Distinguishing spin-orbit coupling and nematic order in the electronic spectrum of iron-based superconductors

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The low-energy electronic states of the iron-based superconductors are strongly affected by both spin-orbit coupling and, when present, by the nematic order. These two effects have different physical origins, yet they can lead to similar gap features in the electronic spectrum. Here we show how to disentangle them experimentally in the iron superconductors with one Fe plane per unit cell. Although the splitting of the low energy doublet at the Brillouin zone center (Γ-point) can be due to either the spin-orbit coupling or the nematic order, or both, the degeneracy of each of the doublet states at the zone corner (M-point) is protected by the space group symmetry even when spin-orbit coupling is taken into account. Therefore, any splitting at M must be due to lowering of the crystal symmetry, such as due to the nematic order. We further analyze a microscopic tight-binding model with two different contributions to the nematic order: d_{xy}/d_{yz} onsite energy anisotropy and the d_{xy} hopping anisotropy. We find that a precise determination of the former, which has been widely used to characterize the nematic phase, requires a simultaneous measurement of the splittings of the Γ-point doublet and at the two low-energy M-point doublets. We also discuss the impact of twin domains and show how our results shed new light on ARPES measurements in the normal state of these materials.

I. INTRODUCTION

In most iron based superconductors [1], the normal state displays two instabilities: a spin-density wave (SDW) transition at T_{SDW} and an orthorhombic/nematic transition at T_{nem} ≥ T_{SDW} [2]. Angle-resolved photoemission spectroscopy (ARPES), being sensitive to the electronic energy-momentum dispersion [3], is an attractive tool to probe how these distinct ordered states manifest themselves in the electronic spectrum [4–12]. However, the close proximity of the different electronic energy scales, together with the multi-orbital character of the band structure, render this task non-trivial [13]. For instance, in several iron pnictides, a partial energy gap of about 50 meV reported in optics experiments, and also observed by ARPES at the points where folded and unfolded bands cross, has been attributed to the formation of the metallic SDW order [14–16]. This is of the same order of magnitude as the energy splitting attributed to the formation of the orthorhombic/nematic phase [4]. As the system is doped towards its maximum superconducting transition temperature, both gaps decrease [16]. Meanwhile, an atomic-like spin-orbit coupling present in the system gives rise to splittings at the Γ point of the order of 10-30 meV in the band structure [17] without any broken-symmetry [13].

Establishing clear criteria to correctly identify the origin of these spectral features is therefore important to advance our understanding of the normal state of the iron superconductors. In principle, the effects of the SDW order – established independently using neutron scattering – on the electronic spectrum can be unambiguously identified, because, being a commensurate density wave, the lattice translational symmetry-breaking is manifested in a folding of the band structure in the momentum space. The case of the nematic splitting is however more subtle, because it involves only rotational symmetry-breaking, without the lattice translational symmetry-breaking, and therefore no zone folding. As an illustration, consider the subspace spanned by the d_{xz} and d_{yz} Fe orbitals only. On the one hand, the nematic order breaks the tetragonal symmetry, giving rise to an additional term in the Hamiltonian: 

\[ \Delta_{\text{nem}} \sum_{k \sigma} \left( c_{xz,k \sigma}^\dagger c_{xz,k \sigma} - c_{yz,k \sigma}^\dagger c_{yz,k \sigma} \right) \]

where the operator \( c_{\alpha,k \sigma} \) destroys an electron at orbital \( \alpha \) with momentum \( k \) and spin \( \sigma \). The result is the splitting between the on-site energies of these two orbitals. On the other hand, the spin-orbit coupling \( \lambda_{\text{SOC}} \) mixes the two orbitals, and splits the energy of the resulting admixtures, without breaking the tetragonal symmetry, via the additional term: 

\[ i \lambda_{\text{SOC}} \sum_{k \alpha} \sigma \left( c_{xz,k \sigma} c_{yz,k \sigma} - c_{yz,k \sigma}^\dagger c_{xz,k \sigma} \right) \]

To distinguish these two features experimentally, one could in principle use spin polarized ARPES or use the fact that while \( \Delta_{\text{nem}} \) has a pronounced temperature dependence, \( \lambda_{\text{SOC}} \) is expected to be nearly temperature-independent. However, the electronic spectral-function’s lifetime, manifested as a broadening of the ARPES data, is also strongly temperature-dependent [18, 19], making this procedure challenging.

