an orbitally selective Mott phase. Evidence for such orbital selectivity has come from angle-resolved photoemission spectroscopy (ARPES) measurements [10,11]. To ascertain how orbital-selective correlations may contribute to superconductivity, it is imperative to address how the orbital selectivity affects the nature and properties of the SC state.

Here we ask how orbital selectivity affects spin resonance excitation, which has been studied for over 20 years in cuprates [12] and has also been studied in iron-based superconductors since the field’s inception [13–16]. The specific approach we will take is motivated by two considerations. First, neutron resonance is generally considered to be a spin-triplet excitonic excitation formed out of the electronic and hole quasiparticles of an unconventional superconductor. Second, in iron pnictides, the orbital weight varies on both the hole Fermi pockets near the center of the Brillouin zone (BZ) and the electron Fermi pockets near the edge of the (one-Fe-unit-cell) BZ. The orbital-weight variation on the hole Fermi pocket is primarily among the degenerate 3d $xz$ and $yz$ orbitals. On the other hand, the orbital-weight variation on the electron pockets involves both the 3d $xz/yz$ and $xy$ orbitals. We can therefore expect that orbital selectivity will be most clearly seen in the variation of the SC gap on the electron pockets.

Despite the isotropic SC gap observed in a number of iron-based superconductors [17–21], recent experiments have also identified an anisotropic gap along the Fermi pockets in several iron pnictides [22–25]. In particular, high-resolution ARPES [22] has revealed an anisotropic SC gap along the electron Fermi pockets in the underdoped Na(Fe1−x,Cox)As; it becomes isotropic when the system reaches the overdoped regime. Our discussions earlier then suggest that the underdoped Na(Fe1−x,Cox)As is an ideal system for the study of the influence of orbital selectivity on SC pairing in general and on neutron resonance in particular.

In this paper, we study SC pairing in a five-orbital $t$-$J_1$-$J_2$ model for iron pnictides. We show that the orbital-selective effects of electron correlations generally give rise to orbital-selective SC gaps. In particular, we emphasize two gaps that are associated with the $xz/yz$ and $xy$ orbitals, respectively, which have the same $A_{1g}$ symmetry but different pairing amplitudes. We show how this orbital-selective pairing naturally leads to a gap anisotropy and double spin resonance excitations, defined as having two peaks in the frequency dependence of the dynamical spin susceptibility at a given wave vector. Finally, we discuss the implication of the results for the ARPES and neutron scattering spectra of several SC iron pnictides.

II. MODEL AND METHOD

We consider a five-orbital $t$-$J_1$-$J_2$ model, which is obtained via a strong-coupling perturbative $w$ expansion about the Mott transition (for a recent review, see Ref. [26]). The Hamiltonian
the SC pairing in the above superconductivity, it only provides higher-order corrections to supplementary methods of Ref. [30].

louin zone. The chemical potential is chosen such that the electron binding model along high-symmetry directions of the one-Fe Brillouin zone is shown in Fig. 1. The nearest-neighbor and next-nearest-neighbor (n.n.n., ⟨ij⟩) exchange interactions also arise from a perturbative band structure. The details of the parametrization are discussed by fitting its local-density approximation (LDA) parameters by fitting its local-density approximation (LDA) continuation.

FIG. 1. (Color online) Band structure of the five-orbital tight-binding model along high-symmetry directions of the one-Fe Brillouin zone. The chemical potential is chosen such that the electron binding model along high-symmetry directions of the one-Fe Brillouin zone is shown in Fig. 1. The nearest-neighbor and next-nearest-neighbor (n.n.n., ⟨ij⟩) exchange interactions also arise from a perturbative band structure. The details of the parametrization are discussed by fitting its local-density approximation (LDA) parameters by fitting its local-density approximation (LDA) continuation.

