



Orbital Selectivity in Electron Correlations and Superconducting Pairing of Iron-Based Superconductors

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Electron correlations play a central role in iron-based superconductors. In these systems, multiple Fe 3d-orbitals are active in the low-energy physics, and they are not all degenerate. For these reasons, the role of orbital-selective correlations has been an active topic in the study of the iron-based systems. In this article, we survey the recent developments on the subject. For the normal state, we emphasize the orbital-selective Mott physics that has been extensively studied, especially in the iron chalcogenides, in the case of electron filling $n \sim 6$. In addition, the interplay between orbital selectivity and electronic nematicity is addressed. For the superconducting state, we summarize the initial ideas for orbital-selective pairing and discuss the recent explosive activities along this direction. We close with some perspectives on several emerging topics. These include the evolution of the orbital-selective correlations, magnetic and nematic orders, and superconductivity as the electron filling factor is reduced from 6 to 5, as well as the interplay between electron correlations and topological band structure in iron-based superconductors.

Keywords: iron-based superconductors, iron selenides, electron correlations, orbital selectivity, orbital-selective pairing

1 INTRODUCTION

Since the discovery of superconductivity in F-doped LaFeAsO [1], the study of iron-based superconductors (FeSCs) has been one of the most active fields in condensed matter physics. The FeSCs feature a large family of materials, which are divided into two major classes, the iron pnictides and iron chalcogenides. The highest superconducting transition temperature (T_c) is at 56 K for the iron pnictides [2, 3] and 65 K or even higher in the single-layer iron chalcogenide [4–8]. It is believed that the high-temperature superconductivity in the FeSCs originates from electron-electron interactions [9–14]. This motivates the consideration of similarities and differences between the FeSCs and other correlated superconductors, especially the cuprates [15]. Similar to the cuprates, most parent compounds of FeSCs have an antiferromagnetically (AFM) ordered ground state [12, 16], and the superconductivity emerges within a certain range of chemical doping. In contrast with the cuprates, most, though not all, parent iron pnictides and iron chalcogenides are metals

[9–14], typically exhibiting electron and hole Fermi pockets as revealed by angle resolved photoemission spectroscopy (ARPES) measurements [17].

These properties raise important questions about the role of electron correlations in the FeSCs and how the correlations interplay with the superconductivity in these materials. In this review, we survey recent developments on the orbital-selective electron correlations in the FeSCs.

1.1 Electron Correlations in the FeSCs

We start by outlining the two important issues regarding the electron correlations of the FeSCs. The first issue concerns the overall strength of the electron correlations. The parent FeSCs are bad metals [18, 19], with the room-temperature electrical resistivities reaching the Mott-Ioffe-Regel limit and corresponding to the product of Fermi wave vector and mean-free path being of order unity. The Mott-Ioffe-Regel criterion [20] signifies a system with a metallic ground state and with strong electron correlations. Further evidence for the bad metal behavior comes from the optical conductivity measurement, which showed that the Drude weight is considerably reduced by the electron correlations [21–25]. In relation to this, the effective mass of the single-electron excitations is much enhanced from their non-interacting counterpart, with the enhancement factor ranging from 3 to 20 across the FeSC families [17, 26–30]. These bad-metal characteristics, together with the existence of a large spin spectral weight observed by neutron scattering experiments (already for the parent iron pnictides [31, 32]) and a number of other characteristics from measurements such as the X-ray emission [33] and Raman scattering [34] spectroscopies, imply that the parent FeSCs possess a considerable degree of electron correlations. Indeed, the integrated spin spectral weight measured from the dynamical spin susceptibility is at the order of $3 \mu_B^2$ per Fe in the parent iron pnictides, which is too large to be generated by particle-hole excitations in the Fermi-surface nesting picture but is consistent with the spin degrees of freedom being dominated by the contributions from the incoherent electronic excitations [32]. The total spin spectral weight is even larger in the iron chalcogenides [11–13].

All of these experimental results suggest that the parent FeSCs are in the bad metal regime which is close to a metal-to-Mott-insulator transition (MIT). This regime can be described by a w -expansion around the MIT within the incipient Mott picture [18, 35, 36], where w is the overall fraction of the electron spectral weight that occupies the coherent itinerant part. To the zeroth order in w , the spin degrees of freedom appear in the form of quasilocalized magnetic moments with frustrated exchange interactions; this picture anchors the description of the AFM order and the associated magnetic fluctuations. The importance of such incoherent electronic excitations to the low-energy physics of the FeSCs has also been emphasized from related considerations [37–48, 50–56].

1.2 Orbital-Selective Correlations and Orbital-Selective Superconducting Pairing

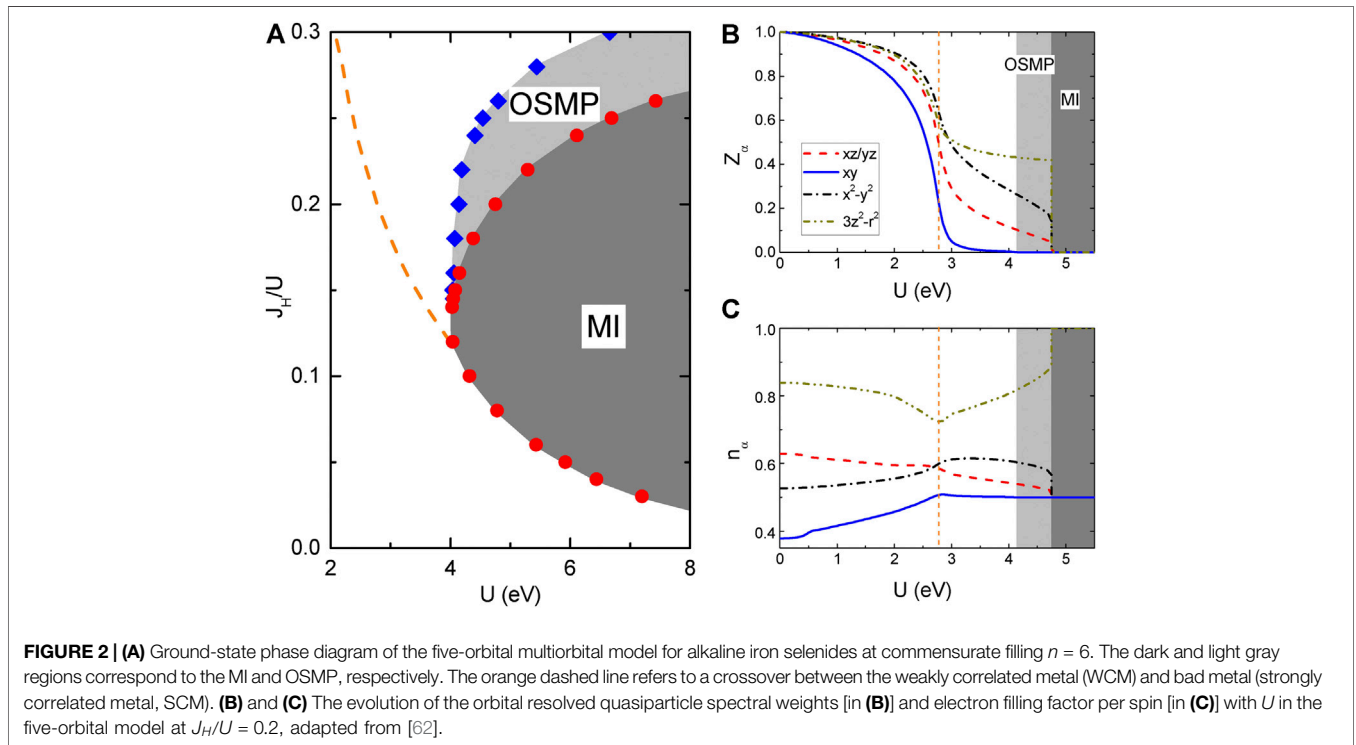
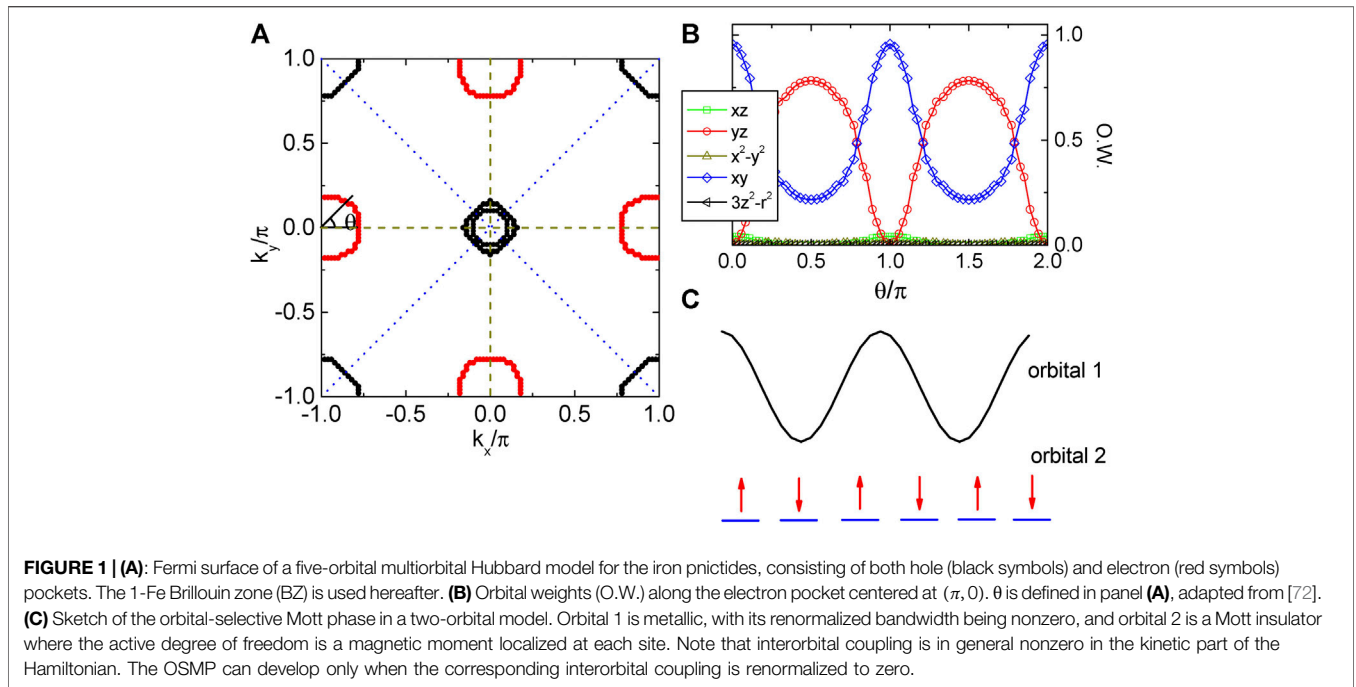
The other, related, issue is the multiorbital nature of the low-energy electronic structure of FeSCs. As illustrated in

