

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

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The origin of the nematic state is an important puzzle to be solved in iron pnictides. Iron superconductors are multiorbital systems and these orbitals play an important role at low energy. The singular C_4 symmetry of d_{zx} and d_{yz} orbitals has a profound influence at the Fermi surface since the Γ pocket has vortex structure in the orbital space and the X/Y electron pockets have yz/zx components, respectively. We propose a low-energy theory for the spin-nematic model derived from a multiorbital Hamiltonian. In the standard spin-nematic scenario, the ellipticity of the electron pockets is a necessary condition for nematicity. In the present model, nematicity is essentially due to the singular C_4 symmetry of yz and zx orbitals. By analyzing the $(\pi,0)$ spin susceptibility in the nematic phase, we find a spontaneous generation of orbital splitting, extending previous calculations in the magnetic phase. We also find that the $(\pi,0)$ spin susceptibility has an intrinsic anisotropic momentum dependence due to the nontrivial topology of the Γ pocket.

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I. INTRODUCTION

Most iron pnictides parent compounds present $(\pi,0)$ 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) in the magnetic and nematic phase are found in the angle-resolved photoemission spectroscopy (ARPES) [27,28] and x-ray absorption spectroscopy [29]. The origin of the nematic phase is widely debated in the literature. There is a controversy on whether nematicity is mostly intrinsic or mostly due to impurity scattering [6,19,24,30–32]. In the intrinsic scenario, it has been discussed in the context of lattice, magnetic, and orbital degrees of freedom (d.o.f) [26,33–51]. Different experiments suggest an electronic origin [2,4,5,17,20,21,27] but due to the spin-orbital interplay, it is difficult to pinpoint between the two.

First-principles calculations and mean-field (MF) approaches in multiorbital Hamiltonians have found OO only inside the $(\pi,0)$ AF phase [35–37,52–55]. Beyond MF, random phase approximation [56,57] or dynamical mean-field theory [58] calculations provide a good description of the spin dynamics in different compounds. However, 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 [8,43–45,49,59–62], in particular, in the context of the spin-nematic (S-N) theory. Within this scenario we have to consider two broken symmetries in the $(\pi,0)$ AF phase: the $O(3)$ spin-rotational symmetry and the Z_2 S-N symmetry between the $(\pi,0)$ and $(0,\pi)$ AF states. The discrete Z_2 S-N symmetry can appear at higher temperature than the magnetic transition. In the work by Fernandes *et al.* [44], 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 effective 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) [44,60]. Ellipticity arguments have also been used to explain experiments [15,44,45,60,63]. In spite of its simplicity, this model helps to understand the interplay between the structural, nematic, and magnetic transitions [44]. However, the absence of microscopic information about the orbital d.o.f 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 X/Y pocket. The particular arrangement of the yz and zx orbitals arises because under a $\pi/2$ rotation the two orbitals transform as $|xz\rangle \rightarrow |yz\rangle$ and $|yz\rangle \rightarrow -|xz\rangle$ [64]. Important features of this singular C_4 symmetry are (i) the yz/zx orbital content in the X/Y pocket and (ii) a nontrivial topology in the Γ pocket with a vorticity equal to 2 in the nonmagnetic phase. Due to this topology, a nodal spin density wave (SDW) with two Dirac cones is formed in the magnetic phase [65,66]. It is essential then to find out the consequences of this low-energy physics in the S-N scenario.

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. The orbital d.o.f. changes the S-N scenario in an essential way: (i) the yz/zx orbital content of the X/Y e pockets gives rise to a finite nematic coupling regardless the value of the ellipticity of the e pockets. Analyzing the $(\pi,0)$ magnetic susceptibility in the nematic phase we find that (ii) the zx , yz degeneracy is spontaneously broken without considering a small crystal field or interactions between the e pockets in the original Hamiltonian and (iii) the spin fluctuations have an anisotropic momentum dependence in the x , y directions due to the spin interaction connecting the Γ pocket with the vorticity two with the topologically trivial X e-pocket. The results obtained are robust for any number of orbitals since they are based on symmetry and topological arguments. To obtain analytical results, we analyze the continuum limit of the d_{yz} - d_{zx} orbital model that displays the fundamental C_4 orbital symmetry. Within this approximation,

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we also consider the ellipticity of the e-pockets perturbatively to compare our results with previous theoretical expectations. We find that the vortex of the Γ pocket gives an anisotropic \mathbf{q} dependence of the $(\pi, 0)$ magnetic susceptibility already at zero order and also affects the contribution proportional to the ellipticity parameter. The calculation of the nematic coupling confirms that, in the limit of validity of the approximation, the dominant contribution is the one coming from the orbital symmetry.

II. EFFECTIVE ACTION FOR THE MULTIORBITAL SYSTEM

We consider a multiorbital Hamiltonian for the FeAs layer including a tight-binding (TB) term plus local interactions as described in [53]. By considering rotational invariance, interactions can be expressed in terms of two coefficients: the intraorbital Hubbard U and the Hund coupling J_H [67]. The TB term can be diagonalized $c_{\eta\mathbf{k}\alpha}^\dagger = \sum_n a_{\eta n}^*(\mathbf{k}) d_{n\mathbf{k}\alpha}^\dagger$ with $a_{\eta n}(\mathbf{k})$ the rotation matrix element between the orbital η and the band basis n . Since we are interested in the low-energy physics, we will restrict our analysis to energies and momenta close to the FS taking into account the h pocket at Γ 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 S-N scenario. Therefore we have $c_{\eta\mathbf{k}\alpha}^\dagger = \sum_m a_{\eta m}^*(\mathbf{k}) d_{m\mathbf{k}\alpha}^\dagger$ with $m = \Gamma, X, Y$ pockets and \mathbf{k} restricted to be close to the FS. Following Ref. [44], we will consider only the spin channel of the interaction of the Hamiltonian and we only consider the spin excitations with momenta near $\mathbf{Q}_1 = (\pi, 0)$ and $\mathbf{Q}_2 = (0, \pi)$. The interaction Hamiltonian is given by

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

$U_{\eta_1 \eta_2}^{\text{spin}} = \frac{8}{3} U \delta_{\eta_1 \eta_2} + 4J_H(1 - \delta_{\eta_1 \eta_2})$ is a matrix in the orbital space. $\vec{S}_{\eta l}(\mathbf{q}) = \sum_{\mathbf{k}} w_{\Gamma l}^{\eta}(\mathbf{k}, \mathbf{k} + \mathbf{q}) \vec{S}_{\Gamma l}(\mathbf{k}, \mathbf{k} + \mathbf{q})$ is the orbital-weighted spin operator for the pocket $l = X, Y$, where $\vec{S}_{\Gamma l}(\mathbf{k}, \mathbf{k} + \mathbf{q}) = \frac{1}{2} \sum_{\alpha\beta} d_{\Gamma\mathbf{k}\alpha}^\dagger \vec{\sigma}_{\alpha\beta} d_{l\mathbf{k}+\mathbf{q}\beta}$. The weight factors $w_{\Gamma l}^{\eta}(\mathbf{k}, \mathbf{k} + \mathbf{q}) = a_{\Gamma\eta}(\mathbf{k}) a_{l\eta}(\mathbf{k} + \mathbf{q})$, relate orbital and pockets basis, while $\vec{\sigma}_{\alpha\beta}$ are the Pauli matrices.