The band structure and the corresponding Fermi surface in the 1-Fe BZ for the tight-binding model at electron doping $x = 0.02$ ($x = n - 6$) are shown, respectively, in Figs. 1 and 2(a). The Fermi surface contains multiple sheets with different orbital characters. The two hole pockets near (0,0) are dominated by the degenerate $xz/yz$ orbitals; the hole pocket near ($\pi, \pi$) has almost completely $xy$ orbital character. The electron pocket near ($\pi, \pi$) [or (0,0)] displays a hybridized $xy$ and $yz$ ($xz$) orbital character [Fig. 2(b)]. The pairing amplitudes are also orbitally-dependent. For $J_1/J_2 \leq 1$, the dominant pairing channel is $s_{\pm, \pm} A_{1g}$ [Fig. 2(c)]. The amplitude of this pairing channel in the $xy$ orbital is larger than that in the $xz/yz$ orbital. The double degeneracy of the $xz$ and $yz$ orbitals gives rise to a subdominant $d_{xz,yz}$ pairing channel with the same $A_{1g}$ symmetry. Its amplitude increases with $J_1/J_2$. The existence of orbital-selective multiple energy scales in pairing is a consequence of the orbital-selective electron correlation effects in the multiorbital model, with the $xy$ orbital typically exhibiting strong correlation effects [4–6]. Correspondingly, the $xy$ orbital has a sizable ratio of $J$ to the renormalized bandwidth, which in turn yields a sizable pairing amplitude [30]. For $J_1/J_2 \gtrsim 1$, the dominant pairing changes to $d_{xz,yz}$ $B_{1g}$, but a similar behavior of the orbital-selective pairing is also found. In the following, we limit our discussion to orbital space [27,33,34]. However, for the purpose of studying possible new characteristics of the spin resonance in the regime where the SC gap is anisotropic through an orbital-selective pairing, we simplify the problem by taking $J_{1(2)}^\alpha = J_{1(2)} \delta_{\alpha \beta}$ (and take $J_2$ to be the energy unit). Correspondingly, we consider intraorbital pairing. For this model, there are then 20 different pairing channels, each with an amplitude and a phase, which are self-consistently determined.

We also calculate the dynamical spin susceptibility in the SC state. At wave vector $q$ and Matsubara frequency $\omega_n$, the spin susceptibility

$$\chi(q,i\omega_n) = \sum_{\alpha \beta} \chi_{\alpha,\beta}(q,i\omega_n),$$

(2)

where

$$\chi_{\alpha,\beta}(q,i\omega_n) = \sum_{\gamma} \left[ (1 + J(q)) \chi^0(q,i\omega_n) \right]_{\alpha,\beta}^{-1} \chi^0_{\gamma,\gamma}(q,i\omega_n),$$

(3)

and

$$\chi^0_{\alpha,\beta}(q,i\omega_n) = \int_{0}^{1/T} dt \ e^{i\omega_n t} \langle T_{\tau} [S_{q\alpha}(\tau) S_{q\beta}^+(0)] \rangle,$$

(4)

Here

$$J(q) = \frac{J_1}{2} (\cos q_x + \cos q_y) + J_2 \cos q_x \cos q_y,$$

(5)

$S_{qq}^\pm = \frac{1}{\sqrt{2}} \sum_{\gamma} e^{i\mathbf{q}\cdot\mathbf{r}} S_{\gamma\gamma}^\pm$, and $\langle \cdots \rangle$ refers to the expectation value with respect to the effective Hamiltonian. The susceptibility at real frequency $\omega$ is then obtained by an analytical continuation $i\omega_n \rightarrow \omega + i0^+$. 