Figures 1A,B, the Fermi surface of the parent FeSCs consists of several pockets, and each pocket contains contributions from multiple Fe $3d$ orbitals. The Fe ion has a valence of +2, corresponding to $n = 6$ electrons occupying its five $3d$ orbitals. These orbitals are not all degenerate, and there are an even number of electrons per Fe site. Thus, the MIT in such systems, if it does take place, is expected to be quite distinct. The common tetragonal structure of FeSCs only preserves the degeneracy between the d_{xz} and d_{yz} orbitals. The partially lifted orbital degeneracy may cause the effects of the electron correlations to be orbital dependent. As a simple example, consider a system with two nondegenerate orbitals. The bandwidths or the electron fillings in these two orbitals are generically different. Thus, even for the same Coulomb repulsion, the degree of electron correlations is expected to be different, and this difference is denoted as orbital selectivity. The case of extreme distinction corresponds to an orbital-selective Mott phase (OSMP): as sketched in **Figure 1C**, orbital 2 becomes a MI where the electrons are fully localized, while orbital 1 remains metallic. The notion that some orbitals can be driven through a delocalization-localization transition while the others remain delocalized can be traced back to the physics of Kondo destruction in f -electron physics [57–59]. For d -electron systems, the OSMP was first considered for $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$ [60] within a multiorbital model whose kinetic part is diagonal in the orbital basis, for which the orbital and band bases are the same.

An important characteristic of the FeSCs is that different orbitals are coupled to each other, as dictated by the crystalline symmetry, and this makes the consideration of the OSMP especially nontrivial. Here, the treatment of the orbital-selective correlation effect in multiorbital models with such interorbital coupling was introduced in [61]. The analysis of [61] sets the stage for realizing

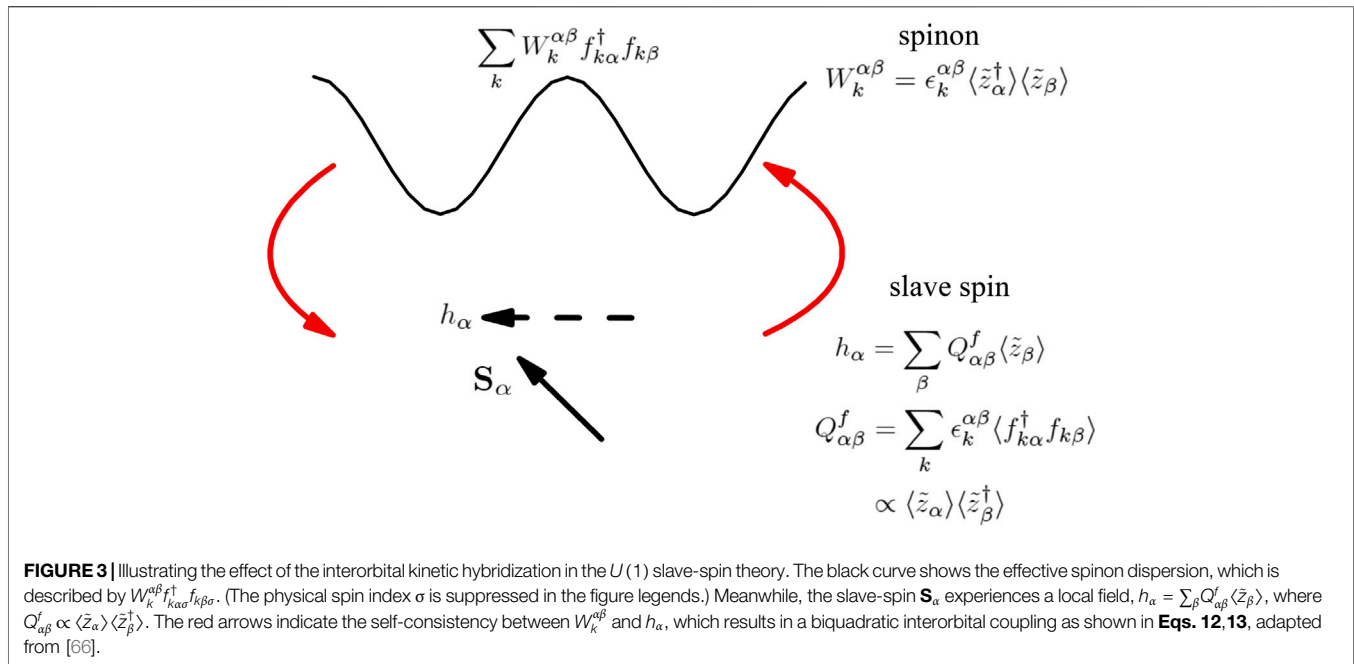
- (1) An OSMP in the multiorbital Hubbard models for the iron chalcogenides [62]. Here, the d_{xy} states are localized while the other $3d$ states are delocalized with nonzero coherent spectral weight. This is so in spite of the fact that the bare Hamiltonian contains a kinetic coupling between the d_{xy} and other $3d$ orbitals of Fe;
- (2) A distinct crossover [dashed line, **Figure 2A**], with the increasing strength of the interactions, from the regime of a weakly correlated metal into an OSMP-proximate regime [62–64]. In this regime, dubbing a “strongly correlated metal” (SCM), all the orbitals remain itinerant but some of the orbitals have substantially reduced and orbitally differentiated quasiparticle weights.

The theoretical work went together with the experimental observation of an OSMP in several iron chalcogenides [29, 30, 65]. The mechanism for the suppression of interorbital coupling by the correlation effects, which allows for the OSMP, is further clarified in terms of a Landau free-energy functional in [66]. (Related microscopic studies have been carried out in [67].) In all these analyses, the interplay between the Hund’s coupling (J_H) and Hubbard interaction (U) plays a crucial role (see the discussions below and in



Figures 2, 3). A complementary approach to the correlation effects describes the localization-delocalization phenomena in the form of orbitally differentiated coherence-incoherence crossover, referred to as Hund’s metal [39, 68, 69]; this approach leads to results that share considerable commonality to those arising from the orbital-selective

Mott physics. Very recently, the low-temperature emergence of the OSMP has been identified in $\text{FeTe}_{1-x}\text{Se}_x$ near the FeTe end ($x \rightarrow 0$) [70]. In addition, the orbital-selective Mott correlations have been advanced as the mechanism for the striking renormalization to the Fermi surface and low-energy electronic dispersion of LiFeAs [71].



The recognition of the orbital-selective correlations has led to the initial work on the orbital-selective pairing [72]. This notion was motivated by—and applied to the analysis of—the properties of the superconducting state in the under-electron-doped NaFeAs [73]. In other theoretical approaches, various forms of orbital-selective pairing were considered in the contexts of the FeSCs [74, 75].

1.3 Perspective and Objective

Because most of the parent compounds are not Mott insulators (MIs), assessing the strength of electron correlations has been an important topic since the beginning of the FeSC field. In principle, the AFM ground state and the superconducting state nearby may originate from the Fermi surface nesting mechanism of a weak-coupling theory [76–80].

