Spin orbital interplay and topology in the nematic phase of iron pnictides

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We derive an effective action for a spin-nematic model starting from a multiorbital Hamiltonian. The singular C4 symmetry of the yz and zx Fe-d orbitals gives rise to a non trivial topology in the Fermi surface of iron superconductors. We find that the spin-nematic order parameter is closely related to this symmetry and that ellipticity is not a necessary condition for nematicity in contrast to what is found in the standard spin-nematic scenario. By analyzing the (π,0) spin susceptibility we find an intrinsic anisotropic momentum dependence and the spontaneous generation of orbital ordering. These results unveil a topological aspect arising from the orbital degree of freedom which is crucial for the understanding of the nematic state of iron superconductors.

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Most iron pnictides parent compounds present (π,0) antiferromagnetism (AF) in the 1-Fe Brillouin zone (BZ) and become superconductors upon doping or pressure. A structural transition takes place before or simultaneously to the AF one. These two transitions enclose the nematic phase characterized by many experimental probes [1–26]. Signatures of ferro-orbital ordering (OO) are found in ARPES experiments in the magnetic and nematic phase [27, 28]. The origin of the nematic phase is widely debated in the literature and has been discussed in the context of lattice, magnetic and orbital degrees of freedom (d.o.f) [29–36, 36–47]. Different experiments seem to indicate that it is electronic in origin [2, 4, 5, 17, 20, 21, 27] but due to the spin orbital interplay it is difficult to pinpoint between the two. There is also a controversy of whether nematicity is mostly intrinsic or mostly due to impurity scattering [6, 19, 24, 48–50].

Some indications about the relation between spin and orbital d.o.f. come from first principle calculations and mean field (MF) approaches in multiorbital Hamiltonians. Within these models OO is generated only when the (π,0) AF sets in [31–33, 51–54]. Beyond MF, Random Phase Approximation [55, 56] or Dynamical Mean Field Theory [57] calculations provide a good description of the spin dynamics in different compounds but the complexity of such calculations makes difficult to sort out the essential physics. On the other hand the Landau approach is very useful to understand the interplay between the structural and magnetic d.o.f and to calculate response functions [8, 39–41, 45, 58–61], in particular in the context of the spin-nematic (S-N) theory. Within this scenario we have to consider two broken symmetries in the (π,0) AF phase: the O(3) spin-rotational symmetry and the Z2 S-N symmetry between the (π,0) and (0, π) AF state. Since the Z2 discrete symmetry belongs to the Ising universality class is less affected by fluctuations and the nematic state can appear before the magnetic transition. In the work by Fernandes et al. [40] the S-N phase is derived from a microscopic Hamiltonian with hole (h-) and electron (e-) pockets without structure in the orbital d.o.f, in the following named orbital-less Landau approach. In this approach the nematic order parameter (OP) crucially depends on the ellipticity of the e-pockets vanishing for circular electron Fermi surfaces (FSs) [40, 59]. Ellipticity is also necessary to explain the evolution of the material with doping [15, 40] and to understand the anisotropy found in inelastic neutron scattering [41, 59, 62]. In spite of its simplicity this model helps to understand the interplay between the structural, nematic and magnetic transitions [40]. However, the absence of microscopic information about the orbital weight of the pockets and the lack of connection between this approach and multiorbital Hamiltonians leaves several important questions open.

Mostly three iron orbitals contribute to the FS of iron superconductors, yz and zx for the Γ pockets and xy, yz/zx for the the X/Y pocket. The particular arrangement of the yz and zx orbitals arises because under a 90 degree rotation the two orbitals transform as |xz⟩→|yz⟩ and |yz⟩→−|xz⟩ [63]. Consequence of this singular C4 symmetry is a non trivial topology in the Γ pocket [63–65]. This pocket can be seen as a doped quadratic band crossing point (QBCP) in the band structure of iron superconductors. QBCP are points in the BZ where two quadratic bands cross. They posses vorticity equal two and have been discussed in other context, specially in bilayer graphene [66]. They are known to be unstable under the renormalization group towards topological and nematic phases [67]. It is essential then to find out the consequences of this non-trivial FS in the S-N scenario.

