Superconductivity in FeSe: The Role of Nematic Order

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Bulk FeSe is a special iron-based material in which superconductivity emerges inside a well-developed nematic phase. We present a microscopic model for this nematic superconducting state, which takes into account the mixing between s-wave and d-wave pairing channels and the changes in the orbital spectral weight promoted by the sign-changing nematic order parameter. We show that nematicity only weakly affects T_c, but gives rise to $\cos 2\theta$ variation of the pairing gap on the hole pocket, whose magnitude and size agrees with angle resolved photoemission spectroscopy and STM data. We further show that nematicity increases the weight of the d_{xz} orbital on the hole pocket, and increases (reduces) the weight of the d_{xy} orbital on the Y (X) electron pocket.

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Introduction.—Superconductivity in FeSe has attracted a lot of attention recently because this material holds the promise to reveal new physics not seen in other Fe-based superconductors [1]. The pairing in FeSe emerges at $T \leq 8$ K from a state with a well-defined nematic order, which develops at a much higher $T_s \sim 90$ K. Because nematic order breaks the C_4 tetragonal symmetry down to C_2, it mixes the s-wave and d-wave pairing channels [2–4]. As a result, the pairing gap on the Γ-centered hole pocket $\Delta(\theta)$ has both s-wave and d-wave components $\Delta(\theta) = \Delta_1 + \Delta_2 \cos 2\theta$, where Δ_1 and Δ_2 are the C_4-symmetric functions of $\cos 4\theta$. This gap form is generic, but the relative sign between Δ_1 and Δ_2 depends on details of the pairing interaction and the structure of the nematic order.

The $\cos 2\theta$ gap anisotropy on the hole pocket ("h" pocket in Fig. 1) has been probed recently by angle resolved photoemission spectroscopy (ARPES) [5–9] and scanning tunneling microscopy (STM) [10,11] measurements. These probes have shown that (i) the gap is larger along the direction towards the X electron pocket made out of d_{yz} and d_{xy} orbitals, than towards the Y pocket made out of d_{xz} and d_{xy} orbitals (Fig. 1), and (ii) the magnitude of the gap on the X pocket correlates with the weight of the d_{yz} orbital component. This led to the proposal [10] that the pairing glue in FeSe is orbital selective and predominantly involves d_{yz} fermions.

To support this argument, Refs. [10,12] analyzed the pairing problem within BCS theory, using the static interaction in the spin channel as the glue. They argued that the observed gap anisotropy can be reproduced only if one phenomenologically sets the interaction on the d_{yz} orbital to be the strongest. This was done by introducing different constant Z factors for each orbital. Constant orbital-dependent Z do not give rise to incoherence, but recalibrate the interactions on different orbitals.

In this Letter we reconsider this issue. We argue that adding different Z factors to d_{xy} and d_{xz}/d_{yz} orbitals is a legitimate way to incorporate high-energy renormalizations, which make interactions on d_{xy} and d_{xz}/d_{yz} orbitals unequal [13–15]. On the other hand, d_{xz} and d_{yz} orbitals become different only in the presence of nematic order. The latter is of order 10 meV (Refs. [10,16,17]), much smaller than the electronic bandwidth. As a result, the d_{xz}/d_{yz} splitting is a low-energy phenomenon which, we believe, should be fully captured within the low-energy model, without introducing phenomenologically $Z_{xz} \neq Z_{yz}$.

In our approach we depart from the tetragonal phase with the Γ/Z-, X-, and Y-centered Fermi pockets in the 1-Fe Brillouin zone. We use the low-energy model of Ref. [18] to parametrize the dispersion near these three points, and

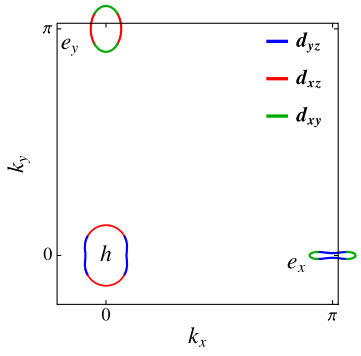

FIG. 1. The Fermi surface and its orbital content in the nematic phase of FeSe. In the 1-Fe Brillouin zone there is a hole (h) pocket centered at $\Gamma/Z = (0, 0)$ and two electron pockets X and Y centered at $(\pi, 0)$ and $(0, \pi)$, respectively. STM and ARPES data [5,10] show that the h pocket is an ellipse elongated along Y, and that the X electron pocket has a peanut-type form with the minor axis along the Y direction.

