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 ∼ 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 Ca$_{2-x}$Sr$_x$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 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 of 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
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 FeTe\(_{1-x}\) 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 \([71]\).

**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 FeTe\(_{1-x}\) 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

![Diagram](https://example.com/diagram.png)
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

\[
H = H_{TB} + H_{int}.
\]

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

\[
H_{TB} = \frac{1}{2} \sum_{i,j,\sigma} t_{ij}^{\sigma} d_i^{\sigma \dagger} d_j^{\sigma} + \sum_i (\Lambda_0 - \mu) d_i^{\alpha \dagger} d_i^{\alpha}.
\]

Here, \( d_i^{\alpha \dagger} \) creates an electron in orbital \((\alpha = 1, \ldots, 5)\) with spin \( \sigma \) at site \( i \), \( t_{ij}^{\alpha \sigma} \), with \( i \neq j \), are the tight-binding parameters, with those for \( \alpha \neq \beta \) describing the interorbital couplings; \( \Lambda_0 \) 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 \( d_{cz} \) and \( d_{cz} \) 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 \( \mu \) 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:

\[
H_{int} = \frac{U}{2} \sum_{i,\alpha,\sigma} n_{i\alpha\sigma} n_{i\alpha\bar{\sigma}} + \sum_{i,\alpha,\beta,\sigma,\bar{\sigma}} \{ U' n_{i\alpha\sigma} n_{i\beta\bar{\sigma}} + (U - J_\parallel) n_{i\alpha\sigma} n_{i\beta\bar{\sigma}} \} - J_\parallel \sum_{i,\alpha,\beta,\sigma,\bar{\sigma}} \{ d_i^{\alpha \dagger} d_i^{\beta \dagger} d_i^{\beta \sigma} d_i^{\alpha \bar{\sigma}} + d_i^{\alpha \dagger} d_i^{\beta \dagger} d_i^{\beta \bar{\sigma}} d_i^{\alpha \sigma} \},
\]

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

### 2.1 The \( U(1) \) Slave Spin Theory

To construct a saddle-point theory, one has to work within 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

\[
d_i^{\alpha \dagger} = S_{i\alpha \dagger} \phi_i^{\alpha \dagger}.
\]

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

\[
S_{i\alpha \dagger} = f_i^{\alpha} S_{i\alpha \dagger} f_i^{\alpha} - \frac{1}{2}
\]

is implemented. This representation contains a \( U(1) \) gauge redundancy corresponding to \( f_i^{\alpha} \rightarrow e^{i\theta} f_i^{\alpha} \) and \( S_{i\alpha \dagger} \rightarrow S_{i\alpha \dagger} e^{i\theta} \). 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:

\[
\tilde{\phi}_{i\alpha} = \phi_{i\alpha} S_{i\alpha}^+ S_{i\alpha} \phi_{i\alpha}^+, \quad \tilde{\phi}_{i\alpha}^+ = \phi_{i\alpha} S_{i\alpha}^+ S_{i\alpha} \phi_{i\alpha}.
\]
where the projectors \( P_i^a = 1/\sqrt{1/2 + \delta \pm S_{i\text{tot}}} \) and \( \delta \) is an infinitesimal positive number to regulate \( P_i^a \). Next we rewrite Eq. 4 with the dressed operator to \( \tilde{d}_{i\text{tot}}^a = \tilde{f}_{i\text{tot}}^a P_i^a \). The Hamiltonian, Eq. 1, is then effectively rewritten as

\[
H = \frac{1}{2} \sum_{(\alpha \beta)} \left( \sum_{i} \left[ \tilde{f}_{i\text{tot}}^\dagger \tilde{c}_{i}^\dagger \tilde{P}_i^\alpha \tilde{c}_{i} \tilde{P}_i^\beta \tilde{f}_{i\text{tot}} \right] \right)^2 + \sum_{i} (\Lambda_i - \mu) \tilde{f}_{i\text{tot}}^\dagger \tilde{f}_{i\text{tot}} - \lambda_{\text{tot}} \left[ \tilde{f}_{i\text{tot}}^\dagger \tilde{f}_{i\text{tot}} \right] - S_{i\text{tot}}^z + H^k_{\text{int}}.
\]

(7)

