Nematic Pairing from Orbital Selective Spin Fluctuations in FeSe

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FeSe is an intriguing iron-based superconductor. It presents an unusual nematic state without magnetism and can be tuned to increase the critical superconducting temperature. Recently it has been observed a noteworthy anisotropy of the superconducting gap. Its explanation is intimately related to the understanding of the nematic transition itself. Here we show that the spin-nematic scenario driven by orbital-selective spin-fluctuations provides a simple scheme to understand both phenomena. Indeed, the pairing mediated by anisotropic spin modes is not only orbital selective but also nematic, leading to stronger pair scattering across the hole and X electron pocket. The delicate balance between orbital ordering and nematic pairing points also to a marked k\textsubscript{z} dependence of the hole-gap anisotropy.

INTRODUCTION

Soon after the discovery of superconductivity in iron-based systems it has been proposed that pairing could be unconventional, i.e. based on a non-phononic mechanism [1, 2]. This proposal has been triggered from one side by the small estimated value of the electron-phonon coupling, and from the other side by the proximity, in the temperature-doping phase diagram, of a magnetic instability nearby the superconducting (SC) one. Within an itinerant-electrons picture pairing could then be provided by repulsive spin-fluctuations between hole and electron pockets, connected by the same wavevector characteristic of the spin modulations in the magnetic phase (see Fig. 1). This suggestion has been supported and confirmed by an extensive theoretical work, aimed from one side to establish why inter-pockets repulsion can overcome the intra-pocket one [3] and from the other side to provide a quantitative estimate of the SC properties starting from RPA-based description of the spin-fluctuation susceptibility [4, 5].

The success of the above scenario has been partly questioned by the discovery of superconductivity in the FeSe system, where a magnetic phase appears only upon doping and superconductivity at T\textsubscript{c} ∼ 9 K emerges in the so-called nematic phase [6]. Here at temperatures below T\textsubscript{S} = 90 K the anisotropy of the electronic properties is far larger than what expected across a standard tetragonal-to-orthorhombic transition, suggesting that it is driven by electronic degrees of freedom [6, 7]. In particular, ARPES experiments clearly show a dramatic change of the Fermi surface (FS) across T\textsubscript{S}, that can be reproduced with an effective crystal-field splitting of the various orbitals [8–16].

In this situation, the explanation of the observed anisotropy of the SC gaps in FeSe becomes intimately related to the understanding of the nematic transition itself. Extensive experimental studies on FeSe-based material, ranging from quasiparticle interference imaging [17, 18] and ARPES measurements [19, 23], to thermal probes [24, 25], suggest that the SC gap in FeSe is highly anisotropic on both hole and electron pockets. By introducing the azimuthal \( \theta \) angle with respect to the center of each pocket one finds that the gap is larger at \( \theta = 0 \) on the Γ pocket, where the predominant character in the nematic phase is \( xz \) [14, 21, 22], and at \( \theta = \pi/2 \) on the X pocket, where the dominant character is \( yz \), see Fig. 1. Thus, accounting for an orbital-dependent SC order parameter is not sufficient to reproduce the observed gap hierarchy, and additional phenomenological modifications of the pairing mechanism must be introduced [17, 21, 26] to describe the experiments.

Among the various attempts to theoretically understand the nematic phase from microscopic models, we have recently emphasized the outcomes of a theoretical approach which correctly incorporates the feedback between orbital degrees of freedom and spin fluctuations [14, 27, 28], which turn out to be sizeable in FeSe as well [29–33]. Indeed, from one side the degree of orbital nesting...
between hole and electron pockets is crucial to determine the temperature scale where spin fluctuations beyond RPA drive the spin-nematic instability [27], making spin fluctuations at \( Q_X = (\pi/a, 0) \) and \( Q_Y = (0, \pi/a) \) anisotropic below \( T_S \) [31]. From the other side the renormalization of quasiparticle dispersions due to the exchange of anisotropic spin modes explains the orbital ordering observed below \( T_S \) as an orbital-selective shrinking mechanism [14]. In this paper we show that such orbital-selective spin fluctuations (OSSF) provide also the key mechanism [14]. In this paper we show that such orbital-selective spin fluctuations (OSSF) provide also the key mechanism [14].

The existence of OSSF provides a natural explanation of the orbital ordering observed in the nematic phase of FeSe. As discussed in [14, 38], the self-energy corrections due to spin exchange imply a chemical-potential shift with opposite sign at the hole and electron pockets, leading in both cases to a shrinking of the FS pockets that explains why experimentally they are always smaller than LDA predictions [14, 39, 40]. The orbital-selective nature of spin fluctuations makes this mechanism also orbital dependent [14]. As a consequence, within a spin-nematic scenario the \( C(4) \) symmetry breaking of spin fluctuations along \( \Gamma X \) and \( \Gamma Y \) explains also the orbital ordering observed in the nematic phase. In Ref. [14] it has been shown that by assuming stronger spin fluctuations at \( Q_X \) below \( T_S \) the self-energy difference \( \Delta \Sigma \) between \( xy \) and \( yz \) and orbitals induced an orbital splitting being positive at \( \Gamma \) and negative at the electron pockets, leading to the observed deformations of the FS below \( T_S \) [6, 10, 12, 14-16]. Even though this orbital-selective shrinking mechanism is generic, a quantitative determination of the nematic splitting requires a phenomenological modelling of the nematic spin modes, as discussed in Ref. [14]. In the present paper we will tune directly the isotropic shrinking and the nematic splittings in order to reproduce the FS measured by ARPES data in the nematic phase above \( T_c \), and to reproduce the \( k_z \) dependence of the hole pocket between the \( \Gamma \) (\( k_z = 0 \)) and \( Z \) (\( k_z = \pi \)) point [11]. The resulting FS at \( k_z = 0 \) is shown in Fig. 1. The effect of the