It is important to keep in mind that the orbital states are not the eigenstates of the electronic Bloch problem [20, 23]. At first, one may think that this feature renders the qualitative distinction between the effects of the spin-orbit coupling and the nematic order less transparent. Indeed, any transformation from the 3d orbital basis of 2 Fe atoms in the crystallographic unit cell to the band basis requires diagonalizing a 20 × 20 matrix in the presence of spin-orbit coupling. The size of the matrix

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The paper is organized as follows: in Section II we introduce the low-energy model in the presence of both spin-orbit coupling and nematic order, and discuss the corresponding band dispersions. In Section III we compare these results to first-principle calculations fitted to a 10-orbital tight-binding model, and to ARPES experiments. Conclusions are presented in Section IV.

II. EFFECTIVE LOW-ENERGY MODEL

The low energy effective Hamiltonian for the states near the Fermi level, corresponding to small hole-like and electron-like pockets, can be obtained from the $k.p$ expansion around the $\Gamma$ and $M$ points of the crystallographic Brillouin zone, which contains 2 Fe atoms [13]. A schematic representation of the corresponding unit cell is shown in Fig. 1: hereafter, $xy$ refer to the Fe-As orthogonal directions (parallel to the crystallographic $ab$ axes), whereas $XY$ refer to the Fe-Fe orthogonal directions. Here, we focus on the $k_z = 0$ plane only, since ARPES measurements have enough resolution to select single $k_z$ values via the energy of the incoming photon. All the orbitals are defined with respect to the Fe-Fe square lattice, i.e. in the notation $d_{xz}$, $d_{yz}$, $d_{xy}$, $d_{x^2-y^2}$, $d_{3z^2-r^2}$ the subscripts should be understood as referring to the $XY$ coordinate system.

At $\Gamma$, the irreducible representations of the $P4/nmm$ space group, suitable for the systems with a single Fe layer per unit cell (i.e. the 111, 1111 and 11111 families) are the same as those of the well known point group $D_{4h}$. Two hole pockets emerge from the $E_g$ doublet, at an energy $\epsilon_1 > 0$, which has degenerate $d_{xz}/d_{yz}$ orbital character (for convenience, we set the chemical potential to zero). Additional hole pockets may or may not emerge from the singlets $A_{1g}$ (with $d_{3z^2-r^2}$ orbital character) and $B_{3g}$ (with $d_{xy}$ character), depending on their position relative to the Fermi level. Because the main qualitative changes caused by the nematic order and the spin-orbit coupling occur in the degenerate states, we focus on the states arising from the $E_g$ doublet only. For each spin projection, $\sigma$, we denote them by a two component spinor $\psi_{\sigma}(k)$.

In contrast, at the $M$ point, the irreducible representations of the space group cannot be mapped onto those of the point group $D_{4h}$. This is a consequence of the fact that $P4/nmm$ is a non-symorphic space group, due to the presence of an $n$-glide plane symmetry, i.e. mirror reflection about the Fe plane followed by the translation by the half unit cell diagonal [13]. Ignoring the spin degeneracy, one finds that all irreducible representations at $M$ are two-dimensional, denoted by $E_M$ in Ref. [13]. The two electron pockets arise from the doublet $E_M$, at an energy $\epsilon_3 < \epsilon_1 < 0$ and with $d_{xz}/d_{yz}$ orbital character, and from the doublet $E_{M3}$, at an energy $\epsilon_5 < \epsilon_1 < 0$ and with $d_{xy}$ orbital character (see Fig. 1b). Out of these 4 states we build two spinors $\psi_{X,\sigma}(k)$ and $\psi_{Y,\sigma}(k)$, whose upper (lower) components transform respectively as $E_{M1}$.
and \( E_{M1}^{Y} \) \( (E_{M5}^{Y}) \) and \( E_{M7}^{Y} \). A schematic representation of
these states is shown in Fig. [1]
Figure 1