As outlined above, the correlation strength of the FeSCs is intermediate: here, the Coulomb repulsion and the bandwidth are similar in magnitude, and the competition between the electrons' itinerancy and localization is the most fierce. Spectroscopy measurements have provided ample evidence that, for the parent compounds of the FeSCs, the incoherent part of the electron spectral weight $(1-w)$ is larger than the coherent counterpart w , which provides a microscopic definition of a bad metal. The full force of the electron correlations in the FeSCs has now become quite apparent [13, 81–98]. In leading toward this understanding, the orbital-selective aspects of the correlations and pairing have played an important role.

Recognizing that the study of the orbital-selective correlations and pairing has had explosive developments in recent years, here we survey the recent theoretical progress on the orbital selectivity for both the normal and superconducting states in multiorbital models for FeSCs. We focus on the MIT at $n = 6$ and show how the Hund's coupling stabilizes a bad metal phase with a large

orbital selectivity. Especially for the iron chalcogenides, an OSMP—with the d_{xy} orbital being Mott localized and the other $3d$ orbitals remaining itinerant—appears in the phase diagram. We further discuss the experimental evidences for the orbital selectivity as well as the implications of the orbital-selective correlations for the magnetism, electronic nematicity, and superconductivity of FeSCs. For the superconducting state, we summarize how the orbital-selective superconducting pairing not only accounts for the strikingly large superconducting gap anisotropy, but also gives rise to novel pairing states. The latter clarifies a number of puzzles in alkaline iron selenides. We note that the orbital-selective correlations correspond to a very broad and active subject. Thus, instead of aiming to be comprehensive, here we review the conceptual and model studies of the orbital-selective Mott physics in the normal state and, relatedly, of the orbital-selective pairing in the superconducting state.

We also note that standard weak-coupling approaches (see, e.g., [99]) do not capture the orbital-selective Mott regime. However, the orbital-selective correlation effects, with some orbitals having substantially reduced and orbitally differentiated quasiparticle weights similar to what we summarize here, have more recently been incorporated in a phenomenological way [100, 101] into the weak-coupling approaches. Some of the limitations of the weak-coupling analyses have been suggested [100, 101] to be remedied by this phenomenological approach, but other issues inherent to the weak-coupling treatments—such as the under-accounting of the spin spectral-weight—remain [31] within the phenomenological approach.

The rest of the manuscript is organized as follows: in **Section 2** we first briefly introduce the multiorbital Hubbard model for FeSCs and outline the $U(1)$ slave-spin theory [63, 66] used for studying the MIT in this model. This approach accounts for the proper symmetry of the involved phases. We also consider a

Landau free-energy functional that demonstrates how an OSMF can be robust in spite of a nonzero bare interorbital kinetic hybridization. We proceed to address the bad metal behavior and the OSMF that is identified in the phase diagram of this model and discuss the implication for the nematic phase of iron selenide. In **Section 3** we set up the multiorbital t-J model for studying the superconductivity of FeSCs and discuss the main results of the orbital-selective superconducting pairing and its implications. In **Section 4** we present a brief summary and an outlook for several emerging directions.

2 ORBITAL-SELECTIVE CORRELATIONS IN THE NORMAL STATE OF IRON-BASED SUPERCONDUCTORS

To study the effects of orbital-selective correlation, we consider a multiorbital Hubbard model for the FeSCs. The Hamiltonian reads

$$H = H_{TB} + H_{int}. \quad (1)$$

Here H_{TB} is a tight-binding model that contains multiple Fe $3d$ orbitals and preserves the tetragonal lattice symmetry of the FeSCs in the normal state. The tight-binding parameters are obtained by fitting to the DFT band structure of specific compounds. A number of tight-binding models, ranging from two to five orbital models, have been proposed for FeSCs [77, 78, 102–106]. In principle, any of these models can be used to illustrate the correlation effects. In practice, we adopt the more realistic five-orbital models, which capture the salient features of the electronic structure and Fermi surface and facilitate a direct comparison to the experimental results. As already stressed, the tetragonal symmetry dictates that interorbital hopping amplitudes are allowed and the fitted tight-binding parameters do show that such hopping amplitudes are nonzero. Specifically, the noninteracting part of the Hamiltonian is written as

$$H_{TB} = \frac{1}{2} \sum_{ij\alpha\beta\sigma} t_{ij}^{\alpha\beta} d_{i\alpha\sigma}^\dagger d_{j\beta\sigma} + \sum_{i\alpha\sigma} (\Lambda_\alpha - \mu) d_{i\alpha\sigma}^\dagger d_{i\alpha\sigma}. \quad (2)$$

Here, $d_{i\alpha\sigma}^\dagger$ creates an electron in orbital ($= 1, \dots, 5$) with spin σ at site i ; $t_{ij}^{\alpha\beta}$, with $i \neq j$, are the tight-binding parameters, with those for $\alpha \neq \beta$ describing the interorbital couplings; and Λ_α refers to the orbital-dependent energy levels, associated with the crystal field splittings, and is diagonal in the orbital basis. In particular, the C_4 symmetry dictates that d_{xz} and d_{yz} are degenerate, but no symmetry enforces any degeneracy between the d_{xy} orbital and the other orbitals. Indeed, for any orbital $\beta \neq xy$, $\Lambda_{xy,\beta} \equiv \Lambda_{xy} - \Lambda_\beta \neq 0$. The chemical potential μ controls the total electron number n that occupies the $3d$ orbitals of each Fe site. In the model, $n = 6$ for the parent (undoped) compound.

The onsite interaction H_{int} takes the following form:

$$H_{int} = \frac{U}{2} \sum_{i,\alpha,\sigma} n_{i\alpha\sigma} n_{i\alpha\bar{\sigma}} + \sum_{i,\alpha < \beta,\sigma} \{ U' n_{i\alpha\sigma} n_{i\beta\bar{\sigma}} + (U' - J_H) n_{i\alpha\sigma} n_{i\beta\sigma} \} - J_H \sum_{i,\alpha < \beta,\sigma} (d_{i\alpha\sigma}^\dagger d_{i\alpha\bar{\sigma}} d_{i\beta\bar{\sigma}}^\dagger d_{i\beta\sigma} + d_{i\alpha\sigma}^\dagger d_{i\alpha\bar{\sigma}}^\dagger d_{i\beta\sigma} d_{i\beta\bar{\sigma}}), \quad (3)$$

where $n_{i\alpha\sigma} = d_{i\alpha\sigma}^\dagger d_{i\alpha\sigma}$. Here, U and U' denote the intraorbital and interorbital repulsion, respectively, and J_H is the Hund's rule exchange coupling. These coupling parameters satisfy $U' = U - 2J_H$ [107].

2.1 The U(1) Slave Spin Theory

The multiorbital system described by the model in **Eq. 1** undergoes a MIT driven by the electron correlations at any commensurate electron filling. This transition can be studied by using a $U(1)$ slave-spin theory [63, 66]. In this subsection we summarize the theoretical approach for the MIT and show that, besides the conventional metallic and Mott insulating phases, there is also an OSMF as the ground state of the system.

Slave-particle (or parton) construction has a long history in the study of correlated systems [108–111]. For the single orbital Hubbard model, the slave boson method of [111] has been successfully applied. But the construction of this theory for an M -orbital Hubbard model would require 4^M slave bosons, which is not feasible for the case of FeSCs where $M = 5$. More recent variations include slave rotor [112] and Z_2 slave-spin [113] formulations. For the purpose of describing the MIT, the Z_2 gauge structure [113–115] is problematic given that the MIT concerns the (de)localization of a $U(1)$ -symmetric charge degrees of freedom [116]. The $U(1)$ slave-spin formulation is more suitable, given that it captures the symmetry of the pertinent phases.

In the $U(1)$ slave-spin formulation [63, 66], the electron creation operator is represented as

$$d_{i\alpha\sigma}^\dagger = S_{i\alpha\sigma}^+ f_{i\alpha\sigma}^\dagger. \quad (4)$$

Here the XY component of a quantum $S = 1/2$ spin operator ($S_{i\alpha\sigma}^+$) is used to represent the charge degree of freedom of the electron at each site i , for each orbital α and each spin flavor σ . Correspondingly, the fermionic “spinon” operator, $f_{i\alpha\sigma}^\dagger$, is used to carry the spin degree of freedom. To restrict the Hilbert space to the physical one, a local constraint

$$S_{i\alpha\sigma}^z = f_{i\alpha\sigma}^\dagger f_{i\alpha\sigma} - \frac{1}{2}, \quad (5)$$

is implemented. This representation contains a $U(1)$ gauge redundancy corresponding to $f_{i\alpha\sigma}^\dagger \rightarrow f_{i\alpha\sigma}^\dagger e^{-i\theta_{i\alpha\sigma}}$ and $S_{i\alpha\sigma}^+ \rightarrow S_{i\alpha\sigma}^+ e^{i\theta_{i\alpha\sigma}}$. In parallel to the slave-rotor approach [112], in this representation, the slave spins carry the $U(1)$ charge. Correspondingly, the $U(1)$ slave-spin theory can naturally describe the MIT, including in multiorbital settings.