In this letter we propose an effective action for the magnetic instability derived from a multiorbital Hamiltonian. The Landau coefficients depend on the orbital content, Hubbard and Hund’s coupling. In our approach we uncover that the orbital d.o.f. changes the S-N scenario in an essential way due to the vorticity of the Γ pocket and the uniquely yz/zx composition of the X/Y e-pockets. We find that (i) the ellipticity of the e-pockets is not mandatory in order to find nematicity in contrast to the orbital-less Landau approach result. (ii) The zx,
$y_z$ degeneracy is spontaneously broken in the $(\pi, 0)$ spin susceptibility in the nematic phase. Due to the interaction between the spin and the charge d.o.f. this orbital anisotropy will induce O-O. (iii) The spin fluctuation in the nematic phase are anisotropic in the $x$, $y$ directions. The results obtained are robust for any number of orbitals since they originate in symmetry and topological arguments. In order to better visualize these mechanisms we will analyze the expression for the spin susceptibility within a simple two-orbital model enough to capture the essence of the singular $C_4$ symmetry and suitable for analytical treatment.

We consider a multiorbital Hamiltonian for the FeAs layer including a tight-binding (TB) term plus local interactions as described in Ref. [52]. By considering rotational invariance, interactions can be expressed in terms of two coefficients: the intra-orbital Hubbard $U$ and the Hund’s coupling $J_{\text{H}}$ [68]. The TB term can be diagonalized $c_{\sigma \kappa} = \sum_m a_{\sigma m}(k) d_{\kappa m}$, with $a_{\sigma m}(k)$ the rotation matrix element between the orbital $\sigma$ and the band basis $n$. Since we are interested in the low energy physics we will restrict to energies and momenta close to the FS taking into account the h-potential at $\Gamma$ and the $X$ and $Y$ e-pockets. For simplicity we do not consider the third pocket found at the $M$ point in the FS since it is parameter sensitive and it is not usually taken into account in the nematic scenario. Therefore we have $c_{\eta \kappa \alpha} = \sum_m a_{\eta m}(k) d_{\kappa m}$, with $m = \Gamma, X, Y$ pockets and $\kappa$ restricted to be close to the FS. Following Ref. [40], we will consider only the spin channel of the interaction of the Hamiltonian and in particular we restrict to the spin excitations with momenta near $Q_1 = (\pi, 0)$ and $Q_2 = (0, \pi)$. The interaction Hamiltonian is given by

$$H_{\text{int}} = -\frac{1}{2} \sum_{\eta_1, \eta_2} \sum_{l=X, Y} U_{\eta_1 \eta_2}^{\text{spin}} \hat{S}_{\eta_1 l}(\mathbf{q}) \cdot \hat{S}_{\eta_2 l}(-\mathbf{q}).$$

$U_{\eta_1 \eta_2}^{\text{spin}} = \frac{8}{3} U \delta_{\eta_1, \eta_2} + 4 J_{\text{H}} (1 - \delta_{\eta_1, \eta_2})$ is a matrix in the orbital space. $\hat{S}_{\eta l}(\mathbf{q}) = \sum_\kappa a_{\eta \kappa l}(\mathbf{k}) \hat{S}_{\eta l}(\mathbf{k} + \mathbf{q})$ is the orbital-weighted spin operator for the pocket $l = X, Y$, where $\hat{S}_{\eta l}(\mathbf{k} + \mathbf{q}) = \frac{1}{2} \sum_{\alpha \beta} \hat{d}_{\eta \kappa \alpha \kappa \beta} \hat{d}_{\kappa \kappa \alpha \beta}$, with $\delta_{\alpha \beta}$ the Pauli matrices.