the model of Ref. [13] for the d_{xz}/d_{yz} pairing interactions in the s-wave and d-wave channels. We introduce a two-component d-wave nematic order parameter $\bar{\Phi} = (n_{d_{xz}} - n_{d_{yz}})/2 = (\bar{\Phi}_h, \bar{\Phi}_e)$, where h and e refer to hole and electron pockets. It reconstructs the Fermi pockets to an ellipsoidal hole pocket elongated along the Y direction, and a peanutlike X electron pocket [5–10,16,17,19] (see Fig. 1). A simple analysis shows that this holds when the nematic order changes sign between hole and electron pockets: $\Phi_h > 0$ and $\Phi_e < 0$. The sign change is consistent with theoretical analysis [13,20–22]. We take as an input the results of earlier studies [13–15,20,23,24] that the largest pairing interaction at low energies is between the hole and electron pockets. This interaction is angle dependent in the band basis and has s^{+-} and $d_{x^2-y^2}$ components U_s and U_d, respectively. U_s is larger, and in the absence of nematicity the system develops an s^{+-} order. We dress up U_s and U_d by coherence factors associated with the nematic order, solve the gap equation, and obtain T_c and the structure of the superconducting gap in the nematic phase [25].

Our results show that T_c is only moderately affected by nematicity, but it gives rise to a sizable anisotropy of the gap on both the hole and electron pockets. This is consistent with the phase diagram of S-doped $FeSe_{1-x}S_x$, which shows that T_c changes little around $x < 0.17$, when nematic order disappears, and with thermal conductivity, specific heat, and STM data [27–30], which show that the gap anisotropy changes drastically between $x < 0.17$ and $x > 0.17$.

For the gap on the hole pocket we find $\Delta(\theta_h) \approx \Delta_h(1 + \alpha \cos 2\theta_h + \beta \cos 4\theta_h)$, where the $\cos 2\theta_h$ term is induced by nematicity. To leading order in $\bar{\Phi}$, $\alpha \propto (4|\Phi_e| - [U_d/U_s]\Phi_h]$, where $\Phi_{h,e}$ are dimensionless orbital orders, normalized to the corresponding Fermi energies [see Ref. [31] and Eq. (5) below]. The Φ_h term reflects the nematicity-induced mixing between the s and d pairing components whereas the Φ_e term is related to the nematicity-induced redistribution of the orbital weight on the electron pockets. We computed $\Phi_{h,e}$ using band structure parameters which fit the ARPES data for the Z pocket ($k_z = \pi$) [31] and found that $\alpha > 0$. A positive α can be interpreted as if nematicity makes the pairing interaction between the Γ and X pockets stronger than between the Γ and Y pockets [10]. We emphasize, however, that this effect is captured within the low-energy model.

In Fig. 2 we show the calculated $\Delta(\theta_h)$ along with the gap anisotropy extracted from the STM data [10,32]. We see that the agreement is quite good. We found equally good agreement with the ARPES data for the Z pocket [5–8]. We also computed the gap at the smaller Γ pocket ($k_z = 0$) and found a smaller gap with a weaker anisotropy. This arises because the dimensionless Φ_h is larger for a smaller pocket and because the whole Γ pocket has predominantly d_{xz} character [31]. A smaller gap at Γ agrees with the ARPES data in Refs. [5,7] but not with Ref. [9].

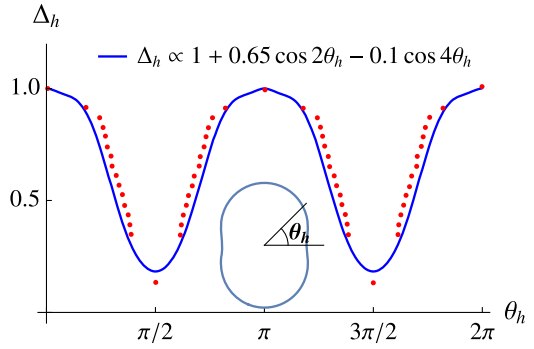

FIG. 2. Angular dependence of the pairing gap on the hole pocket obtained by numerically solving the gap equations with band structure parameters and nematic order parameters fitted to ARPES data above T_c. The gap maximum is along the $\Gamma - X$ direction, consistent with STM and ARPES data [5–10,19]. Points are STM data from Ref. [10]. The gap function $\Delta(\theta_h) = \Delta_h(1 + \alpha \cos 2\theta_h + \beta \cos 4\theta_h)$ has the $\cos 2\theta$ terms induced by nematicity (which we explicitly computed), as well as C_4-symmetric anisotropic $\cos 4\theta$ terms present already in the tetragonal phase due to spin-orbit coupling [18] and/or due to dressing of the pairing interaction by high-energy fermions [13,23].