Let us now introduce the bosonic fields $\vec{\Delta}_{\eta l=X, Y}$ associated to the magnetic d.o.f $\vec{S}_{\eta l=X, Y}$. Via a standard Hubbard-Stratonovich (HS) machinery, we derive the effective action up to the quartic order (for a complete derivation see Appendix A):

$$\begin{aligned} S_{\text{eff}} = & \frac{1}{2} \sum_{l=X, Y} \sum_{\eta_1 \eta_2} r_{\eta_1, \eta_2, l} \vec{\Delta}_{\eta_1 l} \cdot \vec{\Delta}_{\eta_2 l} \\ & + \frac{1}{4} \sum_{\eta_1 \eta_2 \eta_3 \eta_4} \frac{1}{2} u_{\eta_1 \eta_2 \eta_3 \eta_4} \psi_{\eta_1 \eta_2} \psi_{\eta_3 \eta_4} \\ & - \frac{1}{2} g_{\eta_1 \eta_2 \eta_3 \eta_4} \phi_{\eta_1 \eta_2} \phi_{\eta_3 \eta_4} + v_{\eta_1 \eta_2 \eta_3 \eta_4} \psi_{\eta_1 \eta_2} \phi_{\eta_3 \eta_4}, \quad (2) \end{aligned}$$

where $\vec{\Delta}_{\eta_1 X}$, $\vec{\Delta}_{\eta_1 Y}$ are the OPs with ordering momentum either $\mathbf{Q}_1 = (\pi, 0)$ or $\mathbf{Q}_2 = (0, \pi)$ in the Landau action S_{eff} ,

and we decomposed the quartic term using the following parametrization:

$$\psi_{\eta_1 \eta_2} = 2(\vec{\Delta}_{\eta_1 X} \cdot \vec{\Delta}_{\eta_2 X} + \vec{\Delta}_{\eta_1 Y} \cdot \vec{\Delta}_{\eta_2 Y}), \quad (3)$$

$$\phi_{\eta_1 \eta_2} = 2(\vec{\Delta}_{\eta_1 X} \cdot \vec{\Delta}_{\eta_2 X} - \vec{\Delta}_{\eta_1 Y} \cdot \vec{\Delta}_{\eta_2 Y}), \quad (4)$$

where $\phi_{\eta_1 \eta_2}$ is the nematic field in our approach. For a more general parametrization, see Appendix A.

The Landau coefficients are given by

$$r_{l\eta_1 \eta_2} = U_{\eta_1 \eta_2}^{\text{spin}-1} + \frac{1}{4} \sum_k G_{\Gamma} G_l w_{\Gamma l}^{\eta_1} w_{\Gamma l}^{\eta_2}, \quad (5a)$$

$$u_{\eta_1 \eta_2 \eta_3 \eta_4} = \frac{1}{2} \sum_{kl} G_{\Gamma}^2 (G_l w_{\Gamma l}^{\eta_1} w_{\Gamma l}^{\eta_2}) (G_l w_{\Gamma l}^{\eta_3} w_{\Gamma l}^{\eta_4}), \quad (5b)$$

$$\begin{aligned} g_{\eta_1 \eta_2 \eta_3 \eta_4} = & -\frac{1}{2} \sum_{kl} \sum_{s=1(X), -1(Y)} G_{\Gamma}^2 (s G_l w_{\Gamma l}^{\eta_1} w_{\Gamma l}^{\eta_2}) \\ & \times (s G_l w_{\Gamma l}^{\eta_3} w_{\Gamma l}^{\eta_4}), \quad (5c) \end{aligned}$$

$$v_{\eta_1 \eta_2 \eta_3 \eta_4} = \frac{1}{2} \sum_{kl} \sum_{s=1(X), -1(Y)} G_{\Gamma}^2 G_l w_{\Gamma l}^{\eta_1} w_{\Gamma l}^{\eta_2} (s G_l w_{\Gamma l}^{\eta_3} w_{\Gamma l}^{\eta_4}), \quad (5d)$$

with $l = X, Y$. $G_{m, k} = (i\omega_n - \xi_{m, \mathbf{k}})^{-1}$, $m = \Gamma, X, Y$ are the noninteracting single-particle Green's functions. The spin OP $\vec{\Delta}_{\eta l=X, Y}$ is a vector in the orbital space and the effective coefficients of Eq. (2) are matrix/tensor in the same space. If we consider the weight factors $w_{\Gamma l}^{\eta} = 1$, we recover the effective action given by Eq. (7) and the Landau coefficients given by Eq. (8) obtained via the orbital-less approach of Ref. [44].

The effective action, Eq. (2), is invariant under the $O(3)$ symmetry and under the interchange between $\vec{\Delta}_X$ and $\vec{\Delta}_Y$. The quadratic coefficient, Eq. (5a), is the $\eta_1 \eta_2$ component of the quadratic Landau parameter $\hat{r}_{l=X, Y}$. The magnetic susceptibility is defined by $\hat{r}_l(\mathbf{q}, i\Omega_m) = \hat{\chi}_l^{-1}(\mathbf{q}, i\Omega_m)$ and the Néel temperature T_N is fixed by the divergence of $\hat{\chi}_l(0, 0)$. Due to the presence of the orbital d.o.f., the T_N obtained within this formulation is a function of (U, J_H) . The quartic Landau coefficients Eqs. (5b)–(5d) are the elements of the \hat{u} , \hat{g} , and \hat{v} tensors. The \hat{g} tensor coupled to the $(\Delta_X^2 - \Delta_Y^2)$ term is the nematic coupling. By minimizing the action (2), two solutions for $T < T_N$ corresponding to the $(\pi, 0)$ and $(0, \pi)$ magnetic state can be found in a proper range of parameters. To analyze the nematic phase, we need to study how the $\hat{\phi}$ field orders. In Ref. [44], the nematic OP is related with the magnetic susceptibility via a second HS transformation in terms of $\hat{\psi}$ and $\hat{\phi}$ given in Eqs. (3) and (4). A detailed study of the nematic transition goes beyond the aim of this work and it will be the subject of further investigations [68]. We focus on the analysis of the Landau parameters of the effective action (2) that allows us to demonstrate that taking into account the orbital d.o.f changes the S-N picture drastically.

First, let us focus on the quartic coefficients controlling the nematic order. While within the orbital-less Landau approach [44] a finite g requires the e pockets to be elliptical [44, 45, 60] and v is zero unless the interaction between e pockets is taken into account [69], this is no longer true in the present

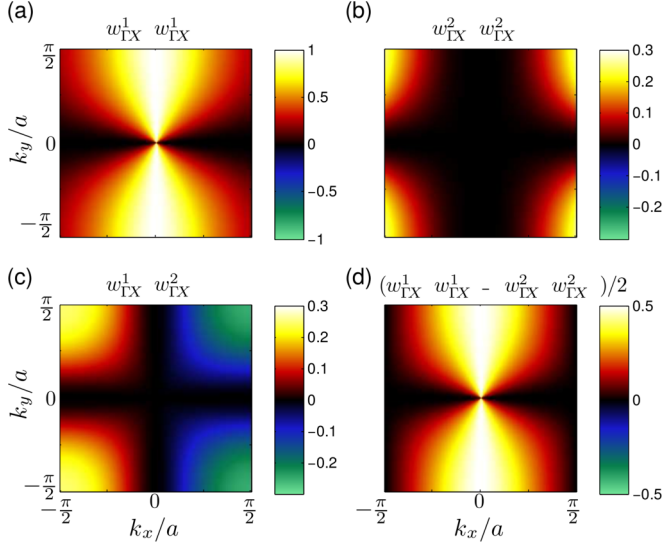


FIG. 1. (Color online) (a)–(c) $w_{\Gamma X}^{\eta_1} w_{\Gamma X}^{\eta_2}$ factors weighting the \mathbf{k} integrals of the magnetic bubble Eq. (7) computed using the same model parameters of [56]. The dominant orbital component is the $w_{\Gamma X}^1 w_{\Gamma X}^1$. The contribution from the orbital 2 is considerably smaller as well as the mixed one $w_{\Gamma X}^1 w_{\Gamma X}^2$. By drawing the \mathbf{k} dependence of the orbital weights for the magnetic fluctuations ΓY , we would find the same results rotated by $\pi/2$ as expected by symmetry. (d) τ_3 weight component $w_{\Gamma X}^3 = \frac{1}{2}(w_{\Gamma X}^1 w_{\Gamma X}^1 - w_{\Gamma X}^2 w_{\Gamma X}^2)$. The τ_3 weight is similar to $\sim w_{\Gamma X}^1 w_{\Gamma X}^1/2$ as found in the simplified model where we assume the contribution of the orbital 2 being zero for the X pocket.

formulation. In fact, regardless of ellipticity, both \hat{g} and \hat{v} , Eqs. (5c)–(5d), are finite due to the yz/zx orbital content of the X/Y e pockets, i.e., $w_{\Gamma Y}^{yz} \sim 0$, $w_{\Gamma X}^{zx} \sim 0$. This result holds for any number of orbitals since it follows from symmetry arguments. This general outcome implies that the nematicity does not necessarily require the ellipticity of the e pockets as expected in the standard S-N scenario. Below, we will address the question about the relative contribution of the orbital C4 symmetry and the ellipticity of the e pockets to the nematic coupling analyzing the simple case of the continuum limit of a two-orbital model.