\[
\langle S \cdot S \rangle (Q_X) \Rightarrow \langle S^{yz}_X \cdot S^{yz}_X \rangle, \quad (6)
\]

\[
\langle S \cdot S \rangle (Q_Y) \Rightarrow \langle S^{xz}_Y \cdot S^{xz}_Y \rangle. \quad (7)
\]

leading in turn to the orbital-selective spin fluctuations (OSSF) at different momenta represented in Fig. 1.

\[
\sum_k (u_X c_{xz} - v_X c_{xz}) \partial u_X e_X
\]

The angular dependence of \( u, v \) factors defined in Eqs. [1-3] identifies the predominant orbital character of each portion of the FS, as shown in Fig. 1. More importantly, by using the identities [1-3] one can establish [27-37] a precise correspondence between the orbital character of the spin operator and the momenta \( Q_X \) or \( Q_Y \) connecting the hole and the \( X/Y \) pockets:

\[
S(X) \equiv S^{xz}_X = \sum_k (u_T h^+_x + v_T h^+_x) \partial u_X e_X \quad (4)
\]

\[
S(Y) \equiv S^{xz}_Y = \sum_k (-u_T h^+_x + v_T h^+_x) \partial u_Y e_Y \quad (5)
\]

In practice, since \( xz \) states are absent at \( X \) the \( S^{xz}_X \) operator has no component at the wavevector \( Q_X \) connecting the \( \Gamma \) and \( X \) pocket, and viceversa for the \( yz \) states, leading in turn to the orbital-selective spin fluctuations (OSSF) at different momenta represented in Fig. 1.

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![Figure 2](image-url)
nematic splitting on the orbital factors when going below \( T_S \) is shown in Fig. 2. Here \( \Delta \Sigma_h = (\Sigma^X - \Sigma^Y)/2 \) denotes the nematic splitting at \( \Gamma \) and \( \Delta \Sigma_e = (\Sigma^X - \Sigma^Y)/2 \) is the nematic splitting at \( M = (X,Y) \). The maximum values are chosen to match the experimental ones \([6,14-16]\), i.e. \( \Delta \Sigma_{h/e} \approx 15 \) meV. The most dramatic changes due to the nematic order are found in the orbital occupation of the hole pocket. Here the presence of a relatively large spin-orbit coupling \( l \approx 20 \) meV implies a mixing of the \( xx \) and \( yy \) orbitals on all the FS. However, below \( T_S \) the \( xx \) character of the hole pocket is strongly suppressed, and the pocket acquires a dominant \( xx \) character even at \( \theta = 0 \), as observed by the polarization dependent ARPES measurements \([12,14,21,22]\). At the same time the nematic splitting enhances the \( yy \) occupation at \( \Gamma \) and suppresses the \( xx \) at \( Y \). As a consequence, one easily understands that the SC gap hierarchy cannot be simply attributed to the FS orbital dependence. Indeed, on the \( X \) pocket the gap is maximum at \( \theta = \pi/2 \), where the band has strong \( yy \) character, while on the \( \Gamma \) pocket it is larger at \( \theta = 0 \), where a dominant \( xx \) character is found. Here we show that the crucial ingredient required to account for the SC properties of FeSe comes indeed from the nematic paring provided by OSSF.

By building up the spin-singlet vertex mediated by the spin fluctuations \([6-28]\) one obtains \([41]\) the pairing Hamiltonian:

\[
H_{pair} = -g_X \sum_{k,k'} v^2_{\Gamma,k} h^\dagger_{\Gamma,k} h_{\Gamma,k'} e_{X,k'} e_{X,k} + \nonumber
-g_Y \sum_{k,k'} v^2_{\Gamma,k} h^\dagger_{\Gamma,k} h_{\Gamma,k'} e_{Y,k} e_{Y,k}.
\]  

