The origin of nematic order in FeSe

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Nematic order in Fe-pnictides and Fe-chalcogenides develops at a temperature $T_s$ that is larger than the magnetic transition (for reviews, see \cite{1}). It spontaneously breaks the tetragonal $C_4$ lattice symmetry down to orthorhombic $C_2$. The origin of this symmetry breaking is currently one of the most intensely debated issues of the Fe-based superconducting materials \cite{2}. In the Fe-pnictides, nematic order occurs reasonably close to the instability towards stripe magnetic order at the Neel temperature $T_N$. Because the stripe order breaks $Z_2$ tetragonal symmetry ($C_4 \rightarrow C_2$) in addition to the $O(3)$ spin-rotational symmetry and because $T_s$ and $T_N$ show similar doping dependencies, it seems reasonable to associate the nematic order with magnetism \cite{2}. Indeed, several groups have argued \cite{3–12} that magnetic fluctuations split the mean-field stripe magnetic transition into two separate $O(3)$ and $Z_2$ transitions. The discrete $Z_2$ symmetry is broken first at $T_s > T_N$, resulting in an intermediate phase, dubbed Ising-nematic, where long-range magnetic order is absent but the $C_4$ lattice symmetry is broken down to $C_2$. Such $Z_2$ order triggers orbital and structural order as all three break the same $C_4$ symmetry.

The magnetic scenario for nematicity in Fe-pnictides is supported by a variety of experimental observations, such as the doping dependencies of $T_N$ and $T_s$ \cite{10}, the scaling between the shear modulus and the spin-lattice relaxation rate \cite{13}, and the sign-change of the in-plane resistivity anisotropy between electron-doped and hole-doped Fe-pnictides \cite{14}. This scenario, however, has been challenged for the Fe-chalcogenide FeSe. This material displays a nematic transition at $T_s \approx 90K$. The properties of the nematic phase in FeSe resemble those in Fe-pnictides: similar softening of the shear modulus \cite{15}, similar orthorhombic distortion and orbital order \cite{16}–\cite{18}, and similar behavior of the resistivity anisotropy upon applied strain \cite{19}. Furthermore, neutron scattering experiment shows that spin fluctuations are peaked at the same ordering vectors as in the Fe-pnictides \cite{20,21}. Yet, in distinction to Fe-pnictides, no magnetic order has thus far been observed in FeSe in the absence of external pressure \cite{22,23}. Moreover, NMR measurements were interpreted as evidence that the magnetic correlation length $\xi$ remains small at $T_s$ \cite{15,24}. Although in the Ising-nematic scenario $\xi$ does not have to be large at $T_s$, this seems to be the case for all Fe-pnictides.

Given these difficulties with the Ising-nematic scenario, spontaneous orbital order has been invoked to explain the nematic state in FeSe \cite{12}–\cite{24}. However, at present, no microscopic theory exists where orbital order appears spontaneously instead of being induced by magnetism \cite{25}–\cite{29}. Alternative scenarios for magnetically-driven nematicity in FeSe have also been proposed, involving the formation of a quantum paramagnet \cite{30}, the onset of spin quadrupolar order \cite{31}, and strong frustration of the magnetic fluctuations \cite{32}. Yet, the issue of why FeSe does not fit into a “universal” theory for the iron-based superconductors still persists.

In this communication, we present an extension of the spin-nematic scenario which explicitly builds on a unique property of the electronic structure of FeSe, namely, the fact that the Fermi energy $E_F$ in this material is small – only a few meV, as seen by ARPES and dH-vA experiments \cite{19,33}. For a system with a small $E_F$, earlier renormalization-group (RG) calculations have shown that there are two density-wave channels whose fluctuations are strong at momenta $(0, \pi)/(\pi, 0)$: a spin density-wave (SDW) channel and a charge-current density-wave (CDW) channel (a CDW with imaginary order parameter, which we denote as iCDW \cite{34}). The relative strength between the two depends on the sign of the inter-pocket exchange interaction ($u_2$ in our notations below). For repulsive $u_2$, the coupling in the SDW channel is larger, while for attractive $u_2$ the coupling in the iCDW channel is larger. In both cases, however, the RG calculations show that the coupling in the subleading channel approaches the one in the leading channel at small energies. The RG process stops at $E_F$, implying that if $E_F$ is larger than the highest instability temperature ($T_s$ for FeSe) the subleading channel is not a strong competitor and for all practical purposes can be neglected. However,
if $E_F \sim T_s$, as in FeSe, the couplings in the two channels become degenerate within the RG. The degeneracy implies that the order parameter manifold increases from $O(3)\times Z_2$, for the three-component SDW, or from $Z_2\times Z_2$, for the one-component iCDW, to a larger $O(4)\times Z_2$. In all cases, the $Z_2$ part of the manifold corresponds to selecting either $(0, \pi)$ or $(\pi, 0)$ for the density-wave ordering vector. While in both $O(3)\times Z_2$ and $O(4)\times Z_2$ models the $Z_2$ symmetry can be broken before the continuous one, in the latter this happens at a significantly smaller correlation length. As a result, at small $E_F$, the nematic order emerges while magnetic fluctuations are still weak. Furthermore, the SDW transition temperature $T_N$ in the $O(4)$ model is additionally suppressed due to the competition with iCDW. We argue that these features explain the properties of the nematic state in FeSe, including non-monotonic pressure dependence of $T_N$ [35, 36].