To construct a saddle-point theory, one has to work within the Schwinger boson representation of the slave spins. A detailed derivation of the saddle-point equations can be found in [63, 66]. Here, for conciseness, we will mostly stay in the slave-spin representation and simply describe the main results. To ensure that the quasiparticle spectral weight in the noninteracting limit is normalized to 1 at the saddle point level, and in analogy to the standard treatment in the slave-boson theory [111], we define a dressed operator:

$$\hat{z}_{i\alpha\sigma}^\dagger = P_{i\alpha\sigma}^+ S_{i\alpha\sigma}^+ P_{i\alpha\sigma}^-, \quad (6)$$

where the projectors $P_{i\alpha\sigma}^\pm = 1/\sqrt{1/2 + \delta \pm S_{i\alpha\sigma}^z}$ and δ is an infinitesimal positive number to regulate $P_{i\alpha\sigma}^\pm$. Next we rewrite **Eq. 4** with the dressed operator to $d_{i\alpha\sigma}^\dagger = \tilde{z}_{i\alpha\sigma}^\dagger f_{i\alpha\sigma}^\dagger$. The Hamiltonian, **Eq. 1**, is then effectively rewritten as

$$H = \frac{1}{2} \sum_{ij\alpha\beta\sigma} t_{ij}^{\alpha\beta} \tilde{z}_{i\alpha\sigma}^\dagger \tilde{z}_{j\beta\sigma} f_{i\alpha\sigma}^\dagger f_{j\beta\sigma} + \sum_{i\alpha\sigma} (\Lambda_\alpha - \mu) f_{i\alpha\sigma}^\dagger f_{i\alpha\sigma} - \lambda_{i\alpha\sigma} [f_{i\alpha\sigma}^\dagger f_{i\alpha\sigma} - S_{i\alpha\sigma}^z] + H_{\text{int}}^S \quad (7)$$

Here, we have introduced the Lagrange multiplier $\lambda_{i\alpha\sigma}$ to enforce the constraint in **Eq. 5**. In addition, H_{int}^S is the interaction Hamiltonian, **Eq. 3**, rewritten in terms of the slave-spin operators [61] as follows:

$$H_{\text{int}}^S = \sum_i \left\{ \frac{U'}{2} \left(\sum_{\alpha\sigma} S_{i\alpha\sigma}^z \right)^2 + \frac{U-U'}{2} \sum_{\alpha} \left(\sum_{\sigma} S_{i\alpha\sigma}^z \right)^2 - \frac{J_H}{2} \sum_{\sigma} \left(\sum_{\alpha} S_{i\alpha\sigma}^z \right)^2 - J_H \sum_{\alpha < \beta} [S_{i\alpha\uparrow}^+ S_{i\alpha\downarrow}^+ S_{i\beta\downarrow}^- S_{i\beta\uparrow}^-] - S_{i\alpha\uparrow}^+ S_{i\alpha\downarrow}^+ S_{i\beta\downarrow}^- S_{i\beta\uparrow}^- + H.c. \right\} \quad (8)$$

One practical way is to neglect the spin flip terms in **Eq. 8** without affecting the qualitative results [63]. The quasiparticle spectral weight is defined as

$$Z_{i\alpha\sigma} = |z_{i\alpha\sigma}|^2 \equiv |\langle \tilde{z}_{i\alpha\sigma} \rangle|^2 \quad (9)$$

A metallic phase corresponds to $Z_{i\alpha\sigma} > 0$ for all orbitals, and a Mott insulator corresponds to $Z_{i\alpha\sigma} = 0$ in all orbitals with a gapless spinon spectrum.

At the saddle-point level, the slave-spin and spinon operators are decomposed and the constraint is treated on average. We obtain two effective Hamiltonians for the spinons and the slave spins, respectively:

$$H_f^{\text{eff}} = \sum_{k\alpha\beta} [\epsilon_k^{\alpha\beta} \langle \tilde{z}_\alpha^\dagger \rangle \langle \tilde{z}_\beta \rangle + \delta_{\alpha\beta} (\Lambda_\alpha - \lambda_\alpha + \tilde{\mu}_\alpha - \mu)] f_{k\alpha}^\dagger f_{k\beta}, \quad (10)$$

$$H_S^{\text{eff}} = \sum_{\alpha\beta} [Q_{\alpha\beta}^f (\langle \tilde{z}_\alpha^\dagger \rangle \langle \tilde{z}_\beta \rangle + \langle \tilde{z}_\beta \rangle \langle \tilde{z}_\alpha^\dagger \rangle) + \delta_{\alpha\beta} \lambda_\alpha S_\alpha^z] + H_{\text{int}}^S, \quad (11)$$

where $\delta_{\alpha\beta}$ is Kronecker delta function, $\epsilon_k^{\alpha\beta} = 1/N \sum_{ij\sigma} t_{ij}^{\alpha\beta} e^{ik(r_i-r_j)}$, $Q_{\alpha\beta}^f = \sum_{k\sigma} \epsilon_k^{\alpha\beta} \langle f_{k\alpha\sigma}^\dagger f_{k\beta\sigma} \rangle / 2$, and $\tilde{z}_\alpha^\dagger = \langle P_\alpha^+ \rangle S_\alpha^+ \langle P_\alpha^- \rangle$. Finally, $\tilde{\mu}_\alpha$ is an effective onsite potential defined as $\tilde{\mu}_\alpha = 2\bar{e}_\alpha \eta_\alpha$, where $\bar{e}_\alpha = \sum_{\beta} (Q_{\alpha\beta}^f \langle \tilde{z}_\alpha^\dagger \rangle \langle \tilde{z}_\beta \rangle + \text{c.c.})$ and $\eta_\alpha = (2n_\alpha^f - 1) / [4n_\alpha^f (1 - n_\alpha^f)]$, with $n_\alpha^f = 1/N \sum_k \langle f_{k\alpha}^\dagger f_{k\alpha} \rangle$.

We study the MIT in the paramagnetic phase preserving the translational symmetry and can hence drop the spin and/or site indices of the slave spins and the Lagrange multiplier in the saddle-point equations, **(10)(11)**. The parameters z_α and λ_α are then solved self-consistently.

2.2 Landau Free-Energy Functional for Orbital-Selective Mott Physics

As described earlier and illustrated in **Figure 1C**, the OSMP can develop only when (at least) one of the orbitals becomes localized,

while the others remain delocalized. How can this be possible in a multiorbital model with nonzero bare interorbital coupling between orbitals? While the $U(1)$ slave-spin approach found an affirmative answer, it is important to ask whether the result of this microscopic approach is robust. To do so, we construct a Landau theory based on the slave-spin formulation [66]. We start from the saddle-point Hamiltonians **Eq. 10**. Consider first **Eq. 10**, where the kinetic hybridization between two different orbitals $\alpha \neq \beta$ is $W_k^{\alpha\beta} f_{k\alpha}^\dagger f_{k\beta}$, with $W_k^{\alpha\beta} = \epsilon_k^{\alpha\beta} \langle \tilde{z}_\alpha^\dagger \rangle \langle \tilde{z}_\beta \rangle \propto \langle \tilde{z}_\alpha^\dagger \rangle \langle \tilde{z}_\beta \rangle$. Because $f_{k\alpha}^\dagger f_{k\beta}$ is conjugate to $W_k^{\alpha\beta}$, from the linear response theory, it is easy to show that $\langle f_{k\alpha}^\dagger f_{k\beta} \rangle \propto W_k^{\alpha\beta} \propto \langle \tilde{z}_\alpha \rangle \langle \tilde{z}_\beta^\dagger \rangle$. As a result, the kinetic hybridization of the spinons is

$$\langle H_f^{\text{eff}} \rangle_{\alpha\beta} = \sum_k \epsilon_k^{\alpha\beta} \langle \tilde{z}_\alpha^\dagger \rangle \langle \tilde{z}_\beta \rangle \langle f_{k\alpha}^\dagger f_{k\beta} \rangle \propto |\langle \tilde{z}_\alpha \rangle|^2 |\langle \tilde{z}_\beta \rangle|^2. \quad (12)$$

Next for **Eq. 11**, we can define an effective field of $h_\alpha = \sum_{\beta} Q_{\alpha\beta}^f \langle \tilde{z}_\beta \rangle$. For similar reasoning as mentioned above, we obtain $Q_{\alpha\beta}^f \propto \langle \tilde{z}_\alpha \rangle \langle \tilde{z}_\beta^\dagger \rangle$, which leads to

$$\langle H_S^{\text{eff}} \rangle_{\alpha\beta} \rightarrow |\langle \tilde{z}_\alpha \rangle|^2 |\langle \tilde{z}_\beta \rangle|^2. \quad (13)$$

Note that **Eq. 13** are natural consequence of **Eq. 11**, and this self-consistent procedure of the saddle-point theory is illustrated in **Figure 3**. Based on **Eq 12** we can construct a Landau free-energy functional in terms of the quasiparticle weights, z_α . For simplicity of notation, we consider a two-orbital model, but our analysis straightforwardly generalizes to the case of more than two orbitals. The free-energy density reads

$$f = \sum_{\alpha=1,2} (r_\alpha |z_\alpha|^2 + u_\alpha |z_\alpha|^4) + \nu |z_1|^2 |z_2|^2, \quad (14)$$

in which the quadratic terms $r_\alpha |z_\alpha|^2$ arise from the kinetic energy of the saddle-point Hamiltonian in **Eq. 11** [as well as in **Eq. 10**]. The biquadratic coupling ν term comes from the kinetic hybridization in **Eq 13**. The biquadratic nature of this intraorbital coupling—as opposed to the bilinear form—is crucial to the stabilization of an OSMP. This can be seen by taking the derivatives of **Eq. 14** with respect to $|z_\alpha|$. Besides the conventional metallic phase with $|z_1| \neq 0$, $|z_2| \neq 0$ and the MI with $|z_1| = |z_2| = 0$, **Eq. 14** supports a third solution with $|z_1| = 0$, $|z_2| = \sqrt{-(r_2/2u_2)}$ (or $|z_2| = 0$, $|z_1| = \sqrt{-(r_1/2u_1)}$), which corresponds to an OSMP.