Here, we have introduced the Lagrange multiplier \( \lambda_{\text{tot}} \) to enforce the constraint in Eq. 5. In addition, \( H^k_{\text{int}} \) is the interaction Hamiltonian, Eq. 3, rewritten in terms of the slave-spin operators [61] as follows:

\[
H^k_{\text{int}} = \sum_k \left\{ \frac{U}{2} \left( \sum_{i} S_{i\text{tot}}^z \right)^2 + \frac{U}{2} \sum_{\alpha < \beta} \left( \sum_{i} S_{i\text{tot}}^z \right)^2 - \frac{J_u}{2} \sum_{\alpha < \beta} \left( \sum_{i} S_{i\text{tot}}^z \right)^2 - J_a \sum_{\alpha < \beta} \left[ S_{i\text{tot}}^\alpha \cdot S_{i\text{tot}}^\beta \right] \right\}.
\]

(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

\[
Z_{\text{tot}} = |z_{\text{tot}}|^2 = \langle |\tilde{z}_{\text{tot}}|^2 \rangle.
\]

(9)

A metallic phase corresponds to \( Z_{\text{tot}} > 0 \) for all orbitals, and a Mott insulator corresponds to \( Z_{\text{tot}} = 0 \) 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:

\[
H^k_{\text{eff}} = \sum_{\alpha \beta} \left[ \epsilon^\alpha_{\beta} \langle \tilde{c}_{\alpha}^\dagger \tilde{c}_{\beta} \rangle + \delta_{\alpha \beta} (\Lambda_i - \lambda_i + \mu_i - \mu) \right] \tilde{f}_{i\text{tot}}^\dagger \tilde{f}_{i\text{tot}},
\]

(10)

\[
H^k_{\text{int}} = \sum_{\alpha \beta} \left[ Q^\alpha_{\beta \gamma} \langle \tilde{c}_{\alpha}^\dagger \tilde{c}_{\beta} \rangle + \delta_{\alpha \beta} \lambda_i S_i^z \right] + H^k_{\text{int}},
\]

(11)

where \( \delta_{\alpha \beta} \) is Kronecker delta function, \( \epsilon^\alpha_{\beta} = 1/N \sum_{\gamma} \epsilon^\alpha_{\gamma} e^{\imath \beta(r, \gamma)} \), \( Q^\alpha_{\beta \gamma} = \sum_k \xi_k \gamma \langle \tilde{f}_{i\text{tot}}^\dagger \tilde{f}_{i\text{tot}} \rangle \)\( \frac{1}{2} \), and \( z_{\text{tot}}^z = \langle \tilde{P}_i^\alpha \rangle S_i^z \langle \tilde{P}_i^\beta \rangle \). Finally, \( \mu_i \) is an effective onsite potential defined as \( \mu_i = 2 \xi_i \eta_i \), where \( \eta_i = (2n_i - 1)/(4n_i(1 - n_i)) \), and \( n_i^\alpha = 1/N \sum_k \langle f_{i\text{tot}}^\dagger f_{i\text{tot}} \rangle \).

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 \( z_{\text{tot}} \) and \( \lambda_i \) 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 \( W_{\beta k} \tilde{f}_{i\beta} \tilde{f}_{i\gamma} \), with \( W_{\beta k} = e^{\alpha_{\beta}} \langle \tilde{z}_{\beta k} \rangle \langle \tilde{z}_{\beta k} \rangle \propto \langle \tilde{z}_{\beta} \rangle \langle \tilde{z}_{\beta} \rangle \). Because \( \tilde{f}_{i\beta} \tilde{f}_{i\gamma} \) is conjugate to \( W_{\beta k} \), from the linear response theory, it is easy to show that \( \langle \tilde{f}_{i\beta} \tilde{f}_{i\gamma} \rangle \propto W_{\beta k} \langle \tilde{z}_{\beta} \rangle \langle \tilde{z}_{\beta} \rangle \). As a result, the kinetic hybridization of the spinons is

\[
\langle \tilde{H}_{\beta k} \rangle_{\text{eff}} = \sum_{k} \langle \tilde{z}_{\beta k} \rangle \langle \tilde{z}_{\beta k} \rangle \langle \tilde{f}_{i\beta} \tilde{f}_{i\gamma} \rangle \propto \langle \tilde{z}_{\beta} \rangle^2 \langle \tilde{z}_{\beta} \rangle^2.
\]

(12)

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

\[
\langle \tilde{H}^k_{\alpha k} \rangle_{\text{eff}} \rightarrow |\langle \tilde{z}_{\alpha} \rangle|^2 |\langle \tilde{z}_{\alpha} \rangle|^2.
\]

(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, \( z_{\alpha} \). 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

\[
f = \sum_{\alpha = 1,2} \left( r_\alpha |z_{\alpha}|^2 + u_\alpha |z_{\alpha}|^4 \right) + v|z_1|^2 |z_2|^2,
\]