Low-energy model.—We consider a quasi-2D model of bulk FeSe, with two corrugated cylindrical d_{xz}/d_{yz} hole pockets, centered at the $k_{x,y} = 0$, with the largest cross section at $k_z = \pi$ and the smallest at $k_z = 0$ (Refs. [5,7,9,16,33]) and two cylindrical d_{yz}/d_{xy} and d_{xz}/d_{xy} electron pockets centered at $(\pi, 0, k_z)$ and $(0, \pi, k_z)$ in the Fe-only Brillouin zone (X and Y pockets). We model the low-energy electronic structure on each pocket by spinors, following Refs. [18,34]. We choose parameters such that in the tetragonal phase the larger hole pocket h has d_{xz} character along the Y direction and d_{yz} character along the X direction, consistent with ARPES experiments [5–7,9,16,19,33].

The band operators for h, X, and Y pockets are expressed in terms of the orbital operators as

$$\begin{aligned} h &= d_{yz} \cos\phi_h + d_{xz} \sin\phi_h, \\ e_X &= -i d_{yz} \cos\phi_X + d_{xy} \sin\phi_X, \\ e_Y &= i d_{xz} \cos\phi_Y + d_{xy} \sin\phi_Y. \end{aligned} \tag{1}$$

In the tetragonal phase, the h pocket is nearly circular and in the absence of spin-orbit coupling (SOC) $\phi_h \approx \theta_h$, where θ_h is the angle measured with respect to the X axis. On electron pockets, to a good approximation $\cos\phi_{X,Y} = A \sin\theta_{X,Y}$, $\sin\phi_{X,Y} = (1 - A^2 \sin^2\theta_{X,Y})^{1/2}$, where $A < 1$ and θ_X (θ_Y) is the angle measured with respect to the X (Y) direction [3,14].

In the nematic phase we introduce momentum-dependent d-wave nematic order with components $\pm\bar{\Phi}_h$ on hole pockets (plus sign on d_{xz} orbital) and $\bar{\Phi}(Y) = -\bar{\Phi}(X) = \bar{\Phi}_e$. For simplicity we neglect the d_{xy}

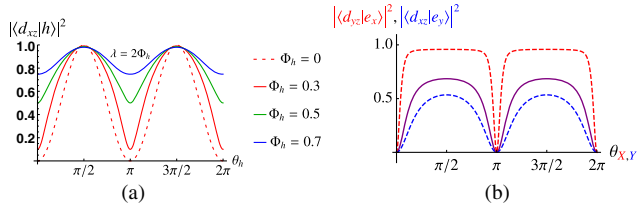

FIG. 3. The change of orbital weight on the hole pocket (a) and on the electron pockets (b) between the tetragonal phase (dashed line) and the nematic phase (solid lines) The angle θ_X (θ_Y) is measured with respect to the X (Y) direction. For the hole pocket, we present the results including the SOC $\bar{\lambda}$ (the band splitting at $k_{x,y} = 0$ is $\pm\sqrt{\bar{\Phi}^2 + \bar{\lambda}^2/4}$). We used $\bar{\lambda} = 2\bar{\Phi}_h$.

component of the nematic order [14,35]. Equations (1) still hold in the presence of nematicity, but the relations between ϕ_h, ϕ_X, ϕ_Y and the angles along the Fermi surfaces become different. For the hole pocket, we define the dimensionless Φ_h via $\cot 2\phi_h = \cot 2\theta_h - 2\Phi_h/\sin 2\theta_h$, again in the absence of SOC (the full expressions with SOC are presented in Ref. [31]). Roughly, $\Phi_h = \bar{\Phi}_h/E_F$. For the same $\bar{\Phi}_h$, Φ_h is larger on the Γ pocket than on the Z pocket, because E_F is smaller at Γ. For the electron pockets we find that the relations $\cos\phi_{X,Y} = A\sin\theta_{X,Y}$ also hold, but A becomes different for X and Y pockets. We define the dimensionless Φ_e via $A_X \approx A(1-\Phi_e)$ and $A_Y \approx A(1+\Phi_e)$.