III. RESULTS

A. Multiorbital nature of the Fermi surface and orbital-selective pairing

The band structure and the corresponding Fermi surface in the 1-Fe BZ for the tight-binding model at electron doping $x = 0.02$ ($x = n - 6$) are shown, respectively, in Figs. 1 and 2(a). The Fermi surface contains multiple sheets with different orbital characters. The two hole pockets near (0,0) are dominated by the degenerate $xz/yz$ orbitals; the hole pocket near ($\pi, \pi$) has almost completely $xy$ orbital character. The electron pocket near ($\pi, \pi$) [or (0,0)] displays a hybridized $xy$ and $yz$ ($xz$) orbital character [Fig. 2(b)]. The pairing amplitudes are also orbitally-dependent. For $J_1/J_2 \leq 1$, the dominant pairing channel is $s_{\pm, \pm} A_{1g}$ [Fig. 2(c)]. The amplitude of this pairing channel in the $xy$ orbital is larger than that in the $xz/yz$ orbital. The double degeneracy of the $xz$ and $yz$ orbitals gives rise to a subdominant $d_{xz,yz}$ pairing channel with the same $A_{1g}$ symmetry. Its amplitude increases with $J_1/J_2$. The existence of orbital-selective multiple energy scales in pairing is a consequence of the orbital-selective electron correlation effects in the multiorbital model, with the $xy$ orbital typically exhibiting strong correlation effects [4–6]. Correspondingly, the $xy$ orbital has a sizable ratio of $J$ to the renormalized bandwidth, which in turn yields a sizable pairing amplitude [30]. For $J_1/J_2 \gtrsim 1$, the dominant pairing changes to $d_{xz,yz}$ $B_{1g}$, but a similar behavior of the orbital-selective pairing is also found. In the following, we limit our discussion to
\[
\frac{J_1}{J_2} \ll 1, \quad \text{where the dominant pairing } s_{xy} : A_{1g} \text{ is consistent with the nodeless sign changing pairing observed in experiments.}
\]

### B. Anisotropic superconducting gap

We now turn to how the orbital-selective pairing amplitudes and the orbital character of the Fermi surface affect the momentum distribution of the SC gaps by inducing gap anisotropy, and how the gap amplitudes and the corresponding anisotropy can be tuned by the degree of magnetic frustration of the system. We discuss and compare the results in the five-orbital \(t-J_1-J_2\) model by taking \(J_1/J_2 = 0.1\) and 0.8 for illustrative purpose. For \(J_1/J_2 = 0.1\), the SC gaps are dominated by the \(s_{xy}\) \(A_{1g}\) pairing channel. The amplitudes of this pairing channel in the \(xy\) and \(xz/yz\) orbitals are significantly different, resulting in two characteristic gaps \(\Delta_{xy} \neq \Delta_{xz/yz}\). The excitation gap of the quasiparticles along each hole pocket is only associated with one of them [see Appendix B, Figs. 5(a) and 5(b)], and is isotropic [Fig. 3(a)] since the dominant orbital character of a hole pocket is uniform in momentum space: \(xy\) for the pocket near \((\pi, \pi)\) and \(xz/yz\) for the pocket near \((0, 0)\). On the other hand, the gaps along the electron pockets are strongly anisotropic [Fig. 3(c)]. This is because the electron pocket has a hybridized \(xy\) and \(xz/yz\) orbital character, and the size of the gap at a particular wave vector depends on the dominant orbital character at that point. The gap anisotropy reflects these two characteristic SC gaps \(\Delta_{xy} \neq \Delta_{xz/yz}\) as shown in Fig. 3(c), the gap cannot be fitted by a single gap function \(\Delta_0 \cos k_x \cos k_y\), although the dominant pairing channel is \(s_{xy}\) \(A_{1g}\). Interestingly, the gap anisotropy reduces with increasing \(J_1/J_2\), and an essentially isotropic gap along the electron pocket is recovered at \(J_1/J_2 = 0.8\) [Fig. 3(d)]. To understand this, note that the pairing amplitude of the subdominant \(d_{x^2-y^2}\) \(A_{1g}\) channel in the \(xz/yz\) orbital increases with \(J_1/J_2\). With the contribution from this subdominant channel, the overall gap in the \(xz/yz\) orbital \(\Delta_{xz/yz} \approx \Delta_{xy}\). This then leads to an essentially isotropic gap along the electron pockets.