Next, we analyze the $(\pi, 0)$ magnetic susceptibility in the nematic phase defined by Eq. (5a) as

$$\chi_{X\eta_1\eta_2}^{-1}(\mathbf{q}) = U_{\eta_1\eta_2}^{\text{spin}-1} + \frac{1}{2}\Pi_X^{\eta_1\eta_2}(q), \quad (6)$$

$$\Pi_X^{\eta_1\eta_2}(q) = \frac{1}{2} \sum_k G_{\Gamma k} G_{Xk+q} w_{\Gamma X}^{\eta_1}(\mathbf{k}, \mathbf{k} + \mathbf{q}) w_{\Gamma X}^{\eta_2}(\mathbf{k}, \mathbf{k} + \mathbf{q}), \quad (7)$$

where $k \equiv (i\omega_n, \mathbf{k})$, $q \equiv (i\Omega_m, \mathbf{q})$, and with ω_n and Ω_m being the fermion and boson Matsubara frequencies, respectively. We restrict our analysis to a two-orbital model [56,65,70] $\eta_{1,2} = yz, zx$. For simplicity, we will use $yz = 1$ and $zx = 2$. The weight factors $w_{\Gamma X}^{\eta_1} w_{\Gamma X}^{\eta_2}$ numerically computed for the d_{yz} - d_{zx} model are shown in Figs. 1(a)–1(c).

The strong \mathbf{k} dependence of the orbital weights modulates the \mathbf{k} integral in Eq. (7). Notice that the contributions to the susceptibility along the k_x direction have zero weight for all

orbital components. Π_X^{11} is the dominant orbital component of the magnetic bubble with the others being suppressed by the small orbital weights.

Let us consider the constant part $q = 0$ of the magnetic susceptibility. By using a Pauli matrices basis to decompose the orbital structure of Eq. (6), we find $\hat{\chi}_X^{-1}(0) \equiv (\tilde{U} + \Pi_X^0)\hat{\tau}_0 - (\tilde{J}_H - \Pi_X^1)\hat{\tau}_1 + \Pi_X^3\hat{\tau}_3$, where $\Pi_X^{0,3} = (\Pi_X^{11} \pm \Pi_X^{22})/4$ and $\Pi_X^1 = \Pi_X^{12}/2$. $\tilde{U} = (8U/3)/\det U^{\text{spin}}$, $\tilde{J}_H = 4J_H/\det U^{\text{spin}}$, where \det indicates the determinant. The τ_0, τ_1 components of the magnetic bubble renormalize U and J_H coupling to a smaller value. Interestingly, a nonzero τ_3 component reflecting the breaking of the orbital degeneracy is spontaneously generated, see Fig. 1(d). The existence of a finite τ_3 component in the spin sector is connected to the orbital splitting in the charge sector. This can be demonstrated deriving the effective action $S_{\text{eff}}[n_{\eta m}, \Delta_{\eta l}]$ that accounts also for the charge d.o.f. at small momentum, $n_{\eta m}$, with $m = \Gamma, X, Y$, and $l = X, Y$. In the nematic phase, the charge susceptibility computed at Gaussian level, $n_{\eta\Gamma}^2$, does not present yz/zx orbital splitting. However, at higher level of the effective action, there are terms coupling the spin mode with broken orbital degeneracy to the charge mode [e.g., $(n_{\eta\Gamma} \Delta_{\eta X})^2$]. Integrating out the spin fluctuations, a τ_3 component is induced in the charge field susceptibility, i.e., orbital splitting is generated into the charge sector. This intrinsic splitting arises because of the effect of the nontrivial yz/zx C4 symmetry at low energy. This mechanism is different from breaking explicitly the yz/zx symmetry by introducing a small crystal field in the Hamiltonian [38,44] or from inferring it assuming X-Y pocket interaction [71]. Our analysis clearly reveals the intrinsic interrelation between spin and orbital d.o.f. in the nematic phase and it extends the MF findings of orbital splitting in the magnetic phase [35–37,52–55].

Finally, we analyze the momentum dependence of the spin susceptibility $\hat{\chi}(\mathbf{q})$, Eq. (6). For perfectly nested pockets and without the orbital structure, one obtains isotropic spin fluctuations $\Pi_X(0, \mathbf{q}) = \Pi_X(0) + c_X^x q_x^2 + c_X^y q_y^2$, where $c_X^i \sim (\partial_{k_i} \xi_{\mathbf{k}})^2$. In the present case, the expansion also involves the \mathbf{k} -dependent orbital weight factors [Figs. 1(a)–1(c)]. Due to the singular orbital symmetry of the problem, we find that the angular dependence introduced by the weights in the magnetic bubble leads to anisotropic component in the spin fluctuations $c_X^x \neq c_X^y$. We discuss quantitatively these results below within a simplified model obtained by the continuum limit of the two-orbital model.

III. QUANTITATIVE DISCUSSION

Our orbital-dependent analysis of the Landau parameters changes qualitatively the S-N picture derived in the orbital-less approach. We have shown that ellipticity is mandatory neither to find a finite nematic coupling \hat{g} nor to have anisotropic spin fluctuations. However, since the e pockets are elliptical we quantify the relative importance of these effects.

We take the continuum limit of the two-orbital model that provides us with simple analytical expressions to be compared to the orbital-less effective action. For simplicity we assume that the X(Y) pocket are exclusively composed by

the 1(2) orbital. Then all the weight factors vanish except $w_{\Gamma X}^1 w_{\Gamma X}^1 = \sin^2 \theta_{\mathbf{k}}$ and $w_{\Gamma Y}^2 w_{\Gamma Y}^2 = \cos^2 \theta_{\mathbf{k}}$ with $\theta_{\mathbf{k}} = \arctan(k_y/k_x)$. These terms reproduce the \mathbf{k} -dependence weights numerically computed in Figs. 1(a)–1(c). The parameter δm , that encodes the ellipticity, is introduced perturbatively via $1/m_{x/y} = (1 \pm \delta m)/m$ with $m_{x/y}$ the e-pocket mass. More details about the model can be found in Appendix B.