In Eq. (10) we used the fact that a spin-nematic scenario implies also a nematic pairing anisotropy with \( g_X > g_Y \), due to the fact that in the nematic phase OSSF along \( \Gamma X \) are stronger than along \( \Gamma Y \). Eq. (10) can be easily solved in the mean-field approximation by defining the orbital-dependent SC order parameters for the hole (\( \Delta_h^{yz}, \Delta_h^{xz} \)) and electron (\( \Delta_e^{yz}, \Delta_e^{xz} \)) pockets. The self-consistent equations at \( T = 0 \) reads:

\[
\Delta_h^{yz} = -g_X \sum_k u^4_{X,k} \Delta_h^{yz} / E_X \quad (9)
\]

\[
\Delta_h^{xz} = -g_Y \sum_k u^4_{Y,k} \Delta_h^{xz} / E_Y \quad (10)
\]

\[
\Delta_e^{yz} = -g_X \sum_k u^2_{\Gamma,k} (u^2_1 \Delta_h^{yz} + u^2_1 \Delta_h^{xz}) / E_{\Gamma} \quad (11)
\]

\[
\Delta_e^{xz} = -g_Y \sum_k u^2_{\Gamma,k} (u^2_1 \Delta_h^{yz} + u^2_1 \Delta_h^{xz}) / E_{\Gamma} \quad (12)
\]

where \( E_l = \sqrt{\xi^2_l + \Delta_l^2} \) with \( l = \Gamma, X, Y \) and the band gap \( \Delta_l \) on each pocket is a convolution of orbital factors and orbital SC order parameters

\[
\Delta_{\Gamma} = u^2_1 \Delta_h^{yz} + u^2_1 \Delta_h^{xz} \quad (13)
\]

\[
\Delta_X = u^2_2 \Delta_e^{yz} \quad (14)
\]

\[
\Delta_Y = u^2_2 \Delta_e^{xz} \quad (15)
\]

**RESULTS**

To get a first intuition on the separate role of the orbital factors and of the pairing anisotropy we show in Fig. 3 the angular averages of the orbital-factors overlaps appearing in Eq.s \([6-12]\). As mentioned above, the nematic splitting on the electron pockets leads to a moderate enhancement of the \( yy \) factor appearing in Eq. (9) with respect to the \( xx \) in Eq. (10), i.e.

![Fig. 3: Nematic-splitting dependence of the angular-averaged orbital-weight overlaps appearing in the SC gap equations Eq.s (6)-(12).](image)

![Fig. 4: Angular dependence of the SC band gap on the hole (top) and electron (bottom) pocket for isotropic pairing \( g_X/g_Y = 1 \) (dashed lines) and nematic pairing \( g_X/g_Y \sim 26 \) (solid lines). The colour code is the same of Fig 1 and accounts for the orbital content of the FS on each pocket. The points are the experimental gap values from Ref. [17].](image)
\[ \langle u_k^X \rangle \gtrsim \langle u_k^Y \rangle \]. Here \( \langle f(k) \rangle \) denotes the angular integration of \( f(k_F(\theta)) \) along the FS wave vector \( k_F(\theta) \) of each pocket. This effect, recently highlighted in Ref. 35, while discussing the \( k_z = \pi \) FS cut (see below), is however too small to account for the observed hole-gap anisotropy at \( k_z = 0 \). Indeed, the strong modification of the hole-pocket orbital factors implies that \( \langle u_k^X \rangle \ll \langle v_k^2 \rangle \). Thus, by neglecting logarithmic corrections in the gap ratios, from Eq.s (9)-(12) one obtains that \( \Delta^x / \Delta^z \simeq g_x \langle v_k^2 \rangle / g_y \langle v_k^2 \rangle \simeq 0.1 (g_x / g_y) \) and \( \Delta^y / \Delta^z \simeq g_y (\langle u_k^X \rangle / \langle u_k^Y \rangle) \simeq 1.8 (g_x / g_y) \Delta^z / \Delta^z \). In this situation an isotropic pairing interaction \( g_X = g_Y \) (as considered in Ref. 35) would lead to \( \Delta^x / \Delta^z \ll \Delta^z / \Delta^z \). Since one also has \( u_k^X \ll v_k^2 \), as shown in Fig. 4, the angular dependence of the hole gap defined in Eq. (13) would be provided by the \( xz \) component, i.e. \( \Delta^X \simeq \Delta^X v_k^2 \). This implies a small modulation of the gap over the FS (see dashed line in Fig. 4), with a relative maximum at \( \theta = \pi/2 \) in contrast with the experimental findings.

The situation is reversed when the OSSF-mediated anisotropic pairing with \( g_X / g_Y \gg 1 \) is considered. In Fig. 4 we report the numerical solutions of Eq.s (9)-(12) along with the experimental data of Ref. 17. The pairing anisotropy provided by nematic spin fluctuations allows one to recover the enhancement of the \( \Delta^X / \Delta^Z \) ratio, leading to the band-gap anisotropy observed experimentally. Also the magnitude and anisotropy of the gap of the \( X \) pocket is overall in agreement with the experimental data. Here we neglected for simplicity the small pairing in the \( xy \) channel, mediated by the spin fluctuations at \( Q = (\pi, \pi) \) connecting the electron pockets 20. When included, it would account for the small but finite SC gap on the \( X \) pocket at \( \theta = 0 \) inferred in 17. It is remarkable that the anisotropy \( g_X / g_Y \) extracted from this analysis is compatible with the anisotropy of the OSSF used in Ref. 14 to reproduce the orbital selective shrinking of the FS in the nematic phase 11.