### C. Spin resonance excitation

The spin excitations in the SC state are also affected by the orbital-selective pairing. We have calculated the dynamical spin susceptibility in the SC state for the \(J_1/J_2 = 0.1\) and 0.8 cases discussed above. The imaginary part of the susceptibility \(\chi''(q, \omega)\) at the antiferromagnetic wave vector \(q = \left(\pi, 0\right)\) exhibits two resonance peaks in the frequency dependence for \(J_1/J_2 = 0.1\) [Fig. 4(a)]. Our detailed analysis finds that the double-peak structure of \(\chi''(q, \omega)\) arises from the different scattering processes that connect two regimes near the electron and hole pockets, as indicated by the arrows in Fig. 2(a). By appearing in the coherence factor of the expression of \(\chi''(q, \omega)\), the different orbital characters of the quasiparticle dispersion put a strong constraint on the scattering processes such that the spin response is enhanced only in certain regimes of the BZ, where the orbital characters of the associated hole and electron bands are compatible. For example, the dominant contribution to the lower-frequency resonance peak at \(\omega_{\|}\) [see Fig. 4(c)] is from scattering between the \(yz\) orbital in regime \(A\) and the \(xy\) orbital in regime \(A'\), as indicated by the dashed arrow in Fig. 2(a). The higher-frequency resonance peak at \(\omega_{\perp}\), on the other hand, is mainly associated with scattering within the \(xy\) orbital between regimes \(B\) and \(B'\) [see Figs. 4(c) and 2(a)]. As a rough estimate, the resonance frequency \(\omega \lesssim E_h + E_e\), where \(E_h\) and \(E_e\) are, respectively, the excitation gaps of
the corresponding hole- and electron-like quasiparticles, i.e., $h = A, B$ and $e = A', B'$. Given the similar orbital character and the proximity to the equivalent points along the Fermi surface, $E'_A \approx E_B$. But the different orbital characters make $E_A \neq E_B$ for $J_1/J_2 = 0.1$. (See Appendix B for more details.)

Therefore, $\omega_L \neq \omega_H$: when this difference is sufficiently large, two resonances appear in the frequency-dependent spectrum. As $J_1/J_2$ increases, both $E_A$ and $E_B$ increase. But due to the subdominant $d_{xz/yz}$ channel in the $xz/yz$ orbital, $E_A$ increases faster, and $E_A \approx E_B$ for $J_1/J_2 = 0.8$. We thus obtain a single resonance peak at $\omega_L \approx \omega_H$, as shown in Figs. 4(b) and 4(d); the multiorbital effect is then reflected in the broadening of the peak.

IV. DISCUSSIONS

Our results elucidate how the orbital selectivity of electron correlations influences superconductivity. We show that the orbital-selective pairing gives rise to gap anisotropy along a Fermi surface with hybridized orbital characters. The magnetic frustration may compete with the orbital selectivity and tune the gap anisotropy. Although we used $J_1/J_2 = 0.1$ to illustrate the simultaneous existence of gap anisotropy and double resonance, this effect persists to $J_1/J_2 \approx 0.5$. This parameter regime is relevant to experiments: we have estimated via a $J_1$-$J_2$-$K$ model that $0.5 \lesssim J_1/J_2 \lesssim 1.5$ for BaFe$_2$As$_2$ [32] and $0.4 \lesssim J_1/J_2 \lesssim 1.2$ for NaFeAs [35]. The range may be further widened with the interorbital exchange couplings. Our results are particularly pertinent to the anisotropic SC gap along the electron pockets in the underdoped Na(Fe$_{1-x}$Co$_x$)$_2$As$_2$ observed in recent ARPES measurements [22]. We are also able to understand the evolution from the anisotropic to the isotropic gap with increasing electron doping: Since the orbital selectivity decreases with electron doping concentration, we expect that the gap will become less anisotropic in the overdoped regime [36].