The model. We consider a quasi-2D itinerant band model with two hole pockets at the $\Gamma$ point and two electron pockets at $(0, \pi)$ and $(\pi, 0)$ in the 1-Fe Brillouin zone [10, 37]. This model can be obtained from an underlying 5-orbital model with Hubbard and Hund interactions and hopping between the Fe 3$d$ orbitals [38, 39].

The quadratic part of the Hamiltonian in the band basis describes the dispersion of the low-energy fermions, and the information about the orbital content along the Fermi pockets is passed onto inter-pocket and intra-pocket interactions, which are the Hubbard and Hund terms dressed by the matrix elements arising from the change from the orbital to the band basis [40]. The angular dependence of the matrix elements leads to angle-dependent interactions. The three interactions relevant for Ising-nematic order are the inter-pocket density-density interaction $u_1$, the exchange interaction $u_2$, and the pair-hopping interaction $u_3$ [41]. To simplify the analysis, we follow earlier works [10] and analyze the Ising-nematic order within an RG procedure that (i) approximates these three interactions as angle-independent and (ii) restricts the analysis to one hole pocket. The extension to two pockets and angle-dependent interactions makes the calculations more involved but does not modify the RG equations in any substantial way and, moreover, leaves them intact if we treat the hole pockets as circular and neglect the $d_{xy}$ orbital component on the electron pockets.

We label the fermions near the hole pocket as $c_{k}$ and the fermions near the electron pockets as $f_{1,k}$ and $f_{2,k}$. The $O(3)$ magnetic order parameter is given by

$$
M_j = \frac{1}{N} \sum_{k_{\alpha\beta}} \left( c_{k_{\alpha},\sigma} c_{f_{j,k_{\beta}},+} + h.c. \right),
$$

whereas the $Z_2$ iCDW order parameter is

$$
\Phi_j = \frac{i}{N} \sum_{k_{\alpha}} \left( c_{k_{\alpha},\sigma} c_{f_{j,k_{+}},\alpha} + h.c. \right),
$$

with $j = 1, 2$ corresponding to the two possible ordering vectors $Q_1 = (\pi, 0)$ and $Q_2 = (0, \pi)$. We show these two ordered states in Fig. 1.

(4) Ising-nematic action. In the Ising-nematic scenario, the $C_1 \rightarrow C_2$ symmetry breaking implies the appearance of a composite order, quadratic in the density-wave order parameters $M_j$ and $\Phi_j$. To analyze this scenario, we need to know the flow of the couplings that drive SDW order, $\Gamma_{sdw} = u_1 + u_3$, and iCDW order, $\Gamma_{icdw} = u_1 + u_3 - 2u_2$ [Ref. 41]. The bare coupling $\Gamma_{sdw} > \Gamma_{icdw}$ when $u_2 > 0$ and $\Gamma_{icdw} > \Gamma_{sdw}$ when $u_2 < 0$. As one integrates out the high-energy degrees of freedom via an RG procedure, the ratio $u_2/(u_1 + u_3)$ decreases as the system flows to lower energies (or temperatures) and approaches zero at the energy/temperature scale in which the system develops SDW/iCDW order. This holds, however, only if this scale is larger than $E_F$. If $E_F$ is larger, the RG flow stops at $E_F$ and the system develops an instability only in the channel with the largest bare coupling.

To illustrate our point, we plot in Fig. 2 a) the RG flow of $\Gamma_{icdw}$ and $\Gamma_{sdw}$ for a particular set of bare couplings $u_1(0) = u_2(0) = 10u_3(0)$, chosen deliberately to give a negative bare $\Gamma_{icdw}$. Under the RG flow, $\Gamma_{icdw}$ becomes positive and approaches $\Gamma_{sdw}$ at the scale where the couplings diverge and the system develops a density-wave order. The Fermi energy $E_F$ sets the scale at which the RG flow stops. In case I (large $E_F$), the RG stops when $\Gamma_{icdw}$ is still small. In case II (smaller $E_F$), the RG stop when $\Gamma_{icdw}$ is comparable to $\Gamma_{sdw}$, and in case III (even smaller $E_F$), the RG flow reaches the $O(4)$ fixed point already at energies larger than $E_F$. We associate case I in Fig. 2 with Fe-pnictides, and cases II/III with FeSe based on the values of $E_F$ obtained by ARPES and quantum oscillations [10, 33].