Recently the gap anisotropy on the hole pocket as a function of \( k_z \) has been investigated in details in Ref. 23. In particular, it has been shown that the \( \Delta^X(\theta) / \Delta^Z(\theta = \pi/2) \) anisotropy increases as one moves from the \( k_z = 0 \) to the \( k_z = \pi \) cut. Even though we did not consider a full 3D model, this effect can be understood by considering the variations of the hole-pocket orbital content when moving from \( k_z = 0 \) to \( k_z = \pi \) (Z point). Indeed, the larger size of the hole pocket at \( Z \) makes its orbital content less sensitive to nematic ordering and spin-orbit mixing, so that is still preserves a marked \( yz \) orbital character around \( \theta = 0 \) 19, 20, 35, with \( u_x \sim \cos \theta \) and \( v_x \sim \sin \theta \) also in the nematic phase. In this situation \( \langle u_k^X \rangle \sim \langle v_k^2 \rangle \), so the enhancement \( \langle u_k^X \rangle > \langle u_k^Y \rangle \) of the orbital factors in the electron pockets is enough to guarantee that \( \Delta^X > \Delta^Z \), leading to a hole-pocket anisotropy compatible with the measurements even when \( g_X = g_Y \), as recently shown in Ref. 35 (see Fig. 4). On the other hand, by retaining the same \( g_X / g_Y > 1 \) ratio extracted from the fitting of the \( k_z = 0 \) gap we find in general an increase of the anisotropy when moving from the \( \Gamma \) to the \( Z \) pocket. While this is consistent with the observations in pure 23 and S-doped 19 FeSe, other groups 20, 21 report instead an overall smaller gap at \( k_z = 0 \). In order to clarify the 3D behavior, an alternative experimental test could be provided by the analysis of superconducting fluctuations above \( T_c \), which are in principle sensitive to a \( k_z \) dependence of the pairing properties 42, 43.

The importance of the nematic spin-fluctuations pairing \( g_X > g_Y \) highlighted in the present work cannot be captured by microscopic models where the spin fluctuations are described at RPA level. Indeed, the \( C(4) \) symmetry breaking of paramagnetic spin fluctuations is a consequence of spin-fluctuations interactions beyond RPA 27, 34. As a consequence, in order to reproduce the experiments previous approaches based on RPA calculations of the spin modes 17, 21, 26 needed to make rather ad hoc assumptions, not clearly supported by theoretical models or other experiments. In particular, the authors of Ref.s 17, 26, 44, extracted from STM data strongly anisotropic orbital-dependent quasi-particle spectral weights, with \( Z_{xy} \ll Z_{xz} < Z_{yz} \). By suppressing the contribution of \( xy \) orbitals and inducing a large \( zz/yz \) quasiparticle spectral-weights anisotropy one actually enhances the spin fluctuations at \( Q_X \), making then effectively \( g_X > g_Y \) in the pairing model of Eq. (16). Even though electronic correlations can indeed cooperate to enhance the \( zz/yz \) orbital differentiation in the nematic phase 35 and reinforce the nematic character of the OSSF itself, the huge quasiparticle spectral-weights anisotropy extracted in Ref.s 17, 26, 44, is not supported by ARPES measurements 21, 23. For exam-
ple the $xz$ and $yz$ components of the hole pockets can be both detected in ARPES, and polarization-dependent measurements clearly establish the orbital-weight evolution across the nematic transition, as discussed above. Analogously, in Ref. [21] the authors remove intentionally the contribution of the $Y$ pocket from the RPA-mediated pairing interaction. This is equivalent to put $g_Y = 0$ in Eqs. (9)-(12), so that $\Delta^x = 0$ and the modulation of the gap at $\Gamma$ follows again the $yz$ orbital weight. However from the experimental point of view there is still a controversy on the possibility to experimentally observe [14, 23] or not [21, 34] the $Y$ pocket. In addition, while the anisotropy of the superconducting couplings is a consequence of the OSSF mediating the pairing, the absence of the $Y$ pocket lacks so far a theoretical justification.

In summary, our work provides a paradigm for the emergence of superconductivity in FeSe from an orbital-selective nematic spin-fluctuations mechanism. By combining the orbital ordering induced by the nematic shrinking of the Fermi pockets below the nematic transition with the anisotropic pairing interaction mediated by nematic spin fluctuations, we explain the gap hierarchy reported experimentally on hole and electron pockets, and its variation with $k_z$. Our findings offer also a fresh perspective on previous attempts to explain the SC properties of FeSe, highlighting from one side the crucial role of spin-mediated pairing, and from the other side clarifying the importance of spin-skin interactions beyond RPA level. This result represents then a serious challenge for a full microscopic approach, that must account self-consistently for the emergence of Ising-nematic spin fluctuations below the nematic transition temperature.

