Effect of disorder on the competition between nematic and superconducting order in FeSe

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Abstract

Crystalline FeSe is known to display strong nematic order below a weak tetragonal-orthorhombic structural transition around $T_n \sim 90$ K, and a superconducting transition at $T_c \sim 9$ K. Recently, it was shown that electron irradiation, which creates pointlike potential scattering defects, has the surprising effect of enhancing $T_c$, while suppressing $T_n$. Here we discuss a possible scenario for such an effect, which postulates a competition between $s_{\pm}$ superconductivity and nematic order. The transition to the nematic state is modeled by a mean field theory of a $d$-wave Pomeranchuk instability, together with a Cooper pairing interaction in both one- and multiband models. The effect of nonmagnetic impurities on both orders is treated on equal footing within the Born approximation. We find evidence that disorder can indeed enhance $T_c$, while suppressing the competing nematic order, but only in a multiband situation. We discuss our results in the context of experimental data on FeSe crystals.

1. Introduction

Fe-based superconductors (FeSC) present a continuing challenge to the condensed matter physics community eight years after their discovery [1]. Pairing is thought to be electronic in nature, and originate from spin fluctuations, treated theoretically in various limits [2–4]. While many aspects of the superconducting state have been understood, the simplest material, FeSe, has proven to be one of the most elusive. It exhibits a tetragonal to orthorhombic structural phase transition at $T_n \sim 90$ K, and displays very strong electronic nematic behavior below this temperature ($T_n$), but never orders magnetically as do the more familiar Fe pnictide systems. While its critical temperature $T_c \sim 9$ K is low for this class of materials, a sharp increase of $T_c$ with a Cooper pairing interaction in both one- and multiband models. The effect of nonmagnetic impurities on both orders is treated on equal footing within the Born approximation. We find evidence that disorder can indeed enhance $T_c$, while suppressing the competing nematic order, but only in a multiband situation. We discuss our results in the context of experimental data on FeSe crystals.

The origin of the nematic order in FeSe has itself been the subject of considerable debate. In general the origin of strong nematic tendencies in the FeSC have been discussed in terms of a competition between fluctuations of structural, orbital, and spin degrees of freedom [10]. At first glance, the lack of long-range magnetic order in the ambient pressure phase diagram seems to suggest that the popular spin nematic scenario [11] might not be appropriate, and that orbital fluctuations might play a more important role [12, 13]. However, the confirmation of a long-range magnetic state under a modest pressure [14, 15] has lent support to other proposals that suggest that the ground state at ambient pressure may be a quantum paramagnetic state [16, 17] or a state with long-range magnetic order of ‘hidden’ quadrupolar type [18, 19]. The very small Fermi surfaces in this system may also be important to prevent long-range ordering [20].

Recently, a new experiment by Teknowijoyo et al [21] measuring $T_c$ and superfluid density $\rho_s$ in FeSe has appeared that may provide an important clue to this puzzle. The authors irradiated their sample with low-energy...
electrons, known to create homogeneously distributed Frenkel pairs of atomic vacancies and interstitials without doping the system [22]. This seems to be the best way to create pure potential disorder in these systems, where chemical substitutions have proven difficult to interpret [23]. In other Fe-based superconductors [24–26], $T_c$ has been strongly suppressed by disorder of this type, as compared to chemical substitution suppression rates. In FeSe, on the other hand, Teknowijoyo et al [21] found an increase of $T_c$ upon irradiation, and concomitant decrease of $T_s$. While these trends are similar to the effect of hydrostatic pressure, the authors argued first that irradiation tended to increase rather than decrease the lattice volume, and that the magnitudes of the changes in lattice constants were in any case an order of magnitude smaller than in pressure experiments. They speculated that impurities might introduce local pair strengthening effects due to the proximity of FeSe to a magnetic transition [27], or that the competition of superconductivity with nematic order might play a role.

An intriguing paradigm to enhance $T_c$ by disorder for an $s_\pm$ state in the presence of competing stripelike $(\pi, 0)$ magnetic order was offered by Fernandes et al [28], who pointed out that both interband and intraband impurity scattering processes would suppress magnetism, while only interband processes would break superconducting pairs. Whether a competition of superconductivity with nematic order can similarly lead to a $T_c$ enhancement is not a priori obvious, given that nematic order is a $q = 0$ distortion of the Fermi surface. In addition, since the gap function in FeSe is known to be highly anisotropic [2], superconductivity will be suppressed by both types of scattering processes, independent of any sign change over the Fermi surface. From these perspectives, the $T_c$ enhancement mechanism of [28] should be irrelevant.