To match ARPES and STM data for the shapes of the h and X pockets, Φ_h must be positive and Φ_e negative. A positive Φ_h increases the d_{xz} spectral weight on the hole pocket, particularly when $\Phi_h > 1/2$; see Fig. 3(a). At $\Phi_h \geq 1$ the hole pocket is almost entirely d_{xz}. A negative Φ_e increases the weight of the d_{yz} orbital on the X pocket and reduces the weight of the d_{xz} orbital on the Y pocket, as shown in Fig. 3(b). We computed the dimensionless $\Phi_{h,e}$ using $\bar{\Phi}_h = 10$ meV, $|\bar{\Phi}_e| \sim 20$ meV (Refs. [10,17,36]) and band structure parameters that fit the ARPES data for the Z pocket [36,37] in the nematic phase above T_c and obtained [31] $|\Phi_e| \sim 0.1$, $\Phi_h \sim 0.3$. For such Φ_h the orbital weight along the Z pocket still interpolates between d_{xz} and d_{yz}. For the Γ pocket, we obtained $\Phi_h \sim 0.7$. The whole h pocket becomes predominantly d_{xz}. In both cases, the orbital content does not depend strongly on the SOC, and to simplify the analysis we neglect SOC in the solution of the gap equations.

Pairing interaction.—We use as an input the results of earlier studies [10,13–15,23] that the largest pairing interaction is the pair hopping between hole and electron pockets, consistent with the observed enhancement of $(\pi,0)/(0,\pi)$ magnetic fluctuations [38–40]. In the band basis, the pair-hopping pairing interaction has the form

$$H_{\text{pair}} = h_k^\dagger h_{-k}^\dagger [U_s(e_{X,p}e_{X,-p}\cos^2\phi_X + e_{Y,p}e_{Y,-p}\cos^2\phi_Y) + U_d\cos 2\phi_h(e_{X,p}e_{X,-p}\cos^2\phi_X - e_{Y,p}e_{Y,-p}\cos^2\phi_Y)], \quad (2)$$

where repeated momentum indices are implicitly summed and spin indices are omitted. In the tetragonal phase, $\cos^2\phi_{X,Y} = A^2(1-\cos 2\theta_{X,Y})/2$, $\phi_h = \theta_h$, and the two terms in Eq. (2) describe pairing interactions in the s-wave and d-wave channels with couplings U_s and U_d, respectively. The ratio $U_s/U_d = (U+J)/(U-J) > 1$ is already at the bare level, where U and J are Hubbard and Hund's interactions, and further increases under RG [13]. Then the leading instability in the absence of nematicity is towards s^{+-} superconductivity.

In the presence of nematic order the situation changes because now $\cos 2\phi_h \approx \cos 2\theta_h - \Phi_h$ and $A_X \neq A_Y$. As a result, the U_d term in Eq. (2) acquires extra terms which have an "s-wave" angular dependence and effectively renormalize the U_s term, making this interaction different for fermions near the X and Y pockets. Substituting the forms of $\cos 2\phi_h$, $\cos 2\phi_X$, and $\cos 2\phi_Y$ into Eq. (2) and restricting to first-order terms in Φ_h and Φ_e, we obtain the pairing interaction in the form

$$H_{\text{pair}} = \frac{A^2}{2}\sum_{j=X,Y} h_k^\dagger h_{-k}^\dagger (A_j + B_j\cos 2\theta_h) e_{j,p}e_{j,-p}, \quad (3)$$

where

$$A_{X,Y} = (1-\cos 2\theta_{X,Y})[U_s(1\mp 2\Phi_e) \mp U_d\Phi_h],$$
$$B_{X,Y} = \pm U_d(1-\cos 2\theta_{X,Y})(1\mp 2\Phi_e). \quad (4)$$

Gap equations.—We use Eqs. (3) and (4) to obtain the linearized gap equations. The gap on the hole pocket is parametrized by $\Delta(\theta_h) = \Delta_h(1+\alpha\cos 2\theta_h)$, (we neglect the $\cos 4\theta$ term to simplify presentation). The computational steps are rather conventional [31]. To linear order in $\Phi_{e,h}$,

$$\alpha \approx \frac{U_s U_d}{U_s^2 - U_d^2/2}\left(4|\Phi_e| - \frac{U_d}{U_s}\Phi_h\right). \quad (5)$$

Notice that α depends only on the ratio U_d/U_s, and not on the strength of the interaction, which is compensated by the Cooper logarithm.

We see that there are two contributions to the gap anisotropy α, originating from the components of the nematic order on hole and electron pockets. Because Φ_h and Φ_e have opposite signs, the sign of α depends on their strength and on the ratio between the interactions U_d/U_s. Because $4|\Phi_e| > \Phi_h$ and $U_d/U_s \leq 1$, we find $\alpha \sim 0.2$ is positive; i.e., the gap $\Delta_h(\theta_h)$ has its maximum along the X direction $\theta_h = 0$. This is consistent with the STM and ARPES data [5–10,19]. The Φ_h term in Eq. (5) is further reduced if we include that the ratio U_s/U_d grows under the renormalization group flow [13].