METHODS

Pairing by Orbital selective spin fluctuations

The OSSF spin-spin interaction Hamiltonian [41] generates an effective interaction in the pairing channel mediated by the spin susceptibilities at the two $Q_{X} = (\pi,0)$ and $Q_{Y} = (0, \pi)$ vectors, such that

$$H_{\text{pair}} = -g_{X} \sum_{k,k'} \hat{h}_{-k} \hat{h}^{\dagger}_{k} \hat{h}_{-k'} \hat{h}^{\dagger}_{k'} u_{X,k} e_{X,k'} e_{X,k'} +$$

$$-g_{Y} \sum_{k,k'} \hat{h}_{-k} \hat{h}^{\dagger}_{k} \hat{h}_{-k'} \hat{h}^{\dagger}_{k'} u_{X,k} e_{X,k'} e_{Y,k'} e_{Y,k'}.$$  

(16)

The $u, v$ factors, defined by Eqs. [1, 3], appearing in the pairing Hamiltonian Eq. (16), imply the orbital selective nature of the SC interaction. Indeed the $\Gamma - X$ interband pairing, $g_X$, is mediated by spin fluctuation peaked at $Q_X$ and involves the $yz$ orbital component only, while the $\Gamma - Y$ interband pairing $g_Y$ at $Q_Y$ involves the $xz$ orbital only. The pairing strength in Eq. (16) scale as the $\omega = 0$ spin-fluctuation propagators, $g_{X/Y} \sim \langle S_{X/Y}^{xx/yy} S_{X/Y}^{xx/yy} \rangle$. While at RPA level the spin modes are always degenerate, taking into account spin-skin interactions beyond Gaussian level [27, 40] one can show that below $T_S$ spin fluctuations break the $Z_2$ Ising degeneracy and they become stronger at a given $Q$ vector. The analysis of the orbital ordering induced by OSSF discussed in [14] and outlined above shows that below $T_S$ one should then have stronger spin fluctuations at $Q_X$, leading then to $g_X > g_Y$.

The mean-field equations for the pairing hamiltonian, Eq. (16), can be easily derived by defining the orbital-dependent SC order parameters for the hole $(\Delta^{h}_{x}, \Delta^{h}_{z})$ and electron $(\Delta^{e}_{x}, \Delta^{e}_{z})$ pockets as:

$$\Delta^{h}_{x} = -g_{X} \langle \hat{u}^2 \Gamma,k_{h} h_{-k} \rangle,$$

$$\Delta^{h}_{z} = -g_{Y} \langle \hat{u}^2 \Gamma,k_{h} h_{-k} \rangle,$$

$$\Delta^{e}_{x} = -g_{X} \langle \hat{u}^2 \Gamma,k_{e} e_{X,k} e_{X, -k} \rangle,$$

$$\Delta^{e}_{z} = -g_{Y} \langle \hat{u}^2 \Gamma,k_{e} e_{Y,k} e_{Y, -k} \rangle.$$  

The corresponding BCS equations at $T = 0$ are the ones reported in the text, Eqs. (9)-(12). In order to reduce the number of fitting parameters and to simplify the calculations we have used constant density of states for all the bands. As long as one observes only the gaps on the $\Gamma$ and $X$ pockets the relative DOS can be reabsorbed in a definition of dimensionless coupling constants, and only the ratio of the dimensionless $g_{X}/g_{Y}$ will matter.

The results of numerical self-consistent calculations of Eqs. (9)-(12) are reported in the text, list of the numerical values of the parameters used can be found in [41].

Data availability

The authors declare that the data supporting the findings of this study are available within the paper and its supplementary information file.

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AUTHOR CONTRIBUTIONS

L.F. conceived the project with inputs from all coauthors. L.F. and L.B. performed the numerical calculations. All the authors contributed to the data analysis, to the interpretation of the theoretical results and to the writing of the text.
Supplementary information

Band structure

To describe the band structure of FeSe above the superconducting (SC) transition, we adapt the orbital model of Ref. [30]. The effective band-mass parameters are extracted from ARPES measurements. These values, considerably smaller than the ones predicted by LDA, are usually reproduced remarkably well by DMFT-based calculations [17]. However, both LDA and DMFT fail in the description of the measured Fermi surface (FS), that are always smaller than expected. Such a FS shrinking [35], present already well above the nematic transition [14, 38], and the nematic splitting, can be explained instead within our low-energy approach by accounting for 

\[ \text{Ref. [14],} \]

the orbital-dependent self-energy corrections of Ref. [36]. The effective band-mass parameters are explained in

\[ \text{Ref. [13],} \]

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For the perfectly circular hole pocket in the paramagnetic phase (\( \Delta \Sigma_h = 0 \)) in the absence of spin-orbit interaction one would simply obtain \( u_\Gamma = \cos \theta \) and \( v_\Gamma = \sin \theta \), where \( \theta \) is the azimuth angle measured with respect to \( k_x = 0 \). Taking into account also the spin-orbit splitting we define the eigenvalues as

\[ E^\pm_1 = h_0^h - |\Sigma^i_0| \pm \sqrt{h_1^{h2} + (h_3^h - \Delta \Sigma_h)^2 + (l/2)^2} \]

while the orbital weight get rescaled, leading to a mixing of the two orbitals all over the FS:

\[ u_\Gamma^2 = \frac{1}{2} \left( 1 + \frac{h_3^h - \Delta \Sigma_h}{\sqrt{h_1^{h2} + (h_3^h - \Delta \Sigma_h)^2 + (l/2)^2}} \right) \]

\[ v_\Gamma^2 = \frac{1}{2} \left( 1 - \frac{h_3^h - \Delta \Sigma_h}{\sqrt{h_1^{h2} + (h_3^h - \Delta \Sigma_h)^2 + (l/2)^2}} \right) \]