First we analyze the momentum dependence of the magnetic fluctuations. Within this approximation the magnetic bubble $\hat{\Pi}_X(q)$, Eq. (7) has only one finite orbital component

$$\Pi_X^{11}(q) = \frac{1}{2} \sum_n \int \frac{d^2 \mathbf{k}}{(2\pi)^2} \frac{\sin^2 \theta_{\mathbf{k}}}{(i\omega_n - \xi_{X,\mathbf{k}})(i\omega_n - \xi_{\Gamma,\mathbf{k}+\mathbf{q}})}. \quad (8)$$

By expanding up to the leading order in momentum we find anisotropic stiffness due to the angular dependence introduced by the $w_{\Gamma X}^1 w_{\Gamma X}^1 \sim \sin^2 \theta_{\mathbf{k}}$: $c_X^x - c_X^y \sim (1 - 4\delta m)v_F^2 N_F/T^2$ with v_F the Fermi velocity and N_F the density of states at the Fermi level (see Appendix B for further details). The $\sin^2 \theta_{\mathbf{k}}$ factor comes from the topological feature of the spin interaction connecting the Γ pocket with vorticity 2 with the topologically trivial X pocket. In the orbital-less effective action $c_X^x - c_X^y \sim (-8\delta m)v_F^2 N_F/T^2$. Therefore the topological feature affects the anisotropic stiffness already at zero order and in addition reduces the contribution proportional to δm that is opposite in sign.

We turn now to the calculation of the Landau parameters. Focusing on the quartic terms of the effective action we notice that, within this approximation, only few components of the \hat{g} , \hat{u} , \hat{v} tensor are finite. Moreover, due to the angular symmetry $u_{2222} = u_{1111} = -g_{1111}$, $u_{1122} = u_{2211} = g_{1122}$, $v_{1111} = -v_{2222} = -g_{1111}$, $v_{1122} = v_{2211} = -g_{1122}$, and $g_{1111} = g_{2222}$, $g_{1122} = g_{2211}$ leaving just two independent components. At finite temperature we find

$$g_{11\eta\eta} = \frac{N_F}{\pi T^2} a_\eta \left(1 + b_\eta \frac{\epsilon_0^2}{T^2} \delta m^2 \right); \quad (9)$$

with a_η and b_η ($\eta = 1, 2$) being numerical factors (see Appendix B). The nematic coupling is finite already at zero order due to the orbital symmetry. The first finite term proportional to δm appears at the second order and it is suppressed by temperature with respect to the zero-order contribution. If the ellipticity is taken into account perturbatively, as usually in the literature, then the effect of the orbital symmetry turns out to be the dominant one. On the other hand, if we are not allowed to expand in δm , the result of Eq. (9) would change and both the effects would contribute on equal footing. Notice, however, that the orbital symmetry is an intrinsic property of the system always present whereas the ellipticity depends on details of the FSs.

IV. CONCLUSIONS

We have derived the effective action for the spin order parameter with Landau coefficients depending on the orbital character, Hubbard and Hund's interaction. This derivation can be adapted for any multiorbital system with spin-orbital interplay. In the context of iron superconductors, this model allows for a good description of the nontrivial low-energy spectra of the system. Important differences are revealed with respect to the orbital-less effective approach: (i) the

nematic coupling is finite due to the yz/zx orbital content of the X and Y pockets regardless of the value of the ellipticity of the e-pocket. (ii) In the nematic phase, the yz/zx degeneracy is spontaneously broken in the spin channel due to the nontrivial C_4 symmetry. This broken symmetry induces orbital splitting in the charge channel revealing the strong spin-orbital interplay. (iii) The spin fluctuations have anisotropic momentum dependence in the x/y directions even in the case of perfect nesting due to the presence of the vortex at the Γ pocket. The vortex also affects the ellipticity contribution. In the light of our results, experiments interpreted in terms of the ellipticity of the e pockets should be revisited including the orbital degree of freedom. We have quantified the general results via the analytical treatment of the continuum limit of the two-orbital model. Since our conclusions are based on topological and symmetry arguments, they are also valid for more realistic models describing iron pnictides. This work is a necessary bridge between multiorbital physics and effective theories of spin fluctuations.

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APPENDIX A: MICROSCOPIC CALCULATION OF THE EFFECTIVE ACTION

The straightforward way to obtain the action in terms of the spin excitations $\bar{\Delta}_{\eta X}$, $\bar{\Delta}_{\eta Y}$ is by means of the Hubbard-Stratonovich (HS) transformation. Here, we summarize the main steps of the derivation of the effective action S_{eff} in Eq. (2). More details about the HS procedure can be found in Refs. [72] and [73] and references therein.

Starting from the microscopic Hamiltonian we can define the microscopic action $S[c_i(\tau)]$ as

$$S[c_i(\tau)] = \int_0^\beta d\tau c_i^\dagger(\tau) [\partial_\tau - \mu] c_i(\tau) + \hat{H}[c_i(\tau)], \quad (A1)$$

τ is the imaginary time and $\beta = 1/T$. Then the partition function of our system can be computed as the integral over Grassmann variables,

$$Z = \int \mathcal{D}c e^{-S[c_i(\tau)]}. \quad (A2)$$

The HS transformation allows us to decouple the quartic term in fermionic operators via the functional identity

$$e^{\frac{\pm a x^2}{2}} = \int \mathcal{D}y e^{-\frac{y^2}{2a} + \sqrt{\pm} y x} \quad a > 0$$

with y an auxiliary variable, i.e., the HS field. At this point the action becomes quadratic with respect to the fermionic

operators so that we can integrate out the fermions from Eq. (A2). The results of this operation are recast back into the exponent and the partition function is expressed in terms of the effective action $S[y]$:

$$Z = \int \mathcal{D}y e^{-S[y]}. \quad (\text{A3})$$

We need to specialize this machinery to the analysis of our case. Pnictide systems have to be described using a multi-orbital Hamiltonian. Typical Hamiltonians include the tight-binding $t_{ij}^{\eta_1\eta_2}$, the crystal field splitting ϵ_{η_1} , and local interactions restricted to the Fe orbitals: the intra-orbital Hubbard's coupling U , the interorbital one U' , the Hund's coupling J_H , and the pairing term J' :

$$\begin{aligned} H = & \sum_{ij\eta_1\eta_2\alpha} t_{ij}^{\eta_1\eta_2} c_{i\eta_1\alpha}^\dagger c_{j\eta_2\alpha} + \text{H.c.} + U \sum_{j\eta_1} n_{j\eta_1\uparrow} n_{j\eta_1\downarrow} \\ & + \left(U' - \frac{J_H}{2} \right) \sum_{j\eta_1 > \eta_2; \alpha\beta} n_{j\eta_1\alpha} n_{j\eta_2\beta} \\ & - 2J_H \sum_{j\eta_1 > \eta_2} \vec{S}_{j\eta_1} \cdot \vec{S}_{j\eta_2} + J' \sum_{j\eta_1 \neq \eta_2} c_{j\eta_1\uparrow}^\dagger c_{j\eta_1\downarrow}^\dagger c_{j\eta_2\downarrow} c_{j\eta_2\uparrow} \\ & - \sum_{j\eta_1\alpha} (\mu - \epsilon_{\eta_1}) n_{j\eta_1\alpha}. \end{aligned} \quad (\text{A4})$$

i, j label the Fe sites in the Fe unit cell, α and β the spin and η_1, η_2 the Fe d orbitals. $c_{i\eta_1\alpha}^{(\dagger)}$ destroys (creates) a fermion with spin α in the η_1 orbital on the i th site, $n_{i\eta_1\alpha} = c_{i\eta_1\alpha}^\dagger c_{i\eta_1\alpha}$ and $\vec{S}_{i\eta_1} = \frac{1}{2} \sum_{\alpha\beta} c_{i\eta_1\alpha}^\dagger \vec{\sigma}_{\alpha\beta} c_{i\eta_1\beta}$, with $\vec{\sigma}_{\alpha\beta}$ the Pauli matrices. Assuming our system rotationally invariant we can use $U' = U - 2J_H$ and $J' = J_H$ leaving only two independent parameters, U and J_H [67]. Repulsion between electrons requires $J_H < U/3$.