In previous theoretical works, the anisotropic SC gaps are discussed within the Fermi surface nesting picture [37,38]. Particularly in the underdoped regime, the coexistence of antiferromagnetism and superconductivity may also lead to an anisotropic gap along the reconstructed Fermi surface [39]. In this scenario, the Fermi surface is reconstructed for both the electron and hole pockets. But experimentally, the gap anisotropy was only observed along electron pockets, and the Fermi surface reconstruction for the gap anisotropy was not observed [22]. It is therefore unlikely that the observed anisotropic gap is primarily driven by the coexistence of superconductivity with antiferromagnetic order.

The anisotropic gap along the electron pocket has also been observed in LiFeAs via ARPES [23], and in hole-doped BaFe$_2$As$_2$ via Raman scattering [25]. Given the very different Fermi surface geometry but similar orbital weights along the electron pocket in these materials, it is likely that the gap anisotropy is associated with orbital selectivity. Particularly for hole-doped BaFe$_2$As$_2$, because hole doping tends to increase the orbital selectivity of electron correlations [40], it is natural to propose that the mechanism advanced here underlies this experimental observation as well.

We have also shown that the frequency dependence of the dynamical spin susceptibility at $(\pi,0)$ displays a resonance whose width is enhanced by the orbital-selective SC gap. When the degree of orbital selectivity is sufficiently strong, the resonance peak may be split into two. Recently, experimental evidence for this has come from neutron-scattering observation of double spin resonances in the electron underdoped NaFeAs system [41]. We stress that the double-resonance feature we have discussed refers to two peaks in the frequency dependence of the dynamical spin susceptibility at one single wave vector. This is very different from weak-coupling calculations. For instance, the calculations of Ref. [42] show only one peak in the frequency dependence at any given wave vector, either at the commensurate $\mathbf{q} = (\pi,0)$ or at an incommensurate $\mathbf{q}$. In our case, the peaks in the frequency dependence appear at the same commensurate wave vector $\mathbf{q} = (\pi,0)$; this wave vector is determined by the $\mathbf{q}$ dependence of $J(\mathbf{q})$. As the wave vector moves away from $\mathbf{q} = (\pi,0)$, the two resonances disperse individually; there are still two peaks in the frequency dependence.

Furthermore, we have become aware of another recent theoretical work [43] which considered the effect of twinning on the spin neutron resonances. In that work, the two resonances at the same wave vector $(\pi,0)$ come from two twinned domains, and in each domain there is still a single resonance at each wave vector.

Finally, the degree of electron correlations remains a central issue in the iron-based superconductors [27,33,44–56]. This issue is typically probed in the normal state, through the bad-metal phenomenology in the optical spectrum [57] or the orbital selectivity in the ARPES spectrum [10,11]. Our theoretical results here suggest that this issue can also be fairly directly probed through the orbital selectivity of the gap function in the SC state. ARPES studies along this direction are already quite realistic [58,59], and we anticipate that a
considerable amount of new insights will be derived through further studies.

V. CONCLUSIONS

Our calculation on the superconducting pairing in a five-orbital \( t-J_1-J_2 \) model for iron pnictides reveals an orbital-selective gap structure due to the strong electron correlation effects. While both gaps have \( s_{\pm 1}, a_1g \) symmetry, the different orbital character gives rise to gap anisotropy along the electron pockets. The orbital-selective pairing leads to a broadened neutron resonance at the antiferromagnetic ordering wave vector \( \mathbf{q} = (\pi, 0) \) in the superconducting state. This resonance may even be split into two peaks if the gap is sufficiently anisotropic. Our results have important implications for the ARPES and neutron measurements on the electron underdoped NaFeAs, as well as the Raman scattering results on the hole-doped BaFe\(_2\)As\(_2\). More generally, our results point to ways of probing electron correlation effects of the iron pnictides through the single-particle and spin responses in their superconducting state.

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APPENDIX A: TIGHT-BINDING PARAMETRIZATION

To obtain the tight-binding parameters, we perform local-density approximation (LDA) calculations for NaFeAs, and we fit the LDA band structure to the tight-binding Hamiltonian.