For the X/Y pockets the general structure is analogous to Eq. (17), provided that the spinors are now defined as

\[ \psi^X = (c_{yz}, c_{xy}) \]

and \( \psi^Y = (c_{zz}, c_{zy}) \). In addition, since the xy orbital is not affected by OSSF, one has in general

\[ \hat{H}^X = \left( \begin{array}{cc} h_0^X + \Sigma^X & h_3^X \frac{-i h^X}{2 h_2^X} \\ i h_2^X & h_0^X - h_3^X \end{array} \right) \]

for the X pocket, with

\[ h_0^X = (h_{yz} + h_{xy})/2 \]

\[ h_3^X = v k_y \]

\[ h_3^X = (h_{yz} - h_{xy})/2 - b (k_x^2 - k_y^2) \]

where \( h_{yz} = -\epsilon_{yz} + a_{yz} k^2 \) and \( h_{xy} = -\epsilon_{xy} + a_{xy} k^2 \). Analogous expressions hold for the Y pocket provided that one exchange the role of \( k_x \) and \( k_y \), \( h_3^X(k_x, k_y) = h_3^X(k_y, k_x) \), and \( \Sigma^X \) is replaced by \( \Sigma^X_{yz} \). At the electron pockets the self-energy corrections are positive, so that the \( \Sigma^{X/Y}_{yz/zz} \) terms lead again to an upward shift of the \( yz/zz \) orbitals. In the spin-nematic state \( \Sigma^X_{yz} > \Sigma^Y_{zz} \) so the \( yz \) sector of the X pocket shrinks further and the \( zz \) part of the Y pocket expands, see Fig. 1 in the main text. The nematic order parameter at the electron pockets is then defined as \( \Delta \Sigma_x = (\Sigma_{yz} - \Sigma_{zz})/2 > 0 \). Notice that in our approach the change of sign of the nematic splitting at the \( \Gamma \) and \( M = (X, Y) \) point is a natural consequence of the self-energy corrections induced by nematic OSSF, as explained in [14]. The X/Y band dispersions are given by

\[ E^{X/Y}_i = h_0^{X/Y} + \Sigma^{X/Y}_i/2 \pm \sqrt{h_1^{X/Y2} + (h_3^{X/Y} - \Delta \Sigma_h^{X/Y})^2} \]

The rotation from the orbital to the band basis is defined by Eq. (20) provided that \( v \Gamma \rightarrow v \Gamma X/Y \), so that the fermionic operators are defined as

\[ c_x = u_x c_{yz} - v_x c_{xy} \]

and \( c_y = c_{zy} \).
\[ u_{y} c_{xz} - iv_{y} c_{xy}, \]

with

\[
u_{x}^{2} = \frac{1}{2} \left( 1 + \frac{h_{x}^{3} - \Sigma_{y z}^{X} / 2}{\sqrt{h_{x}^{3} + (h_{x}^{3} - \Sigma_{y z}^{X} / 2)^{2}}} \right), \]

\[
u_{x}^{2} = \frac{1}{2} \left( 1 + \frac{h_{x}^{3} - \Sigma_{y z}^{X} / 2}{\sqrt{h_{x}^{3} + (h_{x}^{3} - \Sigma_{y z}^{X} / 2)^{2}}} \right), \]

and analogous expressions for \( u_{y}, v_{y} \).

**Orbital Selective Spin Fluctuations Model**

Once established the orbital composition of the low-energy model, one can project the general interacting Hamiltonian including the Hubbard and Hund terms into the low-energy states. As shown in [27, 37] one obtains the effective low-energy interacting terms can be written as

\[ H_{\text{int}} = -\frac{\tilde{U}}{2} \sum_{q} S_{X \times Y}^{ux/yz} \cdot S_{X \times Y}^{ux/yz}. \]

Here \( \tilde{U} \) is the intraorbital interaction renormalized at low energy and the intraorbital spin operators connecting hole and electron pocket are given by Eqs (4)-(5) of the main text, that we rewrite here explicitly

\[ S_{X}^{ux/yz} = \sum_{k} (u_{q} h_{q}^{+} + v_{q} h_{q}^{-}) \sigma_{X} e_{X} \]

\[ S_{Y}^{ux/yz} = \sum_{k} (-v_{q} h_{q}^{+} + u_{q} h_{q}^{-}) \sigma_{Y} e_{Y} \]

The low-energy interacting Hamiltonian in Eq. (25) defines the OSSF: at low energy the hole pockets at \( \Gamma \) and the \( X/Y \) electron pockets share only one orbital, the \( yz/\cdot z \) respectively. Thus the spin interactions along \( x \) and \( y \) has a single orbital character (see Fig 1 in the main text):

\[ \langle S \cdot S \rangle(Q_{X}) \Rightarrow \langle S_{X}^{ux/yz} \cdot S_{X}^{ux/yz} \rangle \]

\[ \langle S \cdot S \rangle(Q_{Y}) \Rightarrow \langle S_{Y}^{ux/yz} \cdot S_{Y}^{ux/yz} \rangle \]