Let us now introduce the bosonic fields $\hat{\Delta}_{\eta l} = \hat{\Delta}_{X l}$ associated to the magnetic d.o.f $\hat{S}_{\eta l} = \hat{S}_{X l}$. Via a standard Hubbard-Stratonovich (HS) machinery [69, 70] we derive the effective action up to the quartic order:

$$S_{\text{eff}} = \sum_{l=X, Y, \eta_1, \eta_2} r_{\eta_1 \eta_2} \hat{\Delta}_{\eta l} \cdot \hat{\Delta}_{\eta l} + \frac{1}{16} \sum_{\eta_1, \eta_2, \eta_3} u_{\eta_1 \eta_2 \eta_3 \eta_4} \psi_{\eta_1 \eta_2} \psi_{\eta_3 \eta_4} + g_{\eta_1 \eta_2 \eta_3 \eta_4} \phi_{\eta_1 \eta_2} \phi_{\eta_3 \eta_4} + 2 v_{\eta_1 \eta_2 \eta_3} \psi_{\eta_1 \eta_2} \phi_{\eta_3}$$

$\Delta_{\eta X}, \Delta_{\eta Y}$ are the OPs with ordering momentum either $Q_1 = (\pi, 0)$ or $Q_2 = (0, \pi)$ in the Landau action $S_{\text{eff}}$ and

$$\psi_{\eta_1 \eta_2} = \frac{1}{2} \left( \Delta_{\eta_1 X} \cdot \Delta_{\eta_2 X} + \Delta_{\eta_1 Y} \cdot \Delta_{\eta_2 Y} \right),$$

$$\phi_{\eta_1 \eta_2} = \frac{1}{2} \left( \Delta_{\eta_1 X} \cdot \Delta_{\eta_2 X} - \Delta_{\eta_1 Y} \cdot \Delta_{\eta_2 Y} \right),$$

where $\phi_{\eta_1 \eta_2}$ is the nematic field in our approach. The Landau coefficients are given by

$$r_{\eta_1 \eta_2} = U_{\eta_1 \eta_2}^{\text{spin}} - 1 + 2 \sum_k G_{\eta l} \omega_{\eta l}^{\eta_1 \eta_2} \omega_{\eta l}^{\eta_2 \eta_1},$$

$$u_{\eta_1 \eta_2 \eta_3 \eta_4} = \frac{1}{2} \sum_{k l} G_{\eta l}^2 \left( G_{\eta l} \omega_{\eta l}^{\eta_1 \eta_2} \omega_{\eta l}^{\eta_2 \eta_1} \right) \left( G_{\eta l} \omega_{\eta l}^{\eta_3 \eta_4} \omega_{\eta l}^{\eta_4 \eta_3} \right),$$

$$g_{\eta_1 \eta_2 \eta_3 \eta_4} = -\frac{1}{2} \sum_{k l, s=1(X), -1(Y)} G_{\eta l}^2 \left( s G_{\eta l} \omega_{\eta l}^{\eta_1 \eta_2} \omega_{\eta l}^{\eta_2 \eta_1} \right) \left( s G_{\eta l} \omega_{\eta l}^{\eta_3 \eta_4} \omega_{\eta l}^{\eta_4 \eta_3} \right),$$

$$v_{\eta_1 \eta_2 \eta_3} = \frac{1}{2} \sum_{k l, s=1(X), -1(Y)} G_{\eta l}^2 \left( s G_{\eta l} \omega_{\eta l}^{\eta_1 \eta_2} \omega_{\eta l}^{\eta_2 \eta_1} \right) \left( s G_{\eta l} \omega_{\eta l}^{\eta_3 \eta_4} \omega_{\eta l}^{\eta_4 \eta_3} \right),$$

with $l = X, Y$. $G_{m,k} = (i \omega_n - \xi_{m,k})^{-1}$, $m = \Gamma, X, Y$ are the non interacting single-particle Green’s functions. The present derivation contains explicitly the orbital d.o.f. The spin OP $\hat{\Delta}_{X l}$ is a vector in the orbital space and the effective coefficients of Eq. (2) are matrix/tensor in the orbital space. If we consider the weight factors $\omega_{\eta l}^{\eta_1 \eta_2} = 1$ we recover the effective action given by Eq. (7) and the Landau coefficients given by Eq. (8) obtained via the orbital-less Landau approach of Ref. [40].