In this paper, we provide a concrete framework for the study of the effect of impurities on the competition between nematic and superconducting order. We first assume that that nematic order may be modeled by a $d$-wave Pomeranchuk instability competing with superconductivity. Such an instability has been argued to qualitatively describe the nematic tendencies of both cuprate [29–31] and Fe-based superconductors [10, 32, 33]. We show here that the nematic order (Pomeranchuk instability) temperature, which we identify with $T_s$, is suppressed naturally by disorder, as found by earlier authors [34]. In addition, however, we find that $T_s$ can actually be enhanced when the nematic order is weakened. Whether $T_c$ is enhanced or suppressed by disorder turns out to depend in a nontrivial way on the interplay of the anisotropy of the superconducting pairing interaction with that of the nematic distortion of the Fermi surface.

We now introduce the mean field treatment of a $d$-wave Pomeranchuk distortion, first within a single band model for pedagogical purposes, and then generalized to multiband Fermi surfaces appropriate to the FeSC. Disorder is then treated in the Born approximation, and the instability temperatures of both nematic and superconducting transitions calculated, for the different model Fermi surfaces, and for different types of anisotropic $s$-wave superconductivity. We present full phase diagrams of superconductivity and nematic order as functions of disorder and temperature, and discuss the comparison with experiment.

2. 1-Band model

2.1. Interplay of superconducting and nematic order

We wish to work with the simplest possible model capturing the competition of superconductivity and nematic order, and allowing for the introduction of the effects of nonmagnetic disorder. We begin therefore with a Hamiltonian describing fermions with an interaction which leads to a Pomeranchuk instability [30],

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{int}},$$

where $\mathcal{H}_0$ describes a noninteracting parabolic band of electrons,

$$\mathcal{H}_0 = \sum_{k} (k^2/(2m) - \mu) c_{k}^\dagger c_k,$$

and

$$\mathcal{H}_{\text{int}} = \frac{V_{\text{nem}}}{4} \sum_{k,k',\sigma\sigma'} (d_k d_{k'}) c_{k\sigma}^\dagger c_{k'\sigma}^\dagger c_{k'\sigma'} c_{k\sigma'}.$$ (1)

where $d_k = \cos 2\phi k, \mu$ is the chemical potential and $\phi$ is the angle around the Fermi surface. In the second line we have made a mean field approximation [30] and defined

$$\Phi_k \equiv \Phi_0 d_k = d_k \sum_{k'} \langle d_{k'} c_{k'\sigma}^\dagger d_{k\sigma} \rangle,$$

which leads to a self-consistency equation for the nematic order parameter

$$\Phi_k = -T d_k \sum_{k', \sigma} \frac{V_{\text{nem}} d_{k'}^\dagger (i \omega_n - \xi_{k'} - \Phi_k)}{\omega_n^2 + (\xi_{k'} + \Phi_k)^2}. $$ (2)

The nematic transition temperature when $\Phi_k \to 0$, $T_{\text{nem}}$, is then given by

$$T_{\text{nem}} = \frac{\mu}{2 \tanh^{-1} (4 \lambda_{\text{nem}}^-)},$$ (3)

where $\lambda_{\text{nem}}^- = m V_{\text{nem}}/2\pi$. It is worth noting that the nematic instability is of the Stoner type: unless $V_{\text{nem}}$ is larger than a threshold value, long range nematic order is not possible.
Next, we study superconductivity in the nematic phase, and show that the interplay of nematicity and superconductivity depends sensitively on the structure of the superconducting pairing. We consider a simple model of a $C_2$-symmetric gap, $\Delta = \Delta_0 (1 + r \cos 2\phi) / \sqrt{1 + r^2} \equiv \Delta_0 \mathcal{Y}(\phi)$, where $\mathcal{Y}(\phi)$ is normalized to 1 over the high temperature Fermi surface.

To study the interplay of such states with nematic order, we introduce the anisotropic pair potential $\mathcal{V}(\phi) \delta_{\mathbf{k}\mathbf{k}'}$ on the Fermi surface, and for the moment assume it to be independent of nematic changes in the Fermi surface itself. The linearized gap equation in the presence of nematic order, $\mathcal{F}_{\phi\phi} > 0$, may then be expressed as

$$1 = 2\pi T_0 \lambda_{\text{nc}} \sum_{\omega_n > 0} \int_0^{2\pi} \frac{d\phi}{2\pi} \mathcal{Y}^2(\phi) \mathcal{P}(\phi, \omega_n),$$

$$\mathcal{P}(\phi, \omega_n) = \frac{1}{\omega_n} \left[ \frac{1}{2} + \frac{1}{\pi} \tan^{-1} \left( \frac{\mu - \Phi_0}{\omega_n} \right) \right].$$

Here the pair bubble $\mathcal{P}(\phi, \omega_n)$ makes the maximum contribution along the long direction ($\phi = \pi/2$) of the deformed Fermi surface. If the minimum of the absolute value of gap function is also along this direction (i.e. $r > 0$), then the deformed Fermi surface will suppress such gap states.