By computing self-energy corrections of the orbital states coming from these OSSF one obtains orbital-dependent self-energy corrections, as shown in Eq. (18) and (22) above. In addition, within a spin-nematic scenario the anisotropy of the spin fluctuations at different \( Q \) vectors translates in the nematic splitting \( \Delta \Sigma_{h} \), \( \Delta \Sigma_{e} \) of the orbitals discussed previously. Here we argue that OSSF can also mediated an orbital-selective nematic pairing. The pairing model derived from the spin-spin interaction Hamiltonian (25) is detailed in the Method Section of the main text, and its outcomes are discussed in the manuscript.

**Model parameters for the FeSe**

We solve self-consistently the set of BCS equations for realistic parameter for the FeSe system in the nematic phase.

Although the physical outcome of this work does not crucially depend on this, instead of using exactly the band parameters of Ref. [14], we will adjust them to fit a smaller value of the nematic splitting of the electron pockets reported afterwards in the literature, \( \Delta \Sigma_{e} \sim 15 \) meV [6, 15]. The list of the band parameters appearing in Eqs (19), (23) and used in the calculations are given in Table I. The spin-orbit coupling is assumed \( \lambda = 20 \) meV. We use \( \Delta \Sigma_{yz/\cdot z} \sim 70/40 \) meV and \( \Delta \Sigma_{X/Y} \sim 45/15 \) meV, in order to have \( \Delta \Sigma_{h/e} \sim 15 \) meV.

| \( \Gamma \) | \( \chi \) |
|---|---|
| \( \epsilon_{\Gamma} \) | 46 |
| \( \epsilon_{\omega} \) | 72 |
| \( \epsilon_{\omega} \) | 55 |
| \( a_{\Gamma} \) | 263 |
| \( a_{\omega} \) | 93 |
| \( a_{\omega} \) | 101 |
| \( b_{\Gamma} \) | 182 |
| \( b \) | 154 |
| \( v \) | 144 |

**TABLE I: Low-energy model parameters for FeSe in the nematic phase at \( k_{z} = 0 \).** All the parameters are in meV, the \( k \) vector is measured in units \( 1/a \sim 0.375 \) Å, where \( \sqrt{2}a = \sqrt{2}a_{\Gamma,Fe} \) is the lattice constant of the 1-Fe unit cell (so that \( a = \sqrt{2}a = 3.77 \) Å is the lattice constant of the 2Fe unit cell).

The \( u, v \), factors defined by Eqs [21], [24], computed using the above set of parameters, are shown in Fig. 2 of the main text. We reproduce the FS and their orbital distribution as experimentally observed by ARPES at \( k_{z} = 0 \) [6, 14], [10, 21], with the hole pocket having \( k_{F}^{h} = 0.056 \) Å\(^{-1}\) and \( k_{F}^{e} = 0.11 \) Å\(^{-1}\), the \( X \) one \( k_{F}^{h} = 0.20 \) Å\(^{-1}\) and \( k_{F}^{e} = 0.051 \) and the \( Y \), \( k_{F}^{h} = 0.10 \) and \( k_{F}^{e} = 0.20 \) Å\(^{-1}\) in the nematic phase.

Using now the \( T = 0 \) BCS equations, Eqs (9)-(12) of the main text, we can fit the experimental data of Ref. [17] using the SC couplings as fitting parameters. The results are shown in Fig. 4 of the main text. Notice that assuming isotropic pairing interactions \( g_{\Gamma} = g_{Y} = 0.84 \) and accounting only for the orbital splitting effects, encoded in the \( u, v \), factors, the SC gap at \( \Gamma \) presents opposite anisotropy with respect the one found in the experiment. On the other hand, considering nematic pairing with \( g_{\Gamma} = 4.77 > g_{Y} = 0.18 \) we reproduce both the absolute values and the angular modulation of the observed gap at \( \Gamma \) and \( X \). It is interesting to compare the value of the anisotropy obtained here with the anisotropy of the OSSF extracted from the analysis of the shrinking effect in Ref. [14]. Since \( g_{\Gamma} \sim (S_{X/Y}^{yz/\cdot z} - S_{X/Y}^{yz/\cdot z}) \) we can in first approximation estimate the ratio as \( g_{\Gamma} \sim (V^{X/Y}(\omega_{X} - \omega_{Y}))^{2} \) where
\( \omega_{X/Y} \) are the masses of the spin fluctuations along \( \Gamma X/Y \) and \( V^{X/Y} \) is the strength of the coupling between the fermions and the spin mode at \( Q_X \) and \( Q_Y \) (see the supplementary material of Ref. [14] for further details). Using the numerical values obtained fitting the ARPES orbital shrinking we found \( g_X/g_Y \sim 20\), that is compatible with the present estimate from fitting the experimental gaps \( g_X/g_Y = 4.77/0.18 \sim 26 \).