We next take the RG results as input and analyze the emergence of a nematic order which spontaneously breaks the symmetry between momenta $Q_1$ and $Q_2$ without breaking any other symmetry. The analysis follows the same steps as for pure SDW order [10]: we introduce $M_j$ and $\Phi_j$ ($j = 1, 2$) as Hubbard-Stratonovich fields which decouple the four-fermion interaction terms, integrate over the fermions, and obtain the effective action in terms of $M_j$ and $\Phi_j$:...
Within a mean-field approximation, $O(4)$ and $Z_2$ are broken at the same temperature. Beyond mean-field, the $Z_2$ symmetry is broken first, and both $M$ and $\Phi$ contribute to it, even if $\Gamma_{\text{sdw}} \neq \Gamma_{\text{idcw}}$. To see this, we treat $M$ and $\Phi$ as fluctuating fields, introduce the composite fields $\psi = u (M_0^2 + \Phi_0^2 + M_y^2 + \Phi_y^2)$ and $\varphi = g (M_x^2 + \Phi_x^2 - M_y^2 - \Phi_y^2)$ to decouple the quartic terms, integrate over the primary fields $M$ and $\Phi$ and obtain the action in terms of $\psi$ and $\varphi$:

$$S_{\text{eff}} [\psi, \varphi] = \frac{\varphi^2}{2g} - \frac{\psi^2}{2u} + \frac{3}{2} \int_q \ln \left[ \left( \chi_c^{-1} + \psi \right)^2 - \varphi^2 \right] + \frac{1}{2} \int_q \ln \left[ \left( \chi_s^{-1} + \psi \right)^2 - \varphi^2 \right]$$

(4)

The field $\psi$ has a non-zero expectation value $\langle \psi \rangle \neq 0$ at any temperature as it does not break any symmetry, but only renormalizes the correlation lengths of the primary fields $M$ and $\Phi$ to $\xi_{\phi} = \xi_{\chi_s} = \xi_{\chi_c}$ respectively. Near $T_\phi$, $\xi_{\phi} \approx \xi_{\chi_s} \approx \xi_{\chi_c}$, a non-zero nematic order parameter $\langle \phi \rangle \neq 0$ emerges when the correlation length $\xi^2 = \pi / g$, or, to logarithmic accuracy in $g \ll 1$, at $T_s = 2 \pi \rho_s / |\log g|$, where $\rho_s$ is the stiffness of the $O(4)$ non-linear $\sigma$ model associated with Eq. (3). It is instructive to compare this result with the case where only $O(3)$ SDW fluctuations are present. In that case, the nematic order emerges when $3 \xi_{\phi}^2 = 4 \pi / g_{O(3)}$, and the transition temperature is $T_\phi = 2 \pi \rho_s / |\log g_{O(3)}|$, where $g_{O(3)}$ is the coupling in the SDW $O(3)$ model. As a result, to obtain the same $T_s$, one needs a much smaller coupling constant $g_{O(3)} \sim g_{O(4)}$. Consequently, at $T = T_s$, the correlation length $\xi_{O(4)}(T)$ in the $O(4)$ case is proportional to $\sqrt{\xi_{O(3)}}$, i.e. it is much smaller than it would be if nematicity was driven solely by SDW fluctuations. This is consistent with NMR [13, 21] and neutron scattering data [21] in the paramagnetic phase of FeSe, which point to the presence of SDW fluctuations, albeit weaker than in the Fe-pnictide compounds. The rapid increase of the correlation lengths below $T_s$, obeying $\xi_{\phi}^2 = \xi_{\chi_s}^2 (T_s - \langle \phi \rangle)$, is also consistent with the increase of $1/T_\phi T$ and the inelastic neutron signal [13, 21, 24].

The $O(4)$ Ising-nematic scenario also addresses why no magnetic order appears down to the lowest temperatures. The SDW and iCDW orders compete via the bi-quadratic term $(u - g) M_j^2 \Phi_j^2$ in the low-energy action of Eq. (3). As a result, for $u_2 > 0$, fluctuations of the sub-leading iCDW channel suppress the transition temperature of the leading SDW channel. Such a suppression
is the largest when the difference between the coupling constants $|\Gamma_{\text{sdw}} - \Gamma_{\text{iCDW}}|$ is the smallest, which happens when the system flows towards $O(4)$ symmetry within RG, i.e. when $E_F$ is small, such as in FeSe.