2.3 Orbital-Selective Mott Physics in FeSCs

We now turn to microscopic studies of the MIT. A realistic microscopic model for FeSCs is described in **Eq. 1**. Owing to its multiorbital nature, the MIT in this model shows unique features. First, the parent compound corresponds to $n = 6$, containing an even number of electrons per Fe ion. Since Mott transition is more readily defined in systems with an odd number of electrons per unit cell, this makes it a nontrivial question whether the model generally supports a MI in the strong correlation limit. Second, besides the Coulomb repulsion U , the Hund's rule coupling J_H also plays a very important role in settling the ground states of the model and, as we will see, plays an important role in realizing an OSMP.

The MIT in the multiorbital model for FeSCs at $n = 6$ has been studied by using the slave-spin methods introduced in **Section 2.1**. In the following, we present the resulting phase diagram for alkaline iron selenides. As shown in **Figures 2A**, a MI is generally stabilized in the phase diagram when the Coulomb repulsion U is sufficiently strong. The critical value U_c for the Mott transition displays a nonmonotonic dependence on the Hund' coupling J_H . This is a general feature of the MIT of the multiorbital Hubbard model away from half-filling and can be understood as follows [63]: naively the MIT takes place when the Mott gap at the atomic limit G_A approaches the bare bandwidth of the tight-binding model D . In the weak J_H limit, the MI is dominated by the low-spin $S = 1$ configuration and correspondingly $G_A \sim U + J_H$. This leads to $U_c \sim D/(1 + J_H/U)$; namely, U_c decreases with J_H/U . On the other hand, for large J_H/U , the high-spin $S = 2$ configuration dominates in the MI state and $G_A \sim U - 3J_H$. Consequently, $U_c \sim D/(1 - 3J_H/U)$ increases with J_H/U .

Importantly, the Hund's coupling already strongly affects the properties of the metallic state. For $J_H/U \geq 0.1$, the system undergoes a crossover from a weakly correlated metal (WCM) to a bad metal with increasing U [shown as the dashed line in **Figure 2A**]. As illustrated in **Figure 2B**, the orbital resolved quasiparticle spectral weight Z_α in each orbital α rapidly drops across this crossover. Inside the bad metal phase, Z_α becomes strongly orbital dependent. This large orbital-selective correlation is rather surprising given that the strength of the onsite interaction is identical for each orbital. To understand the strong orbital selectivity, note that the Hund's coupling suppresses interorbital correlations. For large Hund's coupling, this causes an effective orbital decoupling between any two nondegenerate orbitals and hence promotes the $S = 2$ high-spin configuration in the bad metal regime. As a result of the orbital decoupling, the correlation effect in each nondegenerate orbital depends on its filling factor n_α . This is clearly seen in **Figures 2B,C**: the d_{xy} orbital experiences the strongest correlation effect and n_{xy} is the closest to $1/2$; while the least correlated $3z^2 - r^2$ orbital has the largest filling away from $1/2$.

Further increasing U in the bad metal phase, the system undergoes a transition to the OSMP. In this phase the d_{xy} orbital is fully Mott localized ($Z_{xy} = 0$) whereas the electrons in other Fe $3d$ orbitals are still itinerant ($Z_\alpha > 0$). Besides the aforementioned orbital decoupling effect, several other factors are also important for stabilizing the OSMP. First, the bare bandwidth projected to the d_{xy} orbital is smaller than that of the other orbitals. Second, the orbital fluctuations in the degenerate d_{xz} and d_{yz} orbitals make the threshold interaction needed for their Mott localization larger than that for the nondegenerate d_{xy} orbital, although the filling factors of these three orbitals are all close to $1/2$. Taking into account all these factors, the d_{xy} orbital has the lowest interaction threshold for the Mott transition, at which the OSMP takes place. Because only the d_{xy} orbital is Mott localized, the OSMP survives nonzero doping, while the MI can only be stabilized as a ground state at commensurate fillings. It is worth noting that, for a particular system, whether an OSMP is stabilized depends on the competition of the above factors. For example, the OSMP is stabilized in the model for $K_x\text{Fe}_{2-y}\text{Se}_2$ but not that for LaOFeAs

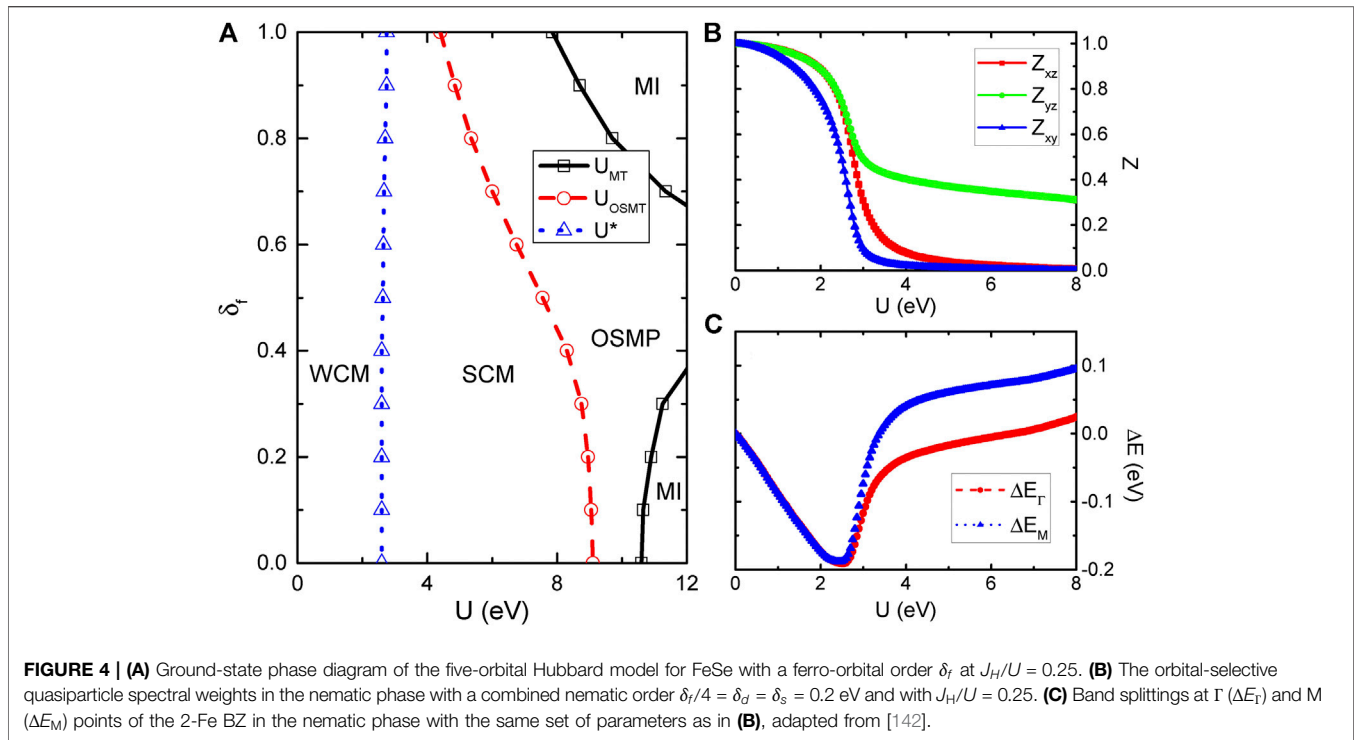
[62, 63]. (However, the OSMP-proximate SCM regime, which displays strong orbital selectivity in the quasiparticle weight, does exist in the model for LaOFeAs [63].) This is mainly because the bare bandwidth of the d_{xy} orbital is sufficiently smaller than that of the other orbitals in $K_x\text{Fe}_{2-y}\text{Se}_2$, but the difference in the bare bandwidths is less pronounced in the case of LaOFeAs . Even though an OSMP is not stabilized as the true ground state for this iron pnictide, it is energetically competitive [63]. As such, the OSMP can be viewed as the anchoring point for the strong orbital-selective correlation effects and the associated bad metal behavior both in the case of the iron selenides and iron pnictides.