Transforming by Fourier and changing the basis from the orbitals to the bands, the tight-binding term can be diagonalized. We are interested in the low-energy physics thus we restrict to energies and momenta close to the FS taking into account the h pocket at Γ and the X and Y e pockets. We consider only the spin channel of the interaction of the Hamiltonian and we restrict our analysis to the spin excitations with momenta near $\mathbf{Q}_1 = (\pi, 0)$ and $\mathbf{Q}_2 = (0, \pi)$. Since the pair-hopping term J' does not contribute to the spin channel, we will not take it into account. The complete microscopic Hamiltonian reads

$$\begin{aligned} H = & \sum_{m=\Gamma, X, Y} \sum_{\mathbf{k}\alpha} \xi_{m\mathbf{k}} d_{m\mathbf{k}\alpha}^\dagger d_{m\mathbf{k}\alpha} \\ & - \frac{1}{2} \sum_{l=X, Y} \sum_{\mathbf{q}} \sum_{\eta_1\eta_2} U_{\eta_1\eta_2}^{\text{spin}} \vec{S}_{\eta_1 l}(\mathbf{q}) \cdot \vec{S}_{\eta_2 l}(-\mathbf{q}). \end{aligned} \quad (\text{A5})$$

Here, $d_{m\mathbf{k}\alpha}^{(\dagger)}$ destroys (creates) a fermion with momentum \mathbf{k} and spin α in the m pocket, $\xi_m = \epsilon_m - \mu$ where ϵ_m is the fermionic dispersion. The spin coupling is $U_{\eta_1\eta_2}^{\text{spin}} = \frac{8}{3} U \delta_{\eta_1\eta_2} + 4J_H(1 - \delta_{\eta_1\eta_2})$, the orbital-weighted spin operator for the pocket $l = X, Y$ is

$$\vec{S}_{\eta l}(\mathbf{q}) = \sum_{\mathbf{k}} w_{\Gamma l}^{\eta}(\mathbf{k}, \mathbf{k} + \mathbf{q}) \vec{S}_{\Gamma l}(\mathbf{k}, \mathbf{k} + \mathbf{q}),$$

where

$$\vec{S}_{\Gamma l}(\mathbf{k}, \mathbf{k} + \mathbf{q}) = \frac{1}{2} \sum_{\alpha\beta} d_{\Gamma\mathbf{k}\alpha}^\dagger \vec{\sigma}_{\alpha\beta} d_{l\mathbf{k}+\mathbf{q}\beta}.$$

The weight factors $w_{\Gamma l}^{\eta}(\mathbf{k}, \mathbf{k} + \mathbf{q}) = a_{\Gamma\eta}(\mathbf{k}) a_{l\eta}(\mathbf{k} + \mathbf{q})$, relate orbital and pockets basis.

We introduce Ψ^\dagger, Ψ six-dimensional creation, destruction operators

$$\Psi_{\mathbf{k}}^\dagger = (d_{\Gamma, \mathbf{k}\uparrow}^\dagger, d_{\Gamma, \mathbf{k}\downarrow}^\dagger, d_{X, \mathbf{k}\uparrow}^\dagger, d_{X, \mathbf{k}\downarrow}^\dagger, d_{Y, \mathbf{k}\uparrow}^\dagger, d_{Y, \mathbf{k}\downarrow}^\dagger). \quad (\text{A6})$$

The auxiliary bosonic fields $\vec{\Delta}_{\eta l}$ coupled to $\vec{S}_{\eta l}(\mathbf{q})$ are our HS fields and play the role of the magnetic order parameters in the Landau functional. Although the presence of a finite interorbital coupling, the U^{spin} matrix is positive defined within the range of validity of the model, $J_H < U/3$, thus we can apply the standard HS transformation. If U^{spin} had develop negative eigenvalues, the HS decoupling would lead to the appearance of an imaginary unit in the effective action that have to be handled properly. For further details we refer to Refs. [74] and [75] where this problem has been analyzed in the context of the superconducting instability.

After the HS transformation the partition function can be written as

$$Z = \int \mathcal{D}\Psi \mathcal{D}\Delta e^{-S[\Psi, \Delta]}, \quad (\text{A7})$$

with

$$\begin{aligned} S[\Psi, \Delta] = & \frac{1}{2} \sum_q U_{\eta_1\eta_2}^{\text{spin}-1} \sum_{l=X, Y} \vec{\Delta}_{\eta_1 l, q} \vec{\Delta}_{\eta_2 l, -q} \\ & + \sum_{kk'} \Psi_k^\dagger \hat{A}_{kk'} \Psi_{k'}. \end{aligned} \quad (\text{A8})$$

We used $k - k' = q$, $k \equiv (\mathbf{k}, i\omega_n)$, $q \equiv (\mathbf{q}, i\Omega_m)$, with ω_n and Ω_m being the Matsubara fermion and boson frequencies, respectively. Hereafter, the repeated orbital indices are summed. The $\hat{A}_{kk'}$ matrix is composed by the blocks

$$\hat{A}_{k, k'}|_{mm} = -\hat{G}_{m, kk'}^{-1} \delta_{kk'}, \quad (\text{A9})$$

$$\hat{A}_{k, k'}|_{\Gamma l} = \frac{1}{4} \hat{\Delta}_{\eta l, k-k'} w_{\Gamma l}^{\eta}(\mathbf{k}, \mathbf{k}'), \quad (\text{A10})$$

where we use a compact notation for the spin sector defining

$$\hat{G}_{m, k} = G_{m, k} \cdot \mathbf{I}, \quad \hat{\Delta}_{\eta l, q} = \vec{\Delta}_{\eta l, q} \cdot \vec{\sigma}$$

with \mathbf{I} the identity matrix and σ^i the Pauli matrices. $G_{m, k} = (i\omega_n - \xi_{m\mathbf{k}})^{-1}$ are the noninteracting single-particle Green's functions.

The exact integration of the fermionic d.o.f in Eq. (A7) gives us an expression for the effective action in terms of the HS field $\Delta_{\eta l}$ only:

$$S_{\text{eff}} = \frac{1}{2} \sum_q U_{\eta_1\eta_2}^{\text{spin}-1} \sum_{l=X, Y} \vec{\Delta}_{\eta_1 l, q} \vec{\Delta}_{\eta_2 l, -q} - \text{Tr} \ln \hat{A}_{kk'}. \quad (\text{A11})$$

It is convenient to decompose the second term of Eq. (A11) by separating in Eqs. (A9) and (A10) the part with the explicit structure of $\delta_{kk'}$ from the rest $\hat{A}_{kk'} = -\hat{G}_0^{-1} + \hat{Y}_{kk'}$.

This separation allows us to rewrite in our action

$$\text{Tr} \ln A_{kk'} = \text{Tr} \ln \hat{\mathcal{G}}_0^{-1} + \text{Tr} \ln (\hat{1} - \hat{\mathcal{G}}_0 \hat{\mathcal{V}}). \quad (\text{A12})$$

Now, we separate the HS fields $\vec{\Delta}_{\eta l, q} = \vec{\Delta}_{\eta l, 0} + \delta \vec{\Delta}_{\eta l, q}$ in its homogeneous and constant part and its fluctuating part. By minimizing the action with respect to $\vec{\Delta}_{\eta l, 0}$, we obtain the mean-field (MF) equations of the magnetic problem that admit nontrivial solutions with a finite magnetization below a critical temperature.