Defining the enlarged spinor \( \Psi_\perp = \begin{pmatrix} \psi_{X,\sigma} \psi_{Y,\sigma} \psi_{\Gamma,\sigma} \end{pmatrix} \), the low-energy Hamiltonian
can be written as
\[
H = \sum_{k,\alpha,\beta} \Psi_(k) H_{\alpha,\beta}(k) \Psi_\beta(k),
\]
where (suppressing \( \alpha, \beta \) and \( k \) the matrix
\[
H = H_0 + H_{SOC} + H_{nem},
\]
is the single-particle Hamiltonian in the nematic-paramagnetic state. The first two terms were obtained
in Ref. [13] and we repeat here the results. For the non-interacting \( H_0 \) part, we obtain:
\[
H_0(k) = \begin{pmatrix} h^+_M(k) & 0 & 0 \\ 0 & h^-_M(k) & 0 \\ 0 & 0 & h^\Gamma(k) \end{pmatrix} \otimes \sigma_0, \tag{3}
\]
with 2 \times 2 matrices:
\[
h^+_M(k) = \sum_{i=1,3} \left( \varepsilon_i + \frac{k^2}{2m_i} \right) \tau_i + v_+(k) \tau_2,
\]
\[
h^\Gamma(k) = \left( \varepsilon_\Gamma + \frac{k^2}{2m_\Gamma} \right) \tau_0 + b k_x k_y \tau_3 + c \left( k_x^2 - k_y^2 \right) \tau_1,
\]
where \( \tau_i = \frac{1}{2} (\tau_0 + \tau_3) \), \( \tau_3 = \frac{1}{2} (\tau_0 - \tau_3) \), and:
\[
v_\pm(k) = v \left( \pm k_x + k_y \right) + p_1 \left( \pm k_x^3 + k_y^3 \right) + p_2 k_x k_y \left( k_x \pm k_y \right) \tag{5}
\]
The Pauli matrices \( \sigma \) refer to the spin space, whereas the Pauli matrices \( \tau \) refer to the spinor space. The
simplicity and generality of this model should be evident when compared to the 10-orbital tight-binding model
with fifth-neighbor hopping parameters. The 13 free parameters are material-dependent, and can be fit to first-
principle calculations. For concreteness, in this paper we use the parameters defined in the first row of Table IX
of Ref. [13]. The corresponding band dispersions and Fermi surfaces are shown as dashed lines in Fig. 2. For
the spin-orbit term \( H_{SOC} \) we have:
\[
H_{SOC}(k) = \begin{pmatrix} 0 & h_{M}^{SOC}(k) & 0 \\ h_{M}^{SOC}(k) & 0 & 0 \\ 0 & 0 & h_{\Gamma}^{SOC}(k) \end{pmatrix}, \tag{6}
\]
with 4 \times 4 matrices:
\[
h_{M}^{SOC}(k) = \frac{\lambda}{4} (\tau_+ \otimes \sigma_1 + \tau_- \otimes \sigma_2),
\]
\[
h_{\Gamma}^{SOC}(k) = \frac{\lambda}{2} \tau_2 \otimes \sigma_3, \tag{7}
\]
and using the usual definition \( \tau_\pm = \tau_1 \pm i\tau_2 \). Here, \( \lambda \) sets
the strength of the spin-orbit coupling, which, without loss of generality, we take to be the same near \( \Gamma \) and \( M \).