By direct inspection of Eq. (2) one finds that $S_{\text{eff}}$ is invariant under the O(3) symmetry and under the interchange between $\hat{\Delta}_X$ and $\hat{\Delta}_Y$. The quadratic coefficient, Eq.(5a), is the $\eta_1 \eta_2$ component of the quadratic Landau parameter $\hat{r}_l = \hat{\Delta}_X$. The magnetic susceptibility is by definition given by $r_l(q, \Omega_m) = \chi_l(q, \Omega_m)$ and the Néel temperature $T_N$ is fixed by the divergence of $\chi_l(0, 0)$. Due to the orbital d.o.f. the $T_N$ obtained within this formulation is a function of $(U, J_{\text{H}})$. The quartic Landau coefficients Eq. (5b)-(5d) are the elements of the $\hat{u}$, $\hat{v}$ tensors in the orbital space. $\hat{\phi}$ is the nematic coupling since it is coupled to the $(\hat{\Delta}_{X X} - \hat{\Delta}_{Y X}^2)$ term. By minimizing the action Eq. (2) with $\hat{\psi}$, $\hat{\phi}$ definite positive and $\hat{\phi}$ small compared to $\hat{\phi}$, two solutions for $T < T_N$ are obtained corresponding to the $(\pi, 0)$ and $(0, \pi)$ magnetic state. As proposed in [40], in order to relate the nematic OP with the magnetic susceptibility it is necessary to go ahead with a second HS transformation in terms of $\psi$ and $\phi$ given in Eq. (3) and in Eq. (4) and minimize the new effective action. However, without going further, it is already clear the importance of taking into account...
explicitly the orbital d.o.f. in the Landau functional. In fact within the orbital-less Landau approach [40] a finite $g$ requires the e-pockets to be elliptical [40, 41, 59] and $v$ is zero unless interaction between e-pockets are taking into account[71]. In the present formulation this is no longer true since both $g$ and $v$ are different from zero even for perfectly nested circular FSs and without considering interactions between the e-pockets. This can be easily checked from Eqs. (5c)-(5d) for any number of orbitals using that the orbital weight is mostly

\[ \chi_{lm\eta_3}(q) = \frac{1}{2} \sum_k G_{l,k} G_{ik+q} \omega_{n_1}^{\eta_3}(k, k + q), \]

where $k \equiv (i\omega_n, k), q \equiv (i\Omega_m, q)$, with $\omega_n, \Omega_m$ fermion, boson Matsubara frequencies respectively and $\eta_1, \eta_2 = y, z, x$. The magnetic bubble $\Pi(q)$ in Eq. (6) differs from the one of [40] in the weight factors $\omega_{n_1}^{\eta_3}$. These terms add a strong $k$ dependency to the standard Green functions integrand (see Fig. 1). We find that the crossed susceptibility is always strongly suppressed by the mixed term $\omega_{n_1}^{\eta_3} \omega_{n_1}^{\eta_2}$ and the contributions to the $\Gamma X (\Gamma Y)$ susceptibility along the $k_x (k_y)$ direction are zero weighted for all orbital components. By using Pauli matrices basis for the orbital space in Eq. (6), we find $\hat{\chi}_l^{-1}(0) \equiv (\hat{U} + \Pi_l^0)^{-1} = (\hat{J}_H - \Pi_l^0) \tau_1 + \Pi_l^0 \tau_3$, with $\hat{U} = (8U/3) / \det (U_{spin})$, $\hat{J}_H = 4|J_H| / \det (U_{spin})$, $\Pi_l^0 = (\Pi_{xyz} = \Pi_{zzzz}) / 2$ and $\Pi_l^3 = \Pi_{yzzz}$. The magnetic bubble $\tau_0, \tau_1$ components renormalize $U, J_H$ coupling to a smaller value. Interestingly, a non-zero $\tau_3$ component reflecting the breaking of the $yz/zx$ degeneracy is spontaneously generated. The weight of this $\tau_3$ component, $\omega_{n_1}^{\tau_3}$, is represented in the last panel of Fig. 1. Let us analyze the physical consequences the finite $\tau_3$ component found in the spin sector. Repeating the present derivation taking into account also the charge d.o.f. at small momentum, $n_{qm}$, we can define the new effective action $S_{eff}[n_{qm}, \Delta n]$. It is easy to check that the charge susceptibility computed at Gaussian level, $n_{qm}^2$, does not present OO component.