We can approximate the effect of nematic order on $T_c$ in the limit of weak deformation of the Fermi surface ($\Phi_0 \ll \mu$),

$$\log \left( \frac{T_{c0}^{\text{nem}}}{T_{c0}} \right) \approx -\frac{\pi r}{2 + r^2} \frac{\Phi_0}{2 \mu}.$$ 

Here $T_{c0}^{\text{nem}}$ ($T_{c0}$) is the superconducting transition temperature in the nematic (tetragonal) phase with no disorder. As expected from the structure of $\mathcal{P}$, the critical temperature $T_c$ depends on the structure of the pairing through the model anisotropy parameter $r$, and can apparently increase or decrease depending on how the anisotropy is oriented with respect to the distorted $C_2$ Fermi surface. When the Fermi surface gets stretched along the direction of gap minima ($r > 0$, figure 1) $T_c$ is suppressed. In contrast, gap minima oriented perpendicularly to the stretched Fermi surface ($r < 0$, figure 1) lead to an increase of $T_c$, since $\mathcal{P}(\phi)$ and $\Delta(\phi)$ have maxima on the same regions of the Fermi surface. This is similar to superconductivity in the presence of spin-density wave order, where gap maxima away from the nesting hot spots is favorable [35].

We note the important role of particle-hole asymmetry for this problem. As seen explicitly from equation (5), in the limit of perfect particle-hole symmetry ($\mu \to \infty$), the coupling between superconducting and nematic order vanishes. Furthermore, the sign of the nematic distortion depends on the sign of $\mu$: thus if one replaces the electron band assumed above with a hole band, the effect will be identical, except that $T_c$ will now be suppressed for $r < 0$. The relative orientation of the gap states described above remains unchanged, however: $T_c$ is suppressed relative to $T_{c0}$ if gap minima are along the stretched direction.

These discussions assume that the nematic/superconducting coexistence solutions discussed above are ground states for the given parameters. However, an examination of the free energy (see appendix) shows that

![Figure 1. Schematic Fermi surface at $T = T_{nem}$ (dashed black curve) and $T = T_{nem}/2$ (solid black), with momentum angle $\phi$ indicated. Superconducting gap with anisotropy given by $r > 0$ (blue) and same with $r < 0$ (red).](image)
those superconducting states with gap minima along the nematic elongation of the Fermi surface are higher energy than the homogeneous nematic state, and are therefore unstable, as illustrated in Figure 2.

### 2.2. Effect of disorder

We first determine the nematic order parameter in the presence of nonmagnetic disorder above $T_c$ by defining a self-energy within the Born approximation,

$$\Sigma_{\text{nem}}(\omega) = n_{\text{imp}} |V_{\text{imp}}|^2 \sum_k G(k', \omega_n),$$

where $n_{\text{imp}}$ is the concentration of impurities with potential $V_{\text{imp}}$, and $G(k, \omega) = (i\omega - \xi_k - \Phi_k + i0^+)^{-1}$ at $T_{\text{nem}}$ and $i\bar{\omega} = i\omega - \Sigma_{\text{nem}}(\omega)$. This renormalizes the single-particle energy and influences the nematic order through its self-consistency equation. Due to the $d$-wave Pomeranchuk form, the $\Phi_k$ itself is not renormalized in this approximation.

To study superconductivity within the same framework, we introduce the disorder self-energy in Nambu space in the same approximation,

$$\hat{\Sigma}(\omega_n) = n_{\text{imp}} |V_{\text{imp}}|^2 \sum_k \hat{G}(k', \omega_n) \equiv \sum_{\alpha=0,3} \sum_{\alpha'} \hat{\tau}_{\alpha\alpha'},$$

where $\hat{G}$ is the Nambu Green’s function

$$\hat{G}(k, \omega_n) = \frac{i\bar{\omega}_n\tau_0 + (\xi_k + \Phi_k)\tau_3 + \hat{\Delta}_k\tau_1}{\hat{\Delta}_n^2 + (\xi_k + \Phi_k)^2 + \hat{\Delta}_k^2}.$$  

Here the renormalized order parameter has the form $\hat{\Delta}_k \equiv \Delta_{\text{iso}} + \Delta_{\text{ani}} d_k$, and we have defined

$$i\bar{\omega}_n = i\omega_n - \Sigma_{\text{nem}}(\omega_n),$$

$$\Delta_{\text{iso}} = \Delta_0/\sqrt{1 + \gamma^2/2} + \Sigma_{\text{iso}}(\omega_