To derive the nematic term \( H_{nem} \), which breaks the tetragonal symmetry along the Fe-Fe directions, it is
enough to find combinations of components of \( \Psi_{\sigma}(k) \) and \( k \), which transform as \( B_{2g} \) invariants, i.e. as
\( k_x k_y \propto K_x^2 - K_y^2 \). Clearly, there can be no bilinear terms which mix the two-component spinors at \( \Gamma \) and \( M \), because
such terms would break the lattice translational symmetry. Meanwhile, nematic is a \( q = 0 \) order. The \( k \) independent
terms near \( \Gamma \) follow immediately from the form of \( h_{\Gamma}(k) \): the only combination of the two components of
\( \psi_{\Gamma,\sigma} \) which transform as \( k_x k_y \) is the combination which
multiplies this term in \( h_{\Gamma}(k) \), because the resulting combination is an invariant, i.e. transforms trivially.
Therefore, near \( \Gamma \), the nematic order induces a \( k \)-independent term
\[
\sim \sum_{k,\sigma} \psi_{\Gamma,\sigma}^\dagger(k) \tau_3 \psi_{\Gamma,\sigma}(k).
\]
Similarly, at \( M \), the \( k \)-
independent combinations which transform as \( B_{2g} \) can be read off from \( h_{M}(k) \). The two independent terms are:
\[
\sim \sum_{k,\sigma} \psi_{X,\sigma}^\dagger(k) \tau_i \psi_{X,\sigma}(k) - \psi_{Y,\sigma}^\dagger(k) \tau_i \psi_{Y,\sigma}(k) \right],
\]
where \( i = 1 \) or \( i = 3 \). We then obtain
\[
H_{nem}(k) = \begin{pmatrix} h_{M}^{nem}(k) & 0 & 0 \\ 0 & -h_{M}^{nem}(k) & 0 \\ 0 & 0 & h_{\Gamma}^{nem}(k) \end{pmatrix} \otimes \sigma_0, \tag{8}
\]
with 2 \times 2 matrices:
\[
h_{M}^{nem}(k) = \frac{\varphi_1}{4} (\tau_0 + \tau_3) + \frac{\varphi_3}{4} (\tau_0 - \tau_3),
\]
\[
h_{\Gamma}^{nem}(k) = \frac{\varphi_2}{2} \tau_3. \tag{9}
\]
Symmetry alone is unable to fix the values of \( \varphi_j \). Nevertheless, because all \( \varphi_j \)'s are nematic order parameters,
they must be related to each other microscopically, although they do not need to be equal to each other. It is
now straightforward to obtain the electronic spectrum in the presence of both nematic order and spin-orbit
coupling. We find splittings in the \( E_g \) doublet at the \( \Gamma \) point (energy \( \epsilon_\Gamma > 0 \)), as well as in the \( E_{M1} \) and \( E_{M5} \) doublets
at the \( M \) point (energies \( 0 < \epsilon_1 < \epsilon_3 \), given by:
\[
\Delta E_g = \sqrt{\lambda^2 + \varphi_2^2},
\]
\[
\Delta E_{M1/3} = \pm \left( \frac{\varphi_1 - \varphi_3}{2} - \frac{1}{2} \sqrt{\lambda^2 + \left( \epsilon_1 - \varphi_1 \right) + \left( \varphi_3 - \epsilon_3 \right)} \right) + 
\]
\[
+ \frac{1}{2} \sqrt{\lambda^2 + \left( \epsilon_1 - \epsilon_3 \right) + \left( \varphi_1 + \varphi_3 \right)} \right)^2, \tag{10}
\]
Red (blue) lines denote the states emerging from the of both spin-orbit coupling and nematic order (solid lines).

The parameters used were \( \lambda = \varphi_1 = 50 \text{ meV} \).

The results derived above are general and independent of the particularities of the band structure. They rely only on the space group symmetry \( P4/mnm \) and its consequences at the doubles at \( \Gamma \) and \( M \). Yet, in order to understand the microscopic meaning of the nematic order parameters \( (\varphi_\Gamma, \varphi_1, \varphi_3) \), it is instructive to compare our results with those obtained from 10-orbital tight-binding models fitted to first-principle calculations. We used the model of Ref. \[26\] for LaFeAsO \[27\] and added two different tetragonal symmetry-breaking terms, while ignoring the spin-orbit coupling. The first is a uniform on-site energy splitting between the \( d_{xz} \) and \( d_{yz} \) orbitals of the form:

\[
H_1 = \frac{\Delta_1}{2} \sum_{\mathbf{k}\sigma} \left( c^\dagger_{\mathbf{xz},\mathbf{k}\sigma} c_{\mathbf{xx},\mathbf{k}\sigma} - c^\dagger_{\mathbf{yz},\mathbf{k}\sigma} c_{\mathbf{yz},\mathbf{k}\sigma} \right),
\]

whereas the second is a hopping anisotropy between the \( d_{xy} \) orbitals of the two Fe atoms. 