Beyond MF, we need to take into account the fluctuation of the magnetic HS fields around their MF value. It is easy to verify that we can expand

$$\text{Tr} \ln (\hat{1} - \hat{\mathcal{G}}_0 \hat{\mathcal{V}}) = \sum_n \frac{1}{n} \text{Tr} (\hat{\mathcal{G}}_0 \hat{\mathcal{V}}_{k-k'})^n$$

in Eq. (A12). We are interested into the nematic d.o.f. so that we need to retain terms up to the quartic order of the expansion in the magnetic HS fields. After a bit of algebra, we obtain the effective action in the nonmagnetic phase:

$$\begin{aligned} S_{\text{eff}} = & \frac{1}{2} \sum_{l=X,Y} \left(U_{\eta_1 \eta_2}^{\text{spin}-1} + \frac{1}{2} \Pi_l^{\eta_1 \eta_2} \right) \vec{\Delta}_{\eta_1 l} \cdot \vec{\Delta}_{\eta_2 l} \\ & + \frac{1}{16} \sum_{l,l'=X,Y} \lambda_{ll'}^{\eta_1 \eta_2 \eta_3 \eta_4} (\vec{\Delta}_{\eta_1 l} \cdot \vec{\Delta}_{\eta_2 l}) (\vec{\Delta}_{\eta_3 l'} \cdot \vec{\Delta}_{\eta_4 l'}), \end{aligned} \quad (\text{A13})$$

where $\Pi_l^{\eta_1 \eta_2}$ is defined as

$$\Pi_l^{\eta_1 \eta_2} = \frac{1}{2} \sum_k G_{\Gamma} G_l w_{\Gamma l}^{\eta_1} w_{\Gamma l}^{\eta_2}, \quad (\text{A14})$$

the $\lambda_{ll'}^{\eta_1 \eta_2 \eta_3 \eta_4}$ are given by

$$\begin{aligned} \lambda_{XX}^{\eta_1 \eta_2 \eta_3 \eta_4} &= \frac{1}{16} \sum_{i w, \mathbf{k}} G_{\Gamma}^2 G_X^2 w_{\Gamma X}^{\eta_1} w_{\Gamma X}^{\eta_2} w_{\Gamma X}^{\eta_3} w_{\Gamma X}^{\eta_4}, \\ \lambda_{YY}^{\eta_1 \eta_2 \eta_3 \eta_4} &= \frac{1}{16} \sum_{i w, \mathbf{k}} G_{\Gamma}^2 G_Y^2 w_{\Gamma Y}^{\eta_1} w_{\Gamma Y}^{\eta_2} w_{\Gamma Y}^{\eta_3} w_{\Gamma Y}^{\eta_4}, \\ \lambda_{XY}^{\eta_1 \eta_2 \eta_3 \eta_4} &= \frac{1}{8} \sum_{i w, \mathbf{k}} G_{\Gamma}^2 G_X G_Y w_{\Gamma X}^{\eta_1} w_{\Gamma X}^{\eta_2} w_{\Gamma Y}^{\eta_3} w_{\Gamma Y}^{\eta_4}, \end{aligned} \quad (\text{A15})$$

and we simplified a bit the notation using $\delta \vec{\Delta}_{\eta l} \rightarrow \vec{\Delta}_{\eta l}$ and dropping the k, q dependencies of the variables. At this point, it is already recognizable the definition for the r coefficient of the gaussian part. For the quartic part, we need to define properly the ψ, ϕ operators. The more general parametrization would be

$$\psi_{\eta_1 \eta_2 \eta'_1 \eta'_2} \sim (\vec{\Delta}_{\eta_1 X} \cdot \vec{\Delta}_{\eta_2 X} + \vec{\Delta}_{\eta'_1 Y} \cdot \vec{\Delta}_{\eta'_2 Y}), \quad (\text{A16})$$

$$\phi_{\eta_1 \eta_2 \eta'_1 \eta'_2} \sim (\vec{\Delta}_{\eta_1 X} \cdot \vec{\Delta}_{\eta_2 X} - \vec{\Delta}_{\eta'_1 Y} \cdot \vec{\Delta}_{\eta'_2 Y}), \quad (\text{A17})$$

so that

$$\vec{\Delta}_{\eta_1 X} \cdot \vec{\Delta}_{\eta_2 X} \sim \psi_{\eta_1 \eta_2 \eta'_1 \eta'_2} + \phi_{\eta_1 \eta_2 \eta'_1 \eta'_2}, \quad (\text{A18})$$

$$\vec{\Delta}_{\eta_1 Y} \cdot \vec{\Delta}_{\eta_2 Y} \sim \psi_{\eta'_1 \eta'_2 \eta_1 \eta_2} - \phi_{\eta'_1 \eta'_2 \eta_1 \eta_2}. \quad (\text{A19})$$

For simplicity, we choose $\eta'_1 \eta'_2 = \eta_1 \eta_2$ in the ψ, ϕ definitions Eqs. (A16) and (A17). Substituting these definitions for writing the quartic terms of Eq. (A13) and reorganizing the various contributions one recovers the expression quoted in the main text for the effective action, Eq. (2).

APPENDIX B: QUANTITATIVE RESULTS FOR THE CONTINUUM LIMIT OF THE TWO-ORBITAL MODEL

We consider a tight-binding model for the d_{yz} and d_{zx} Fe orbitals in an As tetrahedral environment [56,70], which is the minimal model to illustrate how symmetry and topology affect the S-N picture. Taking into account the symmetries of the orbitals and the Fe square lattice, the hoppings fulfill the following relations: $t_1 = t_{yz,yz}^x = t_{zx,zx}^y$, $t_2 = t_{yz,yz}^y = t_{zx,zx}^x$, $t_3 = t'_{zx,zx} = t'_{yz,yz}$, $t_4 = t'_{zx,yz} = -t'_{yz,zx}$, and $t_{zx,yz}^x = t_{yz,yz}^y = 0$ [56,70]. The subscript indicates orbitals, the superscript ' indicates second nearest neighbors, and the superscript x/y the x/y direction. The singular C_4 symmetry between the yz and zx orbitals gives rise to the non-trivial topology of the FS as shown in the following.

We can write the Hamiltonian in the basis of the Pauli matrices with orbital pseudospin $\Psi_{\mathbf{k}}^{\dagger} = (c_{\mathbf{k},yz}^{\dagger}, c_{\mathbf{k},zx}^{\dagger})$:

$$\hat{H}_0 = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^{\dagger} ((h_0(\mathbf{k}) - \mu) \hat{\tau}_0 + \vec{h}(\mathbf{k}) \cdot \vec{\tau}) \Psi_{\mathbf{k}}, \quad (\text{B1})$$

where μ is the chemical potential and

$$h_0(\mathbf{k}) = -(t_1 + t_2)(\cos ak_x + \cos ak_y) - 4t_3 \cos ak_x \cos ak_y,$$

$$h_1(\mathbf{k}) = -4t_4 \sin ak_x \sin ak_y,$$

$$h_3(\mathbf{k}) = -(t_1 - t_2)(\cos ak_x - \cos ak_y).$$

Diagonalizing the Hamiltonian we obtain two bands $E^{\pm}(\mathbf{k}) = h_0(\mathbf{k}) - \mu \pm \sqrt{h_1^2(\mathbf{k}) + h_3^2(\mathbf{k})}$. A generic band structure closed to the Fermi level showing the orbital weights is represented in Fig. 2. Both orbitals contribute to the Γ pockets while the X/Y electron pocket has dominant yz/zx component. The Γ pocket has a vortex structure as it was pointed out in Ref. [65]

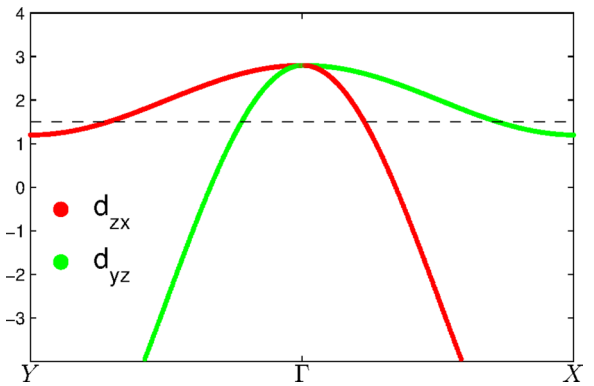


FIG. 2. (Color online) Band structure of the two-orbital d_{yz} d_{zx} model for the same Hamiltonian parameters used in Ref. [56]: $t_1 = -1, t_2 = 1.3, t_3 = t_4 = -0.85$, and $\mu = 1.85$ (dashed line) in units of $|t_1|$. Green (red) stands for the yz (zx) orbital weight. Both orbitals contribute to the Γ pockets while the X/Y pocket is mostly yz/zx .