The OSMP is supported by additional theoretical studies. Orbital differentiation in $K_x\text{Fe}_{2-y}\text{Se}_2$ has also been analyzed in DFT + DMFT calculations [117]. Besides the case of the multiorbital models for $K_x\text{Fe}_{2-y}\text{Se}_2$ and related iron chalcogenides and LiFeAs , strong orbital-selective correlations and OSMP have been evidenced in several other multiorbital models for FeSCs [40, 118, 119]. Additionally, the conclusions of the $U(1)$ slave-spin analysis, regarding both the rapid crossover into the OSMP-proximate SCM regime and the development of the OSMP phase, are confirmed by studies of the multiorbital Hubbard models for the FeSCs based on a Gutzwiller approximation [120]. Note that there has also been theoretical efforts to feed the results of the mechanistic studies on the orbital-selective correlations into the weak-coupling approaches, by incorporating the orbital selectivity in the weak-coupling calculations via phenomenological parameters [100, 101]. Experimentally, ARPES measurements provide clear evidence [29, 30] for OSMP in iron chalcogenides. As temperature goes above about 100 K, the spectral weight for the d_{xy} orbital vanishes, while that for the $d_{xz/yz}$ orbitals does not change much [30]. The behavior is similar for all the iron chalcogenides studied as well as for the alkaline iron pnictide [121], which suggests a universal crossover to the OSMP in FeSCs [30]. Additional evidence for the OSMP has come from THz spectroscopy [122], Hall measurements [123], pump-probe spectroscopy [124], and high-pressure transport measurements [125]. Moreover, a variety of other Fe-based systems have been studied for the orbital-selective Mott behavior [82–87, 98]. We note in passing that related orbital-selective correlation effects have recently been discussed in the multiorbital $5f$ -based actinide systems [126, 127].

2.4 Orbital Selectivity in the Nematic Phase of FeSe

In most iron pnictides, lowering the temperature in the parent compounds gives rise to a tetragonal-to-orthorhombic structural transition at T_s . Right at or slightly below T_s , the system exhibits a transition to a collinear $(\pi, 0)$ AFM state [12]. The origin of the nematicity below T_s has been widely discussed [18, 36, 47–49], and a likely explanation is an Ising-nematic transition of quasilocalized magnetic moments, described by an effective $J_1 - J_2$ -like model [18, 36, 47, 48].

Experiments in bulk FeSe do not seem to fit into this framework. Under ambient pressure, a nematic phase without an AFM long-range order is stabilized in the bulk FeSe below the



structural transition at $T_s \approx 90$ K. This suggests an unusual type of magnetism in the ground state [128, 129]. The nematic order parameter linearly couples to the splitting between the d_{xz} and d_{yz} orbitals, which can be experimentally detected. In the nematic phase of FeSe, ARPES measurements find this splitting to be momentum dependent, and the splittings at both the Γ and M points of the Brillouin zone (BZ) [130–137], ΔE_Γ and ΔE_M , respectively, are relatively small (less than 50 meV). Meanwhile, recent scanning tunneling microscopy (STM) experiments have revealed a strong orbital selectivity [138, 139]. Especially, the estimated ratio of the quasiparticle spectral weights between the yz and xz orbitals is very large: $Z_{yz}/Z_{xz} \sim 4$. Given the small splitting between these two orbitals [131, 136], such a strong orbital selectivity is surprising [140].

To resolve this puzzle, we examine the electron correlation effects in a multiorbital Hubbard model for the nematic phase of FeSe using the $U(1)$ slave-spin theory. To generate a momentum-dependent orbital splitting, besides the momentum-independent ferro-orbital order (δ_f), we have also taken into account a d - and an s -wave bond nematic order (δ_d and δ_s), which corresponds to the nearest-neighboring hopping anisotropy [141]. We add the Hamiltonian H_{nem} that describes the effects of these nematic orders in the d_{xz} and d_{yz} orbital subspace ($\alpha = 1, 2$) into Eq. 1. In the momentum space

$$H_{\text{nem}} = \sum_k \left[-2\delta_d (\cos k_x - \cos k_y) (n_{k1} + n_{k2}) - 2\delta_s (\cos k_x + \cos k_y) (n_{k1} - n_{k2}) + \delta_f (n_{k1} - n_{k2}) \right]. \quad (15)$$

By solving the saddle-point equations, we show that the OSMP is promoted by any of these nematic orders, as illustrated in

Figure 4A. This effect is delicate, because we also find that the full Mott localization of the system depends on the type and strength of the nematic order [142]. Remarkably, we find that, by taking a proper combination of the three types of nematic order, the system can exhibit a strong orbital selectivity with $Z_{yz}/Z_{xz} \sim 4$ while, at the same time, shows a small band splittings at the Γ and M points of the BZ (with $\Delta E_\Gamma, \Delta E_M \lesssim 50$ meV) as a result of a cancellation effect (see **Figures 4B,C**) [142]. These results reconcile the seemingly contradictory ARPES and STM results. The explanation of the unusually large orbital selectivity in the nematic phase of FeSe [138, 139] further shed light to the understanding of the superconductivity in this compound, which we will discuss in **Section 3.3**.

3 ORBITAL-SELECTIVE SUPERCONDUCTING PAIRING

In **Section 2** we have discussed the orbital-selective electron correlations in the normal state of FeSCs. It is natural to ask whether the strong orbital selectivity can affect the pairing symmetry and amplitudes in the superconducting states. The effects of orbital selectivity on superconductivity are two-fold. The orbital selectivity modifies the band structure from its noninteracting counterpart. This has been verified by ARPES measurements [30, 65, 121]. In addition, the orbital selectivity influences the effective interactions projected to the pairing channel. In the following, we study these effects in a frustrated multiorbital t-J model. We show that any interorbital pairing has a negligible amplitude; the structure of the pairing state is then reflected in the pairing amplitude being orbital dependent, which

is denoted as orbital-selective pairing. In FeSCs, this may give rise to superconducting gaps with unexpectedly strong anisotropy as well as new type of pairing states that has no single-orbital counterpart; we will discuss how both types of effects play an important role in several iron pnictide and iron chalcogenide compounds [72, 143, 144].

3.1 Superconducting Pairing in the Multiorbital t-J Model

The bad metal behavior in the normal state implies strong electron correlations in FeSCs. In strongly correlated systems, the effective superconducting pairing has to avoid the penalty from the Coulomb repulsion. Even though the parent compound is not a MI, the superconducting phase in most cases is in proximity to an AFM phase. This suggests that the AFM exchange interaction plays a very important role for superconductivity. It has been shown theoretically that the AFM exchange interaction is enhanced in the bad metal ($0 < Z \ll 1$) regimes near the Mott transition [145]. In a multiorbital correlated system, similar enhancement is anticipated when the system is close to an OSMP. We therefore proceed to study the superconducting pairing within the framework of a multiorbital t-J model, such that the orbital selectivity in the normal state is taken into account.

The effective Hamiltonian of the model has the following form [144].

$$H_{\text{eff}} = \sum_{ij,\alpha\beta\sigma} \left(\sqrt{Z_\alpha Z_\beta} t_{ij}^{\alpha\beta} - \tilde{\lambda}_\alpha \delta_{\alpha\beta} \right) f_{i,\alpha,\sigma}^\dagger f_{j,\beta,\sigma} - \sum_{ij,\alpha\beta} J_{ij}^{\alpha\beta} f_{i,\alpha,\uparrow}^\dagger f_{i,\alpha,\downarrow} f_{j,\beta,\uparrow} f_{j,\beta,\downarrow}. \quad (16)$$

Here, the bands are renormalized by the quasiparticle spectral weights Z_α 's; as we described in the previous section, the orbital (α) dependence of this weight reflects the orbital selectivity in the normal state. In addition, $\tilde{\lambda}_\alpha$ is the effective energy level that takes into account the correlation effect (see Eq. 10); $J_{ij}^{\alpha\beta}$ refers to the orbital-dependent AFM exchange couplings, which can be obtained by integrating out the incoherent single-electron excitations via either the slave-rotor [145] or slave-spin [146] approach. It is generically a matrix in the orbital space. However, the interorbital interactions have been found to generate negligible interorbital pairing [143]. Thus, the most important terms to the pairing are the diagonal interactions in the t_{2g} (d_{xz}, d_{yz}, d_{xy}) orbital subspace. We focus on these spin-exchange interactions between the nearest (J_1^α) and next-nearest neighboring (J_2^α) sites, where the index α enumerates the d_{xz}, d_{yz}, d_{xy} orbitals. We further introduce two ratios to quantify the effects of magnetic frustration and orbital differentiation, respectively, $A_L = J_1/J_2$ and $A_O = J^{xy}/J^{xz/yz}$. In principle A_L and A_O can be determined from the procedure of integrating out high-energy incoherent states [145]. In practice we take them as model parameters, so that a comprehensive understanding on the pairing states can be gained.