Let us finally address the issue of the \( k_z \) gap dependence. As discussed in the main text, a crucial difference when moving from \( k_z = 0 \) to \( k_z = \pi \) is that the orbital character of the hole pocket changes considerably. Since all the FS pockets expand \( [19, 20] \), the effect of the nematic order is less dramatic on the hole pocket, with the consequence that it retains full \( yz \) character at \( \theta = 0 \) [20]. This has already a profound impact on the hole-gap anisotropy, as recently pointed out in Ref. [35]. To highlight the effect of the change of orbital weights on the hole pocket at \( \theta = 0 \) we analyze the BCS solution using a set of realistic band parameters for the \( Z \)-pocket as listed in Table II.

![Diagram](image)

**TABLE II: Low-energy model parameters for the hole-pocket at \( k_z = \pi \) in the nematic phase.**

| \( Z \)   | \( \epsilon_Z \) | \( a_Z \) | \( b_Z \) |
|----------|------------------|----------|----------|
|          | 26               | 473      | 264      |

In the absence of a detailed comparison with the band structure above \( T_S \) as done in Ref. [14], we already include in \( \epsilon_Z \) the effect of the isotropic shrinking, \( (\Sigma_{yz} + \Sigma_{xz})/2 \), and consider separately a further nematic splitting \( \Delta \Sigma_{bh} = 10 \) meV. In Fig. 6 we show the FS shape and composition of the \( Z \) pocket in both the paramagnetic and nematic phase. Notice that even below \( T_S \), the large elliptical \( Z \) pocket, \( k_F = 0.10 \) \( \text{Å}^{-1} \) and \( k_F^* = 0.15 \) \( \text{Å}^{-1} \), retains a marked \( yz \) character at \( \theta = 0 \) in agreement with the ARPES measurements [19, 20]. Moreover given this band structure, the inclusion of a finite spin-orbit coupling does not lead to any significant change, and the \( u_Z, v_Z \) factors defined as Eq.s [21, 24] scale approximately as \( \cos \theta \) and \( \sin \theta \) even below \( T_S \).

Solving the BCS equation in this case one can easily check that, contrary to what found at \( k_z = 0 \), \( \langle u_{0y}^2 \rangle \sim \langle v_{0y}^2 \rangle \), so that the increase of the \( \langle u_{0y}^2 \rangle \) factor over the \( \langle u_{0z}^2 \rangle \) in the nematic phase is enough to have \( \Delta_{\pi y}^2 > \Delta_{\pi z}^2 \). In this case already without nematic pairing one has a larger gap value at \( \theta = 0 \), as observed indeed in Ref. [35] (see also Fig 5 in the main text). As a consequence, if one retains instead the pairing anisotropy \( g_X/g_Y \) extracted from the fitting of the \( k_z = 0 \) gaps the anisotropic effect due to the nematic pairing is amplified now by the orbital factors that cooperates to give the same gap modulation. As a result we would get larger gap values and larger anisotropy when moving from the \( \Gamma \) to the \( Z \) pocket. Recent ARPES experiments investigated the superconducting gaps at \( k_z = \pi \) [19, 21]. While all the experiments confirm the in-plane anisotropy of the gap of the hole-pocket, with a larger gap value at \( \theta = 0 \), the various reports are somehow in disagreement on the \( k_z \) dependence of the gap-magnitude. In fact in Ref.s [19, 21] the absolute value of the gap and its anisotropy are found to be larger at \( k_z = \pi \), while in [20, 21] the authors claimed a decreasing of the gap magnitude when moving from the \( \Gamma \) to the \( Z \) pocket. The present situation calls for a more detailed experimental analysis and specific theoretical studies involving a 3D modeling of the band structure. As a matter of fact details of the 3D band model could change the estimate of the magnitude of the gaps at different \( k_z \), influencing the orbital ordering effects and the balance between such mechanism and the nematic pairing one.

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[1] I. Mazin, D. Singh, M. Johannes, and M. Du, Phys. Rev. Lett. **101**, 057003 (2008).
[2] K. Kuroki, S. Onari, R. Arita, H. Usui, Y. Tanaka, H. Kontani, and H. Aoki, Phys. Rev. Lett. **101**, 087004 (2008).
[3] A. Chubukov, Annual Review of Condensed Matter Physics 3, 57 (2012).
[4] C. Platt, W. Hanke, and R. Thomale, Advances in Physics **62**, 453 (2013).
[5] P. Hirschfeld, Comptes Rendus Physique **17**, 197 (2016).
[6] A. I. Coldea and M. D. Watson, Annual Review of Condensed Matter Physics **9**, 125 (2018).
[7] Y. Gallais and I. Paul, Comptes Rendus Physique **17**, 113 (2016).
[8] T. Shimojima, Y. Suzuki, T. Sonobe, A. Nakamura, M. Sakano, J. Omachi, K. Yoshioka, M. Kuwata-Gonokami, K. Ono, H. Kumigashira, et al., Phys. Rev. B **90**, 121111 (2014).
[9] K. Nakayama, Y. Miyata, G. N. Phan, T. Sato, Y. Tanabe, T. Urata, K. Tanigaki, and T. Takahashi, Phys. Rev. B **90**, 121111 (2014).