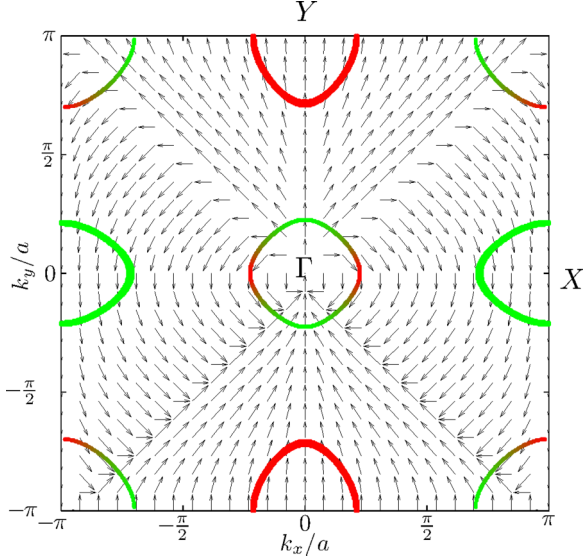


FIG. 3. (Color online) Vortex in the orbital space. The arrows represent the vector field $\vec{n} = \vec{h}(\mathbf{k})/|\vec{h}(\mathbf{k})|$ in the BZ. The FSs of the two-orbital model, whose orbital contribution is shown using the same color code than before (yz green, zx red), are superimposed. Notice the vortex around the Γ point. The vector field around the Fermi surface can be identified in the continuum limit $\vec{n} \sim \vec{n}_\Gamma = (\sin(2\phi_k), \cos(2\phi_k))$, while around the X/Y pockets $\vec{n} \sim \vec{n}_{X/Y} = \pm(0, 1)$. We used the same Hamiltonian parameters of Fig. 2.

for the two- and five-orbital models of iron superconductors. We will identify the vortex in the continuum limit.

We are interested in a low-energy description of the model, i.e., in the behavior of \hat{H}_0 around the Γ , Y , and X points. In the continuum limit, we expand to the lowest order. Around the Γ point, we get

$$h_{0,\Gamma}(\mathbf{k}) \simeq \varepsilon_\Gamma + \alpha_\Gamma \mathbf{k}^2, \quad h_{1,\Gamma}(\mathbf{k}) \simeq -2c k_x k_y,$$

and

$$h_{3,\Gamma}(\mathbf{k}) \simeq b(k_x^2 - k_y^2).$$

This dispersion relation has vorticity equal to two (see Fig. 3) as it has been pointed out in Ref. [65]. For simplicity, we assume $4t_1 \simeq t_1 - t_2 < 0$, so that $b \simeq c > 0$ and around Γ the dispersion relation is isotropic. Around the X/Y point, we get instead

$$h_{0,X/Y}(\mathbf{k}) \simeq \varepsilon_{X/Y} + \alpha_{x/y} k_y^2 + \alpha_{y/x} k_x^2, \\ h_{1,X/Y}(\mathbf{k}) \simeq -2c k_x k_y, \quad h_{3,X/Y}(\mathbf{k}) \simeq \mp d.$$

Where the $\alpha_{x/y}$ coefficients show the opposite ellipticity of the e pockets. All the coefficients $\varepsilon_\Gamma, \varepsilon_X, \varepsilon_Y, \alpha_\Gamma, \alpha_{x/y}$ and b, c, d are functions of the hopping coefficients whose precise dependence is not important at this point.

In general, the Green's function associated to the Hamiltonian (B1) can be written as

$$G(\omega, \mathbf{k}) = \sum_{s=\pm 1} \frac{1}{2} \frac{\tau_0 + s\vec{\tau} \cdot \vec{n}(\mathbf{k})}{\omega - h_0(\mathbf{k}) - s|h(\mathbf{k})|}, \quad (\text{B2})$$

where we fixed for simplicity $\mu = 0$. The vector $\vec{n}(\mathbf{k})$ is defined as $\vec{h}(\mathbf{k})/|\vec{h}(\mathbf{k})|$, and $s = \pm 1$ labels the conduction ($s = 1$) and

valence ($s = -1$) bands. We can particularize this Green's function to each pocket. The vectors \vec{n}_m for $m = \Gamma, X, Y$ are obtained by definitions using the low-energy expansions \vec{h}_m . Within this approximation, the vector field for the Γ pocket is given by $\vec{n}_\Gamma(\mathbf{k}) = (\sin 2\theta_k, \cos 2\theta_k)$, where we use $\theta_k = \arctan k_y/k_x$. The vortex around Γ described by \vec{n}_Γ is represented in Fig. 3. For the X/Y e -pockets we find instead $\vec{n}_X = -\vec{n}_Y = (0, 1)$, which physically means that the orbital weight of the pocket X/Y is only from the d_{yz}/d_{zx} orbital. Using that the Γ point belongs to the valence band ($s = -1$) and the X, Y pockets belong to the conduction ($s = 1$) band, we have

$$\hat{G}_\Gamma(\omega, \mathbf{k}) = \frac{1}{2} \frac{\hat{\tau}_0 - \vec{\tau} \cdot \vec{n}_\Gamma(\mathbf{k})}{\omega - \varepsilon_\Gamma(\mathbf{k})}, \quad (\text{B3a})$$

$$\hat{G}_{X/Y}(\omega, \mathbf{k}) = \frac{1}{2} \frac{\hat{\tau}_0 + \vec{\tau} \cdot \vec{n}_{X/Y}(\mathbf{k})}{\omega - \varepsilon_{X/Y}(\mathbf{k})}. \quad (\text{B3b})$$

By using the \vec{n}_i definitions in Eq. (B3), we can explicitly write down the expressions for the orbital components of the Green's function of each pocket. It is easy to verify that for the X/Y pockets all the orbital components vanish except the yz/zx one,

$$G_{X/Y}^{11/22}(\omega, \mathbf{k}) = (\omega - \varepsilon_{X/Y}(\mathbf{k}))^{-1} \equiv G_{X/Y}(\omega, \mathbf{k}), \quad (\text{B4})$$

by using $yz = 1, zx = 2$, while for the Γ pockets, we have

$$G_\Gamma^{11}(\omega, \mathbf{k}) = \frac{1 - \cos 2\theta_k}{\omega - \varepsilon_\Gamma(\mathbf{k})} \equiv \sin^2 \theta_k G_\Gamma(\omega, \mathbf{k}), \quad (\text{B5})$$

$$G_\Gamma^{12}(\omega, \mathbf{k}) = \frac{\sin 2\theta_k}{\omega - \varepsilon_\Gamma(\mathbf{k})} \equiv \sin 2\theta_k G_\Gamma(\omega, \mathbf{k}), \quad (\text{B6})$$

$$G_\Gamma^{22}(\omega, \mathbf{k}) = \frac{1 + \cos 2\theta_k}{\omega - \varepsilon_\Gamma(\mathbf{k})} \equiv \cos^2 \theta_k G_\Gamma(\omega, \mathbf{k}) \quad (\text{B7})$$

with $G_\Gamma^{21} = G_\Gamma^{12}$ and $G_m(\omega, \mathbf{k}) = (i\omega_n - \varepsilon_m(\mathbf{k}))^{-1}$. In the numerator of each Green's function the orbital content of each pocket is encoded.