To study the superconducting pairing, we decompose the interaction term in Eq. 16 in the pairing channel by introducing the pairing fields in the real space:

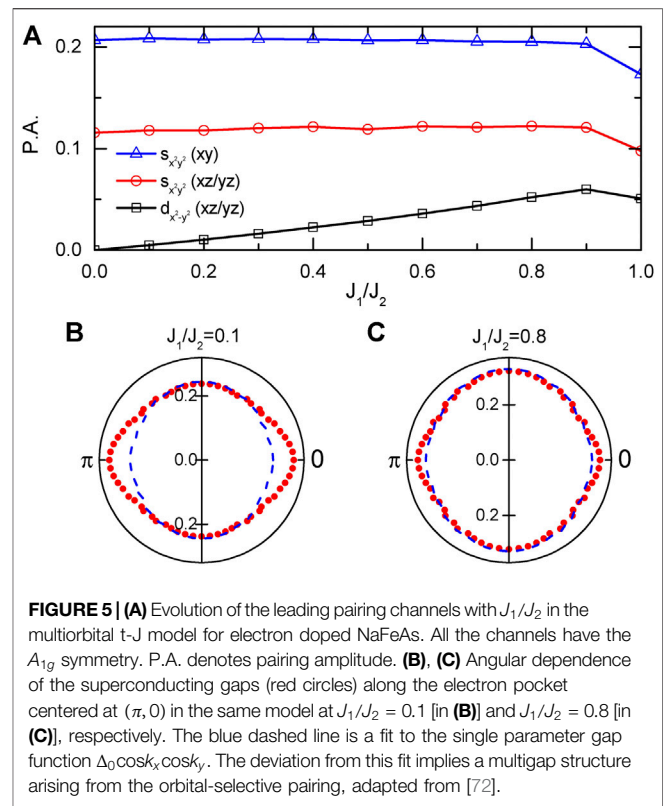
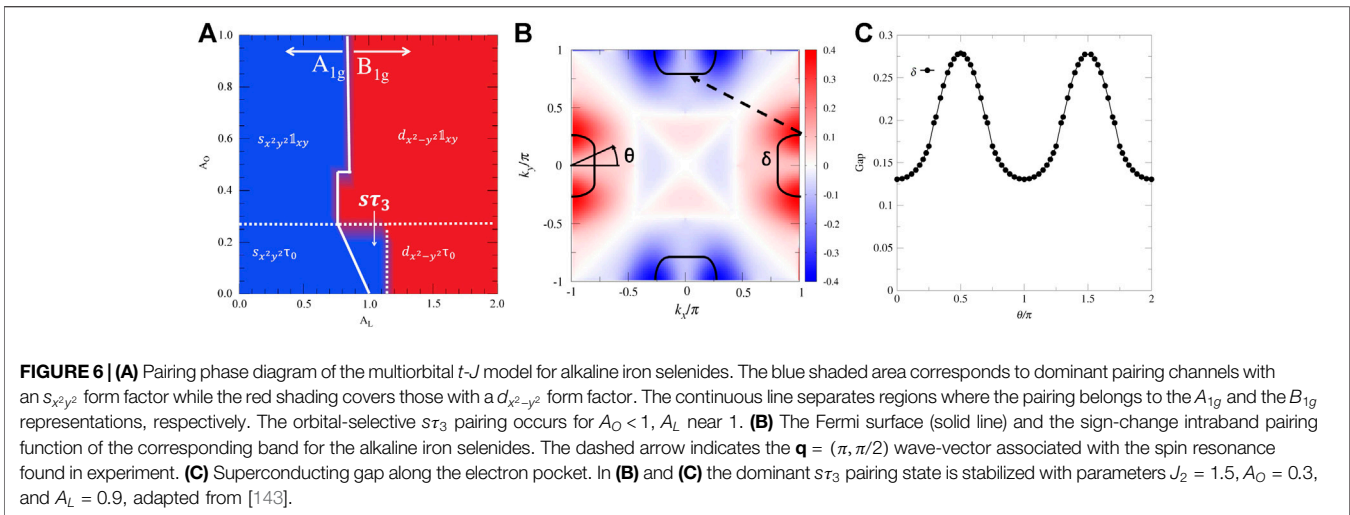


FIGURE 5 | (A) Evolution of the leading pairing channels with J_1/J_2 in the multiorbital t-J model for electron doped NaFeAs. All the channels have the A_{1g} symmetry. P.A. denotes pairing amplitude. **(B), (C)** Angular dependence of the superconducting gaps (red circles) along the electron pocket centered at $(\pi, 0)$ in the same model at $J_1/J_2 = 0.1$ [in **(B)**] and $J_1/J_2 = 0.8$ [in **(C)**], respectively. The blue dashed line is a fit to the single parameter gap function $\Delta_0 \cos k_x \cos k_y$. The deviation from this fit implies a multigap structure arising from the orbital-selective pairing, adapted from [72].

$\Delta_e^\alpha = 1/\mathcal{N} \sum_{\mathbf{e}} f_{i,\alpha,\uparrow} f_{i+\mathbf{e},\alpha,\downarrow}$, where $\mathbf{e} \in \{e_x, e_y, e_{x+y}, e_{x-y}\}$ refers to a unit vector connecting the nearest and next nearest neighboring sites. Transforming to the momentum space we obtain different pairing channels, each of which corresponds to linear combinations of several pairing fields in the real space. In general, the pairing function $\Delta_{g,\alpha,\mathbf{k}} = \Delta_{g,\alpha(\tau_i)} g(\mathbf{k}) (\tau_i)_\alpha$, where $\Delta_{g,\alpha(\tau_i)}$ is the pairing strength of a particular pairing channel. For the nondegenerate d_{xy} orbital, the symmetry of the pairing state is fully determined by the form factor $g(\mathbf{k})$, and the four channels are usually denoted as $s_{x^2+y^2} = \cos k_x + \cos k_y$, $d_{x^2-y^2} = \cos k_x - \cos k_y$, $s_{x^2y^2} = \cos k_x \cos k_y$, and $d_{xy} = \sin k_x \sin k_y$, respectively. In the tetragonal phase, the degeneracy of d_{xz} and d_{yz} orbitals introduces additional pairing channels, and it is necessary to use the 2×2 Pauli matrices τ_i in the orbital isospin space to construct the various possibilities. The pairing channels can be classified according to the one-dimensional irreducible representations of the tetragonal D_{4h} point group to be A_{1g}, B_{1g}, A_{2g} , and B_{2g} . Note that different channels may exhibit the same symmetry, by combining the structure in both the form factor and the orbital structure. For example, both the $d_{x^2-y^2}$ wave channel in the d_{xy} orbital and the $s_{x^2y^2} \tau_3$ channel in the $d_{xz/yz}$ orbitals have the B_{1g} symmetry.

3.2 Orbital-Selective Pairing in FeSCs

Since the discovery of FeSCs, the pairing symmetry of the superconducting state has been one of the most important questions. The s-wave A_{1g} channel has played a particularly important role. In addition, various subleading—in some



cases, nearly-degenerate—pairing channels with compatible symmetry can coexist.

The notion of orbital-selective pairing was introduced [72] in the multiorbital t - J model for electron-doped NaFeAs. With the intraorbital pairing amplitudes being dominant, this leads to a multigap structure, with different pairing components coming from different orbitals. Because the orbital composition varies along each pocket as shown in **Figure 1B**, this orbital-selective pairing can give rise to an anisotropic superconducting gap.

For simplicity, the exchange couplings have been assumed to be orbital independent in the calculation, and the pairing state has an A_{1g} symmetry with a full gap along the Fermi surfaces. The different bandwidths and electron fillings of the d_{xy} and $d_{xz/yz}$ orbitals still make the pairing to be orbital selective. As shown in **Figure 5A**, the pairing amplitude of the leading channel, the $s_{x^2-y^2}$ channel in the d_{xy} orbital, is much larger than those of the subleading channels in the $d_{xz/yz}$ orbitals. This orbital-selective pairing is reflected in an anisotropy of the superconducting gap along the electron pocket, as shown in **Figure 5B**. It turns out that the superconducting gap strongly depends on the magnetic frustration. For $J_1/J_2 = 0.8$ as illustrated in **Figure 5C**, the gap becomes almost isotropic. Here, several competing channels become active, which makes the overall contributions to the gap from the $d_{xz/yz}$ and d_{xy} orbitals comparable. In experiments, an almost isotropic superconducting gap has been reported for the optimally electron doped NaFeAs, but the gap becomes strongly anisotropic along the electron pocket in the underdoped compound [147]. This behavior is understood by the strong orbital-selective pairing [72], which also splits into two the neutron resonance peak as a function of energy in the superconducting state [73, 148]. The orbital-selective pairing is also being explored in other FeSCs [149].