The results shown in Fig. \[3\] for \( \Delta_1 > 0, \Delta_3 = 0 \) and \( \Delta_1 = 0, \Delta_3 > 0 \) reveal that whereas the \( E_g \) and the \( E_M \) doubles are split by \( \Delta_1 \), the \( E_M \) doublet is split by \( \Delta_3 \), with \( \Delta E_g = \Delta E_{M_1} = \Delta_1 \) and \( \Delta E_{M_3} = \Delta_3 \). This is not unexpected, since in our low-energy model the \( E_g \) and \( E_M \) doubles have \( d_{xz}/d_{yz} \) characters, whereas the \( E_M \) doublet has \( d_{xy} \) character \[13\]. Therefore, we can identify \( \varphi_\Gamma = \varphi_1 \) with the on-site \( d_{xz}/d_{yz} \) orbital anisotropy \( \Delta_1 \) and \( \varphi_3 \) to the \( d_{xy} \) hopping anisotropy \( \Delta_3 \). Note that these results are insensitive to the microscopic mechanism behind the tetragonal symmetry breaking, i.e., whether it arises due to orbital \[28, 33\] or spin fluctuations \[2, 50, 40\], or electron-phonon coupling.

III. COMPARISON TO FIRST-PRINCIPLE CALCULATIONS AND ARPES EXPERIMENTS

The results derived above are general and independent of the particularities of the band structure. They rely only on the space group symmetry \( P4/mnm \) and its consequences at the doubles at \( \Gamma \) and \( M \). Yet, in order to understand the microscopic meaning of the nematic order parameters \( (\varphi_\Gamma, \varphi_1, \varphi_3) \), it is instructive to compare our results with those obtained from 10-orbital tight-binding models fitted to first-principle calculations. We used the model of Ref. \[26\] for LaFeAsO \[27\] and added two different tetragonal symmetry-breaking terms, while ignoring the spin-orbit coupling. The first is a uniform on-site energy splitting between the \( d_{xz} \) and \( d_{yz} \) orbitals of the form:

\[
H_1 = \frac{\Delta_1}{2} \sum_{\mathbf{k}\sigma} \left( c^\dagger_{\mathbf{xz},\mathbf{k}\sigma} c_{\mathbf{xx},\mathbf{k}\sigma} - c^\dagger_{\mathbf{yz},\mathbf{k}\sigma} c_{\mathbf{yz},\mathbf{k}\sigma} \right),
\]

whereas the second is a hopping anisotropy between the \( d_{xy} \) orbitals of the two Fe atoms. 

The results shown in Fig. \[3\] for \( \Delta_1 > 0, \Delta_3 = 0 \) and \( \Delta_1 = 0, \Delta_3 > 0 \) reveal that whereas the \( E_g \) and the \( E_M \) doubles are split by \( \Delta_1 \), the \( E_M \) doublet is split by \( \Delta_3 \), with \( \Delta E_g = \Delta E_{M_1} = \Delta_1 \) and \( \Delta E_{M_3} = \Delta_3 \). This is not unexpected, since in our low-energy model the \( E_g \) and \( E_M \) doubles have \( d_{xz}/d_{yz} \) characters, whereas the \( E_M \) doublet has \( d_{xy} \) character \[13\]. Therefore, we can identify \( \varphi_\Gamma = \varphi_1 \) with the on-site \( d_{xz}/d_{yz} \) orbital anisotropy \( \Delta_1 \) and \( \varphi_3 \) to the \( d_{xy} \) hopping anisotropy \( \Delta_3 \). Note that these results are insensitive to the microscopic mechanism behind the tetragonal symmetry breaking, i.e., whether it arises due to orbital \[28, 33\] or spin fluctuations \[2, 50, 40\], or electron-phonon coupling.
domain types, reflecting the dependence of the hole-pockets dispersions are very similar for the two twin domains, resulting in an effective doubling of the number of bands – even though the number of bands is not a consequence of translational symmetry. Moreover, the doubling of the number of bands may be difficult to resolve the different domain contributions near the $M$ point. As a result, it is more likely for ARPES to be able to resolve the two domains contributions near the $M$ point.