The dispersion relations within this approximation can be expressed by $\varepsilon_\Gamma(\mathbf{k}) \simeq \varepsilon_0 - \frac{\mathbf{k}^2}{2m_\Gamma}$, $\varepsilon_{X/Y}(\mathbf{k}) \simeq -\varepsilon_0 + \frac{k_x^2}{2m_{x/y}} + \frac{k_y^2}{2m_{y/x}}$, where ε_0 is the offset energy. To better compare with previous results, we treat the ellipticity perturbatively analogously to what is discussed in Ref. [44]. We assume an isotropic mass for the h pocket as $m_\Gamma = m$ and we use the parameter δm encoding the ellipticity, such that the anisotropic e pocket mass reads as $1/m_{x/y} = (1 \pm \delta m)/m$. Near the Fermi energy and for small ellipticity, the dispersions can be approximated by $\varepsilon_\Gamma = -\varepsilon$ and $\varepsilon_{X/Y} = \varepsilon \pm \varepsilon_0 \delta m \cos 2\theta_k$.

1. Magnetic susceptibility in the nematic phase.

In general, the spin susceptibility depends on four orbital indices but in the spin-nematic scenario the spin susceptibility, Eqs. (6) and (7) of the main text, depends just on two orbital indices [76]. In the continuum limit, the magnetic $(\pi, 0)$ bubble is given by

$$\Pi_X^{\eta\eta'}(q) = \frac{1}{2} \sum_k G_\Gamma^{\eta\eta'}(k) G_X^{\eta'\eta}(k+q), \quad (\text{B8})$$

where there is no summation in η, η' and we compact the notation using the quadrivectors $k \equiv (i\omega_n, \mathbf{k})$, $q \equiv (i\Omega_m, \mathbf{q})$, and $\sum_k \equiv T \sum_{\omega_n} \int \frac{d^2\mathbf{k}}{4\pi^2}$. By replacing the Green's functions by Eqs. (B4)–(B7), we obtain that the only finite component is

$$\Pi_X^{11}(q) = \frac{1}{2} \sum_k \sin^2 \theta_{\mathbf{k}} G_{\Gamma}(k) G_X(k+q). \quad (\text{B9})$$

By comparison of the above equation with the expression for the bubble defined in terms of the orbital weights $\omega_{\Gamma X}^{\eta_1} \omega_{\Gamma X}^{\eta_1}$, Eq. (7) of the main text, we identify

$$\omega_{\Gamma X}^1 \omega_{\Gamma X}^1 = \sin^2 \theta_{\mathbf{k}}, \quad \omega_{\Gamma X}^1 \omega_{\Gamma X}^2 = \omega_{\Gamma X}^2 \omega_{\Gamma X}^2 = 0. \quad (\text{B10})$$

By analogous analysis of the $(0, \pi)$ bubble $\Pi_Y^{\eta'}$, we obtain

$$\omega_{\Gamma Y}^2 \omega_{\Gamma Y}^2 = \cos^2 \theta_{\mathbf{k}}, \quad \omega_{\Gamma Y}^1 \omega_{\Gamma Y}^2 = \omega_{\Gamma Y}^1 \omega_{\Gamma Y}^1 = 0. \quad (\text{B11})$$

Let us focus now on the hydrodynamic limit of the static $(\pi, 0)$ bubble (B9) in the nematic phase,

$$\Pi_X^{11}(0, \mathbf{q}) = \Pi_X^{11}(0) + c_X(\theta_{\mathbf{q}}) \mathbf{q}^2 + \mathcal{O}(\mathbf{q}^3). \quad (\text{B12})$$

To study the \mathbf{q} -dependent part, we have to expand up to \mathbf{q}^2 the $G_X(k+q)$ Green's function in Eq. (B9) also taking into account the ellipticity of the X pockets. The constant part and the momentum dependent one can be computed explicitly separating the momentum integral in the one over the angular variable $\theta_{\mathbf{k}}$ and the other over the modulus $\int dk^2 \simeq N_F \int d\varepsilon$ with N_F being the density of states at the Fermi level.

The constant part is negative and at perfect nesting diverges logarithmically as $\Pi_X^{11}(0) \simeq -N_F \ln(\Lambda/2T)/(4\pi) + \dots$, with Λ being the upper cutoff for the low-energy theory. The term is the standard logarithm appearing in the problem of the antiferromagnetic instability.

The \mathbf{q} -dependent part can be written as $c_X(\theta_{\mathbf{q}}) \mathbf{q}^2 = c_X^x q_x^2 + c_X^y q_y^2$, where

$$c_X^x = -\frac{v_F^2 N_F}{256\pi T^2} (1 + \delta m), \quad c_X^y = -\frac{v_F^2 N_F}{256\pi T^2} (3 - 7\delta m). \quad (\text{B13})$$

Thus we found that the stiffness of the magnetic bubble is anisotropic already at the level of zero ellipticity $\delta m = 0$ due to the angular modulation $\sin^2 \theta_{\mathbf{k}}$ introduced by the vortex in Eq. (B9). Notice that the finite term and the one proportional to δm have a competing role in making the magnetic stiffness anisotropic. Equation (B9) reproduces exactly the magnetic

bubble obtained via the orbital-less approach [44] once $\sin^2 \theta_{\mathbf{k}}$ is eliminated. The momenta analysis for this case leads to

$$c_X^x = -\frac{v_F^2 N_F}{64\pi T^2} (1 + 2\delta m), \quad c_X^y = -\frac{v_F^2 N_F}{64\pi T^2} (1 - 2\delta m), \quad (\text{B14})$$

and the anisotropic stiffness is found only at order δm . In addition, the dependence on δm of the $c_X^{x/y}$ coefficients is different with respect to the one obtained by retaining the orbital information; Eq. (B13) highlights that the vortex also affects the terms accounting for the ellipticity.

Notice that in the paramagnetic phase the tetragonal symmetry is respected since the anisotropic properties found for the Π_X hold for the Π_Y having into account the orbital exchange yz/xz , i.e., $c_Y^x \equiv c_X^y$ and $c_Y^y \equiv c_X^x$. Once is entered in the nematic phase, the two modes are no longer equivalent and the momentum dependence of the spin fluctuations is actually anisotropic as we discussed above.

2. Quartic coefficients.

We start directly from the definition of the orbital nematic coefficients \hat{g} , Eq. (5c) of the main text. By using the expressions (B10) and (B11) for the orbital weights, we have

$$g_{1111} = -\frac{1}{2} \sum_k \sin^4(\theta_{\mathbf{k}}) G_{\Gamma}^2(k) G_X^2(k), \quad (\text{B15a})$$

$$g_{1122} = \frac{1}{2} \sum_k \sin^2(\theta_{\mathbf{k}}) \cos^2(\theta_{\mathbf{k}}) G_{\Gamma}^2(k) G_X(k) G_Y(k). \quad (\text{B15b})$$

Expanding $G_{X/Y}$ in powers of δm and computing explicitly the integrals, we obtain

$$g_{11\eta\eta} = \frac{N_F}{\pi T^2} a_{\eta} \left(1 + b_{\eta} \frac{\epsilon_0^2}{T^2} \delta m^2 \right); \quad (\text{B16})$$

with a_{η} and b_{η} ($\eta = 1, 2$) being numerical factors: $-a_1 = 3a_2 = 3/2^9$ and $b_1 = 7b_2 = 7/2^6$. The following equations hold: $g_{1111} = g_{2222}, g_{1122} = g_{2211}$. The tensor elements of the nematic coupling are finite, also assuming circular pockets (i.e., $\delta m = 0$), while the first finite contribution in δm appears at the second order. All the other quartic coefficients \hat{u}, \hat{v} are related to the above ones by angular symmetry. Also, $u_{2222} = u_{1111} = -g_{1111}$, $u_{1122} = u_{2211} = g_{1122}$, $v_{1111} = -v_{2222} = -g_{1111}$, and $v_{1122} = v_{2211} = -g_{1122}$, while all the other components are zero.

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