To go beyond this analytic expansion in powers of $\Phi_{e,h}$, we solved the gap equations numerically for the same set of parameters, but not restricting to first order in $\Phi_{h,e}$.

We found the same gap structure but somewhat larger $\alpha \approx 0.65$. The result is shown in Fig. 2 along with the STM data from Ref. [10]. For this plot, we added to $\Delta(\theta_h)$ an additional $\beta \cos 4\theta_h$ term with $\beta = -0.1$. The $\cos 4\theta_h$ dependence arises already in the tetragonal phase and is determined by details beyond our model.

The sign of the gap anisotropy can be interpreted as the indication that in the nematic state the pairing interaction between the h and X pockets becomes stronger than between the h and Y pockets. Because the positive contribution to α comes from Φ_e, the increase of the h-X interaction can be traced back to the increase of d_{yz} orbital weight on the X pocket. In this respect, qualitatively our results agree with Refs. [10,12], where the increase of the d_{yz} orbital weight was introduced phenomenologically, via an orbital dependent constant Z factor. However, in our theory the modification of the d_{xz}/d_{yz} orbital weights naturally emerges within the low-energy model and does not require the inclusion of additional Z factors.

On the electron pockets, to leading order in $\Phi_{h,e}$, the gaps have the forms $\Delta_{X,Y} = -\Delta_h \gamma_{X,Y}(1 - \cos 2\theta_{X,Y})$, where $\gamma_{X,Y} = \gamma[1 \pm (2|\Phi_e| - U_d/U_s \Phi_h + \alpha/2)]$ and $\gamma > 0$ is a number whose value depends on the electronic structure. The vanishing of the gaps at $\cos 2\theta_{X,Y} = \pm 1$ is an artifact of neglecting the d_{xy} orbital in the pairing problem. In reality, the gaps $\Delta_{X,Y}$ tend to small but finite values along the X and Y directions, respectively. The ARPES and STM data reported an anisotropic, but still sign-preserving gap on the X pocket, with gap maximum at $\theta_X = \pi/2$, consistent with our formulas. The overall sign of $\Delta_{X,Y}$ is opposite to that of Δ_h. The dependence of $\gamma_{X,Y}$ on the nematic order shows that the gap magnitude is larger on the X pocket than on the Y pocket. We propose to verify this in future experiments.

Fermionic self-energy.—The STM data indicate that in the nematic phase the Y pocket is less visible than the X pocket, and in some ARPES studies [9,41] this Y pocket has not been observed. To understand this feature, we computed the self-energy on both electron pockets to second order in U_s and U_d and extracted the actual quasiparticle residues $Z_{X,Y}$ on each electron pocket [31]. We find $Z_Y > Z_X$ simply because the effective interaction is larger for fermions on the X pocket (we recall that larger interaction leads to a smaller Z). If this was the only effect, we would expect the Y pocket to become more visible. However, like we said, nematic order also increases the d_{yz} spectral weight of the X pocket and decreases the d_{xz} orbital spectral weight of the Y pocket (see Fig. 3). If the d_{xy} orbital excitations are not observed in STM and ARPES because of matrix elements, or if the d_{xy} orbital is more incoherent than the d_{xz}/d_{yz} orbitals [26,42–44], then the Y pocket should indeed become less visible in the nematic phase. We caution, however, a recent ARPES study [9] did not find d_{xy} excitations on the X pockets to be more incoherent that d_{yz} excitations, so the reason why the Y pocket is less visible in STM and some ARPES studies is not yet understood.

Conclusions.—In this Letter we argued that the experimentally observed anisotropy of the superconducting gap in bulk FeSe can be explained within the low-energy model for nematic order, without adding phenomenologically different quasiparticle weights for the d_{xz}/d_{yz} orbitals. Our key result is that T_c is not strongly affected by the nematic order, but nematicity mixes s-wave and d-wave pairing channels and gives rise to a $\cos 2\theta_h$ gap anisotropy on the hole pocket The sign of the $\cos 2\theta_h$ term is determined by the interplay between the nematic order parameters on hole and electron pockets, which are of different sign, and the relative strength of s-wave and d-wave components of the pairing interaction. On the Z pocket, we found a sizable $\cos 2\theta_h$ gap anisotropy with the gap maximum along the X direction, in agreement with the data. In our calculations the gap on the Γ pocket is smaller and less anisotropic. On the peanutlike X pocket, the gap is found to be maximal along the minor axis, which is also in agreement with the data. We also argued that nematicity decreases the weight of the d_{xy} orbital on the X pocket and increases it on the Y pocket. This may potentially explain why the Y pocket is less visible in STM and in some ARPES data.

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