(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 \( v \) 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’s 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 \( J_H/U > 0.1 \), 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 \( Z_r \) in each orbital rapidly drops across this crossover. Inside the bad metal phase, \( Z_r \) becomes strongly orbital dependent. This large orbital-selective correlation is rather surprising given that the strength of the onsite \( J_H \) coupling already strongly affects the metallic state

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 [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 $\Gamma$ and $M$ points of the Brillouin zone (BZ) [130–137], $\Delta E_\Gamma$ and $\Delta E_M$, 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 ($\delta_f$), we have also taken into account a $d$- and an $s$-wave bond nematic order ($\delta_d$ and $\delta_s$), which corresponds to the nearest-neighbor hopping anisotropy [141]. We add the Hamiltonian $H_{nem}$ that describes the effects of these nematic orders in the $d_{sz}$ and $d_{xz}$ orbital subspace ($\alpha = 1, 2$) into Eq. 1. In the momentum space

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

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 $\Gamma$ 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

**FIGURE 4 |** (A) Ground-state phase diagram of the five-orbital Hubbard model for FeSe with a ferro-orbital order $\delta_f$ at $J_{HF} / U = 0.25$. (B) The orbital-selective quasiparticle spectral weights in the nematic phase with a combined nematic order $\delta_f/4 = \delta_d = \delta_s = 0.2$ eV and with $J_{HF}/U = 0.25$. (C) Band splittings at $\Gamma$ ($\Delta E_\Gamma$) and $M$ ($\Delta E_M$) points of the 2-Fe BZ in the nematic phase with the same set of parameters as in (B), adapted from [142].
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 ≪ 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].

$$H_{\text{eff}} = \sum_{\langle i,j \rangle \alpha \beta} \left( Z_{ij} \hat{a}_{i \alpha}^\dagger \hat{a}_{j \beta} + \text{H.c.} \right) + \sum_{\langle i,j \rangle \alpha \beta} \left( \lambda_{ij} \hat{a}_{i \alpha}^\dagger \hat{a}_{j \beta} + \text{H.c.} \right),$$

(16)

Here, the bands are renormalized by the quasiparticle spectral weights $Z_{ij}$'s; as we described in the previous section, the orbital ($\alpha$) dependence of this weight reflects the orbital selectivity in the normal state. In addition, $\lambda_{ij}$ is the effective energy level that takes into account the correlation effect (see Eq. 10); $Z_{ij}$ 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 $t_{ij}$ ($d_{xz}, d_{yz}, d_{xy}$) orbital subspace. We focus on these spin-exchange interactions between the nearest ($t_{ij}^0$) and next-nearest neighboring ($t_{ij}^1$) sites, where the index $i$ 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, $A_I = t_{ij}^0 / t_{ij}^1$ and $A_O = t_{ij}^0 / t_{ij}^{1y}$. In principle $A_I$ 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:

$$\Delta^{\text{eff}} = \frac{1}{\sqrt{N}} \sum f_{\alpha \beta,1} \sum_{\tau \tau'} \delta_{\tau \tau'} g(\mathbf{k}) (\tau_\alpha \tau_\beta),$$

where $e \in \{e_x, e_y, e_{xy}, e_{x-y}\}$ 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 $\Delta_{\alpha \beta(\tau)} = \Delta_{\alpha \beta}(\mathbf{k}) (\tau_\alpha \tau_\beta)$, where $\Delta_{\alpha \beta} (\tau_\alpha)$ 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 $s_{d_{xy}} = \cos k_x + \cos k_y$, $d_{x^2-y^2} = \cos k_x - \cos k_y$, $s_{d_{xy}} = \cos k_x \cos k_y$, and $s_{d_{xy}} = \sin k_x \sin k_y$, respectively. In the tetragonal phase, the degeneracy of $d_{xy}$ and $d_{yz}$ orbitals introduces additional pairing channels, and it is necessary to use the $2 \times 2$ Pauli matrices $\tau_1$ 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 $s_{d_{xy}} \tau_1$ channel in the $d_{yz}$ orbital 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, $s_{3/2}$ pairing, with s-wave form factor but $A_{1g}$ 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 $s_{3/2}$ 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 $d + id$ pairing. The latter allows the state to contrast with the more familiar $d + id$ pairing in a way that the $^3$He-B superfluid state contrasts with $^3$He-A state [157]. This understanding elevates the $d + id$ pairing to the status of a natural multiorbital pairing state. We note in passing that an analogous $s_{3/2}$ pairing has been constructed for the first unconventional superconductor CeCu$_2$Si$_2$ [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 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 $AFe_2As_2$ ($A=K, Rb, Cs$), 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
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 and the possible Majorana zero mode in the superconducting FeSCs. Such correlation effects and the spin-orbit coupling affects the 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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