In the following we focus on the analysis of the magnetic susceptibility defined by the effective action Eq. (2) in the nematic phase. Our analysis is completely general and model independent since it is based on symmetry and topological arguments. A simple two-orbital model (see for example Ref. [73]) is enough to capture the $C_4$ symmetry of the FS [63, 64] and it is suitable for computing analytical expressions. From Eq. (5a) we have

\[ \chi_{lm\eta_3}(q) = U^{spin} \chi_{lm\eta_3}(q), \]

where $l \equiv (i\omega_m, l), q \equiv (i\Omega_n, q)$, with $\omega_m, \Omega_n$ fermion, boson Matsubara frequencies respectively and $\eta_1, \eta_2 = y, z, x$. The magnetic bubble $\Pi(q)$ in Eq. (6) differs from the one of [40] in the weight factors $\omega_{n_1}^{\eta_3}$. These terms add a strong $k$ dependency to the standard Green functions integrand (see Fig. 1). We find that the crossed susceptibility is always strongly suppressed by the mixed term $\omega_{n_1}^{\eta_3} \omega_{n_1}^{\eta_2}$ and the contributions to the $\Gamma X (\Gamma Y)$ susceptibility along the $k_x (k_y)$ direction are zero weighted for all orbital components. By using Pauli matrices basis for the orbital space in Eq. (6), we find $\hat{\chi}_l^{-1}(0) \equiv (\hat{U} + \Pi_l^0)^{-1} = (\hat{J}_H - \Pi_l^0) \tau_1 + \Pi_l^0 \tau_3$, with $\hat{U} = (8U/3) / \det (U_{spin})$, $\hat{J}_H = 4|J_H| / \det (U_{spin})$, $\Pi_l^0 = (\Pi_{xyz} = \Pi_{zzzz}) / 2$ and $\Pi_l^3 = \Pi_{yzzz}$. The magnetic bubble $\tau_0, \tau_1$ components renormalize $U, J_H$ coupling to a smaller value. Interestingly, a non-zero $\tau_3$ component reflecting the breaking of the $yz/zx$ degeneracy is spontaneously generated. The weight of this $\tau_3$ component, $\omega_{n_1}^{\tau_3}$, is represented in the last panel of Fig. 1. Let us analyze the physical consequences the finite $\tau_3$ component found in the spin sector. Repeating the present derivation taking into account also the charge d.o.f. at small momentum, $n_{qm}$, we can define the new effective action $S_{eff}[n_{qm}, \Delta n]$. It is easy to check that the charge susceptibility computed at Gaussian level, $n_{qm}^2$, does not present OO component.

However at higher level of the effective action due to the coupling, $n_{qm}^2 \Delta n^2$, between the spin channel with broken $yz/zx$ degeneracy and the charge bosonic mode, a $\tau_3$ component will be induced in the charge field susceptibility i.e. OO will be generated into the charge sector. Our analysis clearly reveals the intrinsic interrelation between spin and orbital d.o.f. in the nematic phase. Notice that this intrinsic OO generation is different from breaking explicitly the $yz/zx$ symmetry by introducing a small crystal field in the Hamiltonian [34, 40]. This results extend to the nematic state the MF findings of OO only within the magnetic phase [31–33, 51–54].

In the following we study the topological aspects. Within the continuum limit of the two-orbital TB Hamiltonian the $\Gamma$ pocket takes the typical form of a QBCP with vorticity equal 2, $\Pi_{x,y}(k) = 2b_k k_y \tau_1 + a(k_x^2 - k_y^2) \tau_3$, where $a$ and $b$ depend on the hopping (see SI). We can define the vector $\vec{n}_v = (\sin(2\phi_k), \cos(2\phi_k))$ with $\phi_k = \arctan \frac{k_x}{k_y}$. For the X/Y pocket we have $\vec{n}_x \sim (0, 1)$ and $\vec{n}_y \sim (0, -1)$ (see Fig. 2). Within this approximation the magnetic bubble $\Pi_{x,y}(q = 0)$ has only the $\eta_1 = \eta_2 = yz$ component, $\Pi_{x}^1 = 0$ and $\Pi_{y}^1 = \Pi_{x}^3 = \frac{1}{2} \Pi_{x,y}^{yz}$ where

\[ \Pi_{x,y}^{yz}(0) = T \sum_{n} \int \frac{d^2k}{(2\pi)^2} \frac{\sin^2 \phi_k}{(i\omega_n - \xi_{x,y}(k))(i\omega_n - \xi_{x,y}(k))} \]