**Experimental signatures.** We know discuss the experimental consequences of the Ising-nematic order. The breaking of the $Z_2$ symmetry between the $j = 1$ and $j = 2$ components of the $O(4)$ field implies the breaking of $C_4$ lattice rotational symmetry down to $C_2$. This instantaneously triggers structural order due to the coupling to lattice. To investigate how $Z_2$ order affect the electronic states, we return to the original four-pocket model (with fermions near the two hole pockets described by the operators $c_{1,k}$ and $c_{2,k}$) and include the explicit angle-dependence introduced by the matrix elements for the transformation between orbital and band basis. This transformation has the particularly simple form $c_{1,k} = d_{xz} \cos \theta_k - d_{yz} \sin \theta_k$, $c_{2,k} = d_{xz} \sin \theta_k + d_{yz} \cos \theta_k$ if one considers circular hole pockets and neglects the $d_{xy}$ orbital component on the electron pockets [42].

The feedback effect of the Ising-nematic order on the fermions takes place via the self-energy corrections involving the unequal susceptibilities of the primary SDW and iCDW fields at momenta $Q_1$ and $Q_2$. These corrections not only shift the chemical potentials of the $f_1$ and $f_2$ electron pockets in opposite directions $\langle f_{1,k}^\dagger f_{1,k} \rangle - \langle f_{2,k}^\dagger f_{2,k} \rangle \propto \langle \varphi \rangle$, but also give rise to a $d$-wave like distortion of the $c_1$ and $c_2$ hole pockets: $\langle c_{1,k}^\dagger c_{1,k} \rangle - \langle c_{2,k}^\dagger c_{2,k} \rangle \propto \langle \varphi \rangle \cos 2\theta_k$ (see Fig2). In the orbital basis, the latter corresponds to ferro-orbital order $\langle d_{xz}^\dagger d_{xz} \rangle - \langle d_{yz}^\dagger d_{yz} \rangle \propto \langle \varphi \rangle$ [42]. Note that besides the changes in the dispersions proportional to $\langle \varphi \rangle$, there is an overall shift of the chemical potential, symmetric for the two electron and the two hole pockets.

The behavior of hole pockets in the Ising-nematic scenario is consistent with the existing ARPES data that show a $d$-wave type elongation of one of the hole pockets, whereas the other hole pocket sinks below the Fermi level [15]. The behavior of the electron pockets in the 2-Fe Brillouin zone is also consistent with the splitting of the chemical potentials of the $f_1$ and $f_2$ fermions.

We also investigate how pressure affects the nematic transition temperature $T_s$. Within our approach, $T_s$ is defined by the condition $3\xi_s^2 + \xi_c^2 = 4\pi g$. Upon pressure, the Fermi pockets become bigger, and the Fermi energy increases. As a result iCDW becomes less competitive and $\xi_c$ decreases, while $\xi_s$ increases. The combination of these two opposite tendencies in general gives rise to a non-monotonic behavior of $T_s$. This is illustrated in Fig. 3 using a simple modeling in which $\xi_j^2 \approx T - T_J$, with $T_J$ denoting the bare transition temperatures for SDW and iCDW (see caption).

Note that in our analysis so far we considered $u_2(0) > 0$. If on the other hand this interaction is attractive, $u_2(0) < 0$, the iCDW phase is the leading instability, and the ground state manifold is $Z_2 \times Z_2$. In this case, the nematic and iCDW transitions are expected to be simultaneous [10]. Although at present no microscopic mechanism is known to give $u_2(0) < 0$ [24], this could be another possibility to explain the existence of nematic order without magnetic order in FeSe. Such an iCDW phase could be detected via its time-reversal symmetry breaking, which would be manifested in, e.g., $\mu$SR measurements. The phase diagram under pressure can be explained by assuming that under pressure $u_2$ would change sign and SDW would become the leading instability.

**Summary** In summary, we propose a natural extension of the Ising-nematic scenario to explain the puzzling nematic state observed in FeSe. Our scenario relies on the smallness of $E_F$ and explains the onset of nematic order far from magnetism due to the near degeneracy between the SDW channel and an iCDW charge-current density wave channel. This near-degeneracy could result in the nucleation of local iCDW order in the presence of point-like impurities, which favor iCDW against SDW order [42]. While these fluctuations cooperate with magnetic ones to break the tetragonal symmetry, they compete for long-range order and reduce both $T_N$ and the magnetic correlation length at the onset of nematic order. We argue that this Ising-nematic scenario can also explain the observed non-monotonic dependence of the nematic transition temperature $T_s$ upon pressure.

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