We can now discuss the implications of our results to the interpretation of ARPES experiments in the nematic-paramagnetic state, which takes place in the temperature range $T_{SDW} < T < T_{nem}$ for unstrained samples and in the temperature range $T_{SDW} < T$ for detwinned samples. The observed splitting of the $E_M$ doublet has been mostly attributed to an anisotropy in the onsite energies of the $d_{xz}$ and $d_{yz}$ orbitals (ferro-orbital order), which in our model is given by $\varphi_3$. However, our results in Eq. (11) show that this splitting depends also on the nematic order parameter $\varphi_3$, corresponding to anisotropic $d_{xy}$ hopping, and on the spin-orbit coupling $\lambda$. Thus, to properly disentangle these three contributions $\varphi_1 = \varphi_3$, and $\lambda$ we argue that it is necessary to measure simultaneously the splitting of the two doublets at the $M$ point and of the doublet at the $\Gamma$ point. The interplay between these three parameters may also explain why the doublet splittings are different at these two high-symmetry points, as observed experimentally.

Applied to twin samples, our results reveal important distinctions in the twin-domains dispersions near the $\Gamma$ and $M$ points, as shown in Fig. 4. Specifically, while at $\Gamma$ the dispersions are very similar for the two twin domains, at $M$ they are significantly different, since only in the latter the nematic order gives rise to a bonding and an anti-bonding orbital mixing. Moreover, the doubling of the number of bands is not a consequence of translational symmetry-breaking, since the nematic order is a $q = 0$ order.

Finally, we comment on the application of our results to the 122 materials, whose space group is $I4/mmm$ instead of $P4/nmm$. In contrast to the latter, the former space group is symmorphic. In the limit of no coupling between the Fe layers, this distinction is irrelevant, and the results derived here for the 1111, 111, and 11

Figure 3: Band dispersion along the $\Gamma$-$M$ direction (in meV) for the 10-orbital model of Ref. [20] in the presence of (a) an onsite energy anisotropy between the $d_{xz}/d_{yz}$ orbitals, $\Delta_1 = 50$ meV, and (b) a hopping anisotropy between $d_{xy}$ orbitals of nearest-neighbor Fe atoms, $\Delta_3 = 50$ meV. Dashed lines represent the dispersions for $\Delta_1 = \Delta_3 = 0$.

Figure 4: Band dispersions along the $\Gamma$-$M$ direction (in meV) for two different types of nematic domain. Solid (dashed) lines correspond to the domain with $\varphi_3 = 50$ meV ($\varphi_3 = -50$ meV). In both cases, $\lambda = 50$ meV.
families would also apply to the 122 family. Turning on a weak inter-layer coupling should lead to small changes, mixing states at \( k_z = \pi \) to \( k_z = 0 \). Although such an additional mixing could complicate the analysis proposed here, it remains to be seen whether it can be resolved by current ARPES experiments.

### IV. CONCLUSIONS

In summary, we used a low-energy model that respects all symmetries of the \( P4/\overline{mmm} \) iron superconductors to reveal the interplay between nematic order and spin-orbit coupling in the electronic spectrum of these materials. The simple expressions obtained for the splittings of the three doublets located at the high-symmetry points of the crystallographic Brillouin zone, Eq. (11), enables one to distinguish unambiguously using ARPES experiments not only these two physical effects, but also the two different contributions to the nematic order—namely the \( d_{xz}/d_{yz} \) orbital and \( d_{xy} \) hopping anisotropies. These criteria to disentangle spin-orbit and nematicity, being independent of details of the band dispersions, open an interesting route to systematically study the energy scales and the relevance of these two physical effects to the normal state of different iron-based superconductor families.

We thank S. Borisenko, A. Chubukov, V. Cvetkovic, I. Eremin, and R. Valenti for fruitful discussions. RMF is supported by the Department of Energy under Award Number DE – SC0012336. OV is supported by the NSF CAREER award under Grant No. DMR-0955561. We would also like to thank the KITP-UCSB Research Program, “Magnetism, Bad Metals and Superconductivity”, where this work was initiated, for hospitality. KITP is supported in part by NSF Grant No. NSF PHY11-25915.

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$$2 \tilde{t} \sum_{\sigma} c_{s^2(1), \sigma}^\dagger c_{s^2(2), \sigma} \left[ \cos \left( \frac{k_x + k_y}{2} \right) + \cos \left( \frac{k_x - k_y}{2} \right) \right]$$

with $\tilde{t} = -3$ meV.

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