By direct inspection of Eq. (8) is trivial to verify that the suppression of the integrand along the $k_x$ direction (Fig. 1) is simply due to $\sin^2 \phi_k$. This angular dependence arises from the different vorticity of the $\Gamma$ and X pockets connected by the spin interaction.
Finally we analyze the anisotropic properties of the spin susceptibility $\chi(\Omega = 0, \mathbf{q})$, Eq. (6). For perfect nested pockets and without the orbital structure one obtains isotropic spin fluctuations $\Pi_X(0, \mathbf{q}) = \Pi_X(0) + c\mathbf{q}^2$ where $c \sim (\partial_{\mathbf{k}} \xi)_{Y}^2$. However in the present case the expansion involves also the $\mathbf{k}$-dependent orbital weight factors. This introduces an anisotropic component in the spin fluctuations

$$\Pi_X(0, \mathbf{q}) = \Pi_X(0) + c\mathbf{q}^2 + \delta c_x q_x^2 + \delta c_y q_y^2,$$

(9)

with $\delta c_x / y \propto \partial_{\mathbf{k}} \xi_{x/y} \omega^{x-y}(\mathbf{k})\partial_{\mathbf{k}} \xi_{x/y}$ where we used $\omega^{x-y} \propto 0$ so that as before the only non-zero term of $\Pi_X(0, \mathbf{q})$ is the $yz$ one. This anisotropy can also be computed in the continuum limit where the analogous to $\omega^{y-x}(\mathbf{k})$ is the angular dependence $\phi_{k}$ of the spin susceptibility as already discussed for the $q = 0$ term (see Eq. 8). Again this anisotropy arises because the spin interaction is connecting the $\Gamma$ pocket with vorticity $2$ with the $X/Y$ pockets that are trivial. The anisotropic character of the AF fluctuation above $T_N$ found here is consistent with experiments in neutron scattering [25, 26, 56, 62, 74]. In Ref. [62, 74] the anisotropy is linked to the ellipticity of the e-pockets. We however found that even by considering circular pockets an anisotropic component is present consistently with Ref. [25, 56]. This is a robust result with topological origin and does not depend on details of the band structure or disorder effects. Interestingly in the $(\pi, 0)$ AF phase in iron superconductors the connection of the $\Gamma$ pocket with vorticity $2$ with the $X/Y$ pockets, gives rise to a metallic nodal spin density wave [64]. In Ref. [32] it was found that this particular magnetic reconstruction of the FS is realized for small magnetic moment and gives rise to the experimental Drude anisotropy. This anisotropy found for the nodal spin density wave is likely related with the scenario proposed in this letter [72].

In a realistic band structure, at low energy there are two (or three) h-pockets at the $\Gamma$ point. The $\mathbf{k}$-structure of the orbital content of the h-pockets gives rise to a different vorticity $-2, -2$ (0) for each one, while the trivial topology of the e-pockets is not changed. Within the S-N approach, the e-pockets interact stronger with the h-pocket more nested by the $\Gamma$ pocket with opposite vorticity where the opposite anisotropy is now expected. This suggests a possible explanation for the sign-reversal of the in-plane resistivity anisotropy found in h-doped compounds. [15] More detailed analysis is beyond the scope of this work, however since the former arguments are based on robust properties of the system, symmetry and topology, the qualitative discussion are not expected to change.