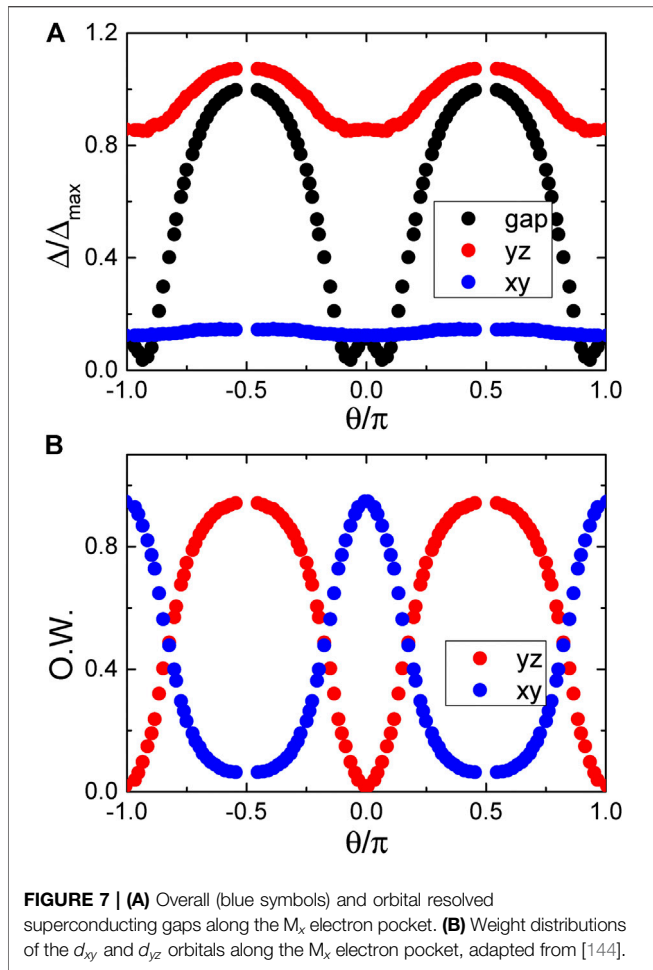
Besides the gap anisotropy, strong orbital selectivity may give rise to novel pairing states. In a multiorbital t - J model for the electron-doped alkaline iron chalcogenide compounds with only electron Fermi pockets, with orbital independent exchange couplings, the dominant pairing symmetry has been found to

be either an s -wave A_{1g} channel when J_2 is dominant or a d -wave B_{1g} channel for dominant J_1 coupling [150, 151]. In the regime where the two types of pairing states are quasidegenerate, a novel orbital-selective pairing state, $s\tau_3$ pairing, with s -wave form factor but B_{1g} symmetry in the $d_{xz/yz}$ orbital subspace can be stabilized as the leading pairing channel [143] (see **Figure 6A**). However, its nontrivial orbital structure makes it distinct from the other two pairing channels, and this successfully explains the unconventional superconductivity in alkaline iron chalcogenides [143]. It produces a full gap but the pairing function has a sign change between the two electron pockets, which causes a spin resonance around the wave vector $(\pi, \pi/2)$, as shown in **Figures 6B,C**. These features are compatible with both the ARPES and neutron scattering measurements [152–156].

Importantly, the $s\tau_3$ pairing corresponds to an irreducible representation of the crystalline point group. Nonetheless, in the band basis, this multiorbital superconducting state has the form of a multiband $d + d$ pairing. The latter allows the state to contrast with the more familiar $d + id$ pairing in a way that the $^3\text{He-B}$ superfluid state contrasts with $^3\text{He-A}$ state [157]. This understanding elevates the $d + d$ pairing to the status of a natural multiorbital pairing state. We note in passing that an analogous $s\tau_3$ pairing has been constructed for the first unconventional superconductor CeCu_2Si_2 [157], which provides a natural understanding of the recently discovered low-temperature behavior in this heavy fermion compound [158].

3.3 Orbital-Selective Pairing in the Nematic Phase of Iron Selenide

As we discussed in **Section 2.4**, recent STM measurements in the nematic phase of FeSe have uncovered not only a surprisingly large difference between the quasiparticle weights of the d_{xz} and d_{yz} orbitals, but also an unusually strong anisotropy of the superconducting gap [138, 139]. These experimental findings provide evidence for a strongly orbital-selective superconducting state.



Theoretically, the pairing structure in the nematic phase of FeSe has been investigated within the framework of the multiorbital t-J model in Eq. 16. The slave-spin calculation [142] produces $Z_{xz} : Z_{yz} : Z_{xy} = 1 : 4 : 0.5$; an orbital-selective pairing was shown, with the leading pairing channel in the d_{yz} orbital. Taking into account the mixed orbital character of both hole and electron pockets, such an orbital-selective pairing naturally leads to a large gap anisotropy as shown in Figure 7. This orbital-selective pairing not only provides the understanding of the experimental observations [133–135, 138], but also sheds new light on the interplay among the pairing state, Mott physics, and the nematic order, all of which appear to be important ingredients for the unconventional superconductivity in FeSCs. Experimentally, other signatures of orbital-selective superconductivity in nematic FeSC are also being explored [159].

4 SUMMARY AND OUTLOOK

Since the discovery of superconductivity in FeSCs, clarifying the underlying microscopic physics of these materials has been the goal of extensive research, and considerable progress has been achieved. By now it has become abundantly clear that electron

correlations play a key role. This includes both the Hubbard and Hund’s couplings, which combine to cause the normal state of the FeSCs to be a bad metal in proximity to a Mott transition. Theoretical studies on the pertinent microscopic models for the FeSCs not only confirm the existence of the bad metal in the phase diagram, but also reveal a strong orbital selectivity in this phase, which is anchored by an orbital-selective Mott phase. In this manuscript we have reviewed recent theoretical progress on the orbital selectivity. It has been found that the orbital selectivity not only is a universal property of the normal state of FeSCs, but also shows intriguing interplay with the nematicity. Equally important, it can strongly affect the superconducting states of the system.

It is worth reiterating that the FeSCs consist of a large family of materials, and superconductivity has been found over a broad range of tuning parameters, such as pressure and electron filling. For example, many electron-doped iron chalcogenides have a simpler Fermi surface, with only electron pockets, and the electron filling is $n \sim 6.1 - 6.2$. Even so, superconductivity is also discovered and, indeed, it is in this category of materials that the highest- T_c FeSC belongs. Here, the strong orbital selectivity is shown to be universal in these systems and has been extensively studied.

Also of note is the case of extremely hole-doped iron pnictides, which likewise displays superconductivity. A prototype class of materials in this category is $A\text{Fe}_2\text{As}_2$ ($A = \text{K, Rb, Cs}$), which contains hole pockets only, and the electron filling is at $n = 5.5$. As illustrated in Figure 8, they are far from both the $n = 6$ and $n = 5$ MIs. Although the superconducting T_c observed in these systems is much lower than that of the other iron-based systems, a number of recent experiments prompt the consideration of a completely different type of antiferromagnetism and nematicity [161–167], which are possibly associated with the Mott physics in

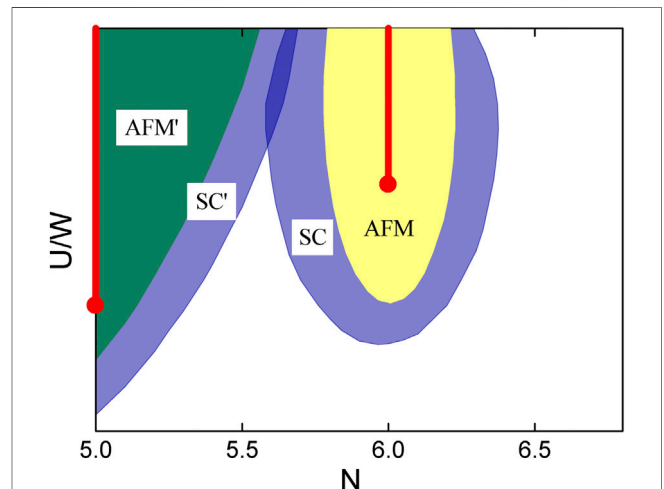


FIGURE 8 | Schematic phase diagram as a function of U/W (the ratio of the Coulomb interaction to bandwidth) and the electron filling n . Here the red lines denote the MIs at electron filling $n = 6$ and $n = 5$, respectively. AFM marks the $(\pi, 0)$ AFM order near the $n = 6$ MI, while AFM’ represents the AFM order near the $n \rightarrow 5$ limit [64]. SC and SC’ denote two superconducting states near the two AFM phases, adapted from [160].

the $n = 5$ limit. In particular, the d_{xy} orbital is shown to be closer to the Mott localization with reducing the total electron filling. Therefore, a systematic study on the evolution of orbital-selective correlations with doping from $n = 6$ to $n = 5$ would be important in clarifying the underlying physics and the connection to superconductivity in these heavily hole-doped materials.

A topic of considerable recent interest in the area of FeSCs is the indication for a topologically nontrivial band structure and the possible Majorana zero mode in the superconducting iron chalcogenides [168]. This highlights the important role of spin-orbit coupling in these systems. Given the compelling evidence for the strongly orbital-selective correlations we have discussed here, it would be highly desirable to clarify how the interplay between the correlation effects and the spin-orbit coupling affects the topological properties of the electronic band structure. Such efforts promise to elucidate the extent to which the topological band structure develops in the various families of FeSCs.

AUTHOR CONTRIBUTIONS

All authors listed have made a substantial, direct, and intellectual contribution to the work and approved it for publication.

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Conflict of Interest: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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