We use the form of the five-orbital tight-binding Hamiltonian given in Ref. [47]. The tight-binding parameters so derived are listed in Table I.

Figure 1 shows the band structure of the five-orbital tight-binding model at \( n = 6.02 \). (a) and (b) Inner and outer hole pockets near \((0, 0)\); (c) hole pockets near \((\pi, \pi)\); (d) electron pocket near \((0, \pi)\).

APPENDIX B: MOMENTUM DISTRIBUTION OF THE EXCITATION GAP OF THE QUASIPARTICLES

In the conventional BCS theory for a single-band model with \( s\)-wave pairing symmetry, the superconducting gap \( \Delta \) is momentum-independent, and the excitation gap for the BCS quasiparticles is \( E(k) = \sqrt{(\xi_k - \mu)^2 + \Delta^2} \), where \( \xi_k \) and \( \mu \) are, respectively, the dispersion and chemical potential of

| \( t_{\alpha}^{\beta} \) parameters of the five-orbital for NaFeAs. |
|-----------------|-----------------|-----------------|-----------------|-----------------|
| \( \epsilon_{\alpha} \) | \( a = 1 \) | \( a = 2 \) | \( a = 3 \) | \( a = 4 \) |
| \( -0.10818 \) | \( -0.10818 \) | \( -0.40863 \) | \( 0.14158 \) | \( -0.40471 \) |
| \( t_{\alpha}^{\mu} \) | \( \mu = x \) | \( \mu = y \) | \( \mu = xy \) | \( \mu = xx \) |
| \( a = 1 \) | \( 0.01398 \) | \( -0.42534 \) | \( 0.24665 \) | \( -0.02238 \) |
| \( a = 3 \) | \( 0.34046 \) | \( -0.08566 \) | \( 0.01052 \) | \( 0.01023 \) |
| \( a = 4 \) | \( 0.16907 \) | \( 0.12337 \) | \( 0.00955 \) | \( -0.02595 \) |
| \( a = 5 \) | \( -0.04400 \) | \( -0.04958 \) | \( 0.01441 \) | \( -0.05132 \) |

- FIG. 5. (Color online) Orbital weights along the Fermi surface of the five-orbital tight-binding model at \( n = 6.02 \). (a) and (b) Inner and outer hole pockets near \((0, 0)\); (c) hole pockets near \((\pi, \pi)\); (d) electron pocket near \((0, \pi)\).
the tight-binding model. For the five-orbital $t$-$J_1$-$J_2$ model, considering the multiorbital nature of the model and the complicated structure of the superconducting pairing function, the excitation gap has a complicated momentum distribution, which can only be obtained numerically. We show the momentum distribution of the excitation gap for $J_1/J_2 = 0.1$ in Fig. 6. Note that due to the momentum-dependent pairing function and the nonzero interorbital hopping, the excitation gap at regime $B$ ($E_B$) is smaller than that along the hole pocket centered at $(\pi, \pi)$. But still $E_B > E_A$ at $J_1/J_2 = 0.1$.

FIG. 6. (Color online) (a) Fermi surface of the five-orbital tight-binding model at $n = 6.02$. Different symbols represent the dominant orbital characters of the pockets. (b) Momentum distribution of the excitation gap of the quasiparticles in the five-orbital $t$-$J_1$-$J_2$ model for $n = 6.02$ and $J_1/J_2 = 0.1$. The black circles show the Fermi surface of the tight-binding model at the same filling. The arrows illustrate the scattering processes that contribute the most to the spin susceptibility in the superconducting state.

[36] More generally, in a model with both orbital-dependent exchange couplings and hopping parameters, whether an anisotropic gap shows up depends on how different the ratio of exchange coupling to the renormalized electronic bandwidth, $I_D^\alpha/D^\alpha$, is among the different orbitals, and this ratio will be tuned by the strength of electron correlations.