In conclusion, we derived the effective action for the spin order parameter with Landau coefficients depending on the orbital character, Hubbard and Hund’s interaction. This derivation is valid for any multiorbital system, not just for iron pnictides and it represents the starting point of many possible studies. In the context of iron superconductors, important differences are revealed with respect to the orbital-less Landau approach due to the non trivial topology of the Fermi surface: (i) the nematic coupling is different from zero even for perfect nesting due to the different orbital content of the $X$ and $Y$ pockets. (ii) In the spin susceptibility it is found that the $yz/xz$ degeneracy is spontaneously broken in the spin channel. This broken symmetry will induce ferro-orbital ordering in the charge channel. The result reveals the strong spin orbital interplay. (iii) The spin fluctuations are anisotropic in $x/y$ direction even for the case of perfect nesting. We have shown analytical results for the spin susceptibility by considering the two-orbital model but since our conclusions are based in topological and symmetry arguments, they are also valid for more realistic models describing iron pnictides. At the light of our results experiments interpreted using the ellipticity of the e-pockets should be revisited with the information in the orbital degree of freedom. This work highlights for the first time a clear connection between microscopic nematicity and topology.

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Supplementary Material
Spin orbital interplay and topology in the nematic phase of iron pnictides
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To calculate the spin susceptibility we have considered a tight-binding model for the \(d_{yz}\) and \(d_{xz}\) Fe orbitals with indirect hopping through the As as the one studied in Ref. [1]. In the following we discuss some of the technical aspects used in the main text.

The two orbital model is enough to illustrate the symmetry and topological arguments. Considering the symmetries of the orbitals and the Fe square lattice with tetrahedral environment, the hoppings fulfill the following relations: \(t_1 = t'_{xHy} = t'_{Hyx}, t_2 = t'_{xZx}, t_3 = t'_{xZy}, t_4 = t'_{yZy}, t_5 = t'_{yZx}, \) and \(t_{xHy} = t_{yZy} = 0\) [1]. The subscripts indicate orbitals, the superscript \('\) indicates second nearest neighbors and the superscript \(x/y\) indicates second nearest neighbors and the superscript \(x/y\)-direction. This non-trivial \(C_4\) symmetry between the \(yz\) and \(zr\) orbitals gives rise to the non-trivial topology of the FS.

We can write the Hamiltonian in the basis of the Pauli matrices with orbital pseudospin \(\Psi_\mathbf{k} = (\alpha_{kYZ}, \alpha_{kZX})^T\):

\[
\hat{H}_0 = \sum_\mathbf{k} \Psi_\mathbf{k}^+ \left( h_0(\mathbf{k}) \tau_0 + \hat{\mathbf{h}}(\mathbf{k}) \cdot \mathbf{\tau} \right) \Psi_\mathbf{k}, \quad (S1)
\]

with

\[
h_0(\mathbf{k}) = -(t_1 + t_2)(\cos ak_x + \cos ak_y) - 4t_3 \cos ak_x \cos ak_y, \quad (S2)
\]

\[
h_3(\mathbf{k}) = -(t_1 - t_2)(\cos ak_x - \cos ak_y), \quad (S3)
\]

and

\[
h_1(\mathbf{k}) = -4t_4 \sin ak_x \sin ak_y. \quad (S4)
\]

Diagonalizing the Hamiltonian we arrive to the two bands \(E^\pm(\mathbf{k}) = h_0(\mathbf{k}) \pm \sqrt{h_0^2(\mathbf{k}) + h_3^2(\mathbf{k})}\). A generic band structure closed to the Fermi level showing the orbital weights is represented in Fig. S1. There is a QBCP at the hole \(\Gamma\) pocket just above the FS and the \(X/Y\) electron pocket has dominant \(yz/xx\) component.

We are interested in the behavior of \(H_0\) around \(\Gamma\), \(Y\) and \(X\) points. In the continuum limit we expand to lowest order. Around the \(\Gamma\) point we get: \(h_{0,\Gamma}(\mathbf{k}) \simeq \varepsilon_\Gamma + \alpha_\Gamma k^2\), \(h_{1,\Gamma}(\mathbf{k}) \simeq -2ck_xk_y\) and \(h_{3,\Gamma}(\mathbf{k}) \simeq b(k_x^2 - k_y^2).\) Assuming \(4t_3 \simeq t_1 - t_2\), we have \(b \simeq c\), and around \(\Gamma\) the dispersion relation is isotropic. Since we discuss topological arguments the results are not dependent on this approximation. The \(\Gamma\) pocket has the typical dispersion relation of a QBCP with vorticity equal 2 [2]. Around the \(X/Y\) point \(X/Y(\mathbf{k}) \simeq \varepsilon_\Gamma + \alpha_\Gamma k_x^2 + \alpha_\Gamma k_y^2\). The QBCP is seen at the \(\Gamma\) point just above the FS. It is observed that \(X/Y\) pocket is mostly \(yz/xx\).

FIG. S1: (Color online) Band structure of the two orbital model. Green (red) stands for the \(yz/xx\) orbital weight.

In general, the Green function associated to the Hamiltonian (S1) can be written as

\[
\hat{G}(\omega, \mathbf{k}) = \frac{1}{2} \sum_{s = \pm 1} \frac{\tau_0 + \mathbf{\tau} \cdot \hat{n}(\mathbf{k})}{\omega - s|\hat{h}(\mathbf{k})|}, \quad (S5)
\]

with \(\hat{n}(\mathbf{k}) = \hat{h}(\mathbf{k})/|\hat{h}(\mathbf{k})|\), and \(s = \pm 1\) labels the conduction \((s = 1)\) and valence \((s = -1)\) bands. If we define \(\theta_\mathbf{k} = \arctan(k_y/k_x)\) then \(\hat{n}(\mathbf{k}) = (\sin 2\phi_\mathbf{k}, \cos 2\phi_\mathbf{k})\). We can particularize this Green function to each pocket. In our case, the \(\Gamma\) point belongs to the valence band \((s = -1)\) and the \(X, Y\) pockets belong to the conduction \((s = 1)\) band.

\[
\hat{G}_\Gamma(\omega, \mathbf{k}) = \frac{1}{2} \frac{\tau_0 - \mathbf{\tau} \cdot \hat{n}_\Gamma(\mathbf{k})}{\omega - \varepsilon_0 + \frac{k^2}{2m}}, \quad (S6a)
\]

\[
\hat{G}_{X/Y}(\omega, \mathbf{k}) = \frac{1}{2} \frac{\tau_0 + \mathbf{\tau} \cdot \hat{n}_{X/Y}(\mathbf{k})}{\omega - \varepsilon_0 - \frac{k_x^2}{2m_x} - \frac{k_y^2}{2m_y}}, \quad (S6b)
\]
where we have approximated the dispersion relations of the $\Gamma$, $X$, and $Y$ points as $E_\Gamma (k) \simeq \varepsilon_0 - \frac{k^2}{2m_\Gamma}$, $E_X (k) \simeq -\varepsilon_0 + \frac{k_x^2}{2m_x} + \frac{k_y^2}{2m_y}$, and $E_Y (k) \simeq -\varepsilon_0 + \frac{k_x^2}{2m_y} + \frac{k_y^2}{2m_x}$, respectively and $\varepsilon_0$ is an energy offset. Notice that in general the dispersion relations of the $X, Y$ are elliptical with opposite ellipticity. For the $X/Y$ electron pockets we take the approximation $\hat{n}_X = -\hat{n}_Y = (0, 1)$. The physical meaning is that the orbital weight of the pocket $X/Y$ is from the $d_{yz}/d_{zx}$ orbital. In general the spin susceptibility depend on four orbital indices but in the spin-nematic scenario the spin-susceptibility depends just on two orbitals (Eq. (7) in the text). In the continuum limit is given by

$$\Pi_{\eta\eta'}(0, q) = -\frac{1}{\beta} \sum_{\omega_n} \int \frac{d^2 k}{4\pi^2} G^\eta_{\Gamma}(i\omega_n, k) G^\eta'_{X}(i\omega_n, k + q),$$

$$\tag{S7}$$

where there is no summation in $\eta, \eta'$. For $q = 0$ and replacing the Green’s functions by expressions Eq. S6 we obtain the expression quoted in the text for $\Pi_{XYYZ}(0)$. To calculate $\Pi_{\eta\eta'}(0, q)$ we have used zero ellipticity to isolate the effect of the of the spin interaction connecting the vortex in the $\Gamma$ pocket with the $X/Y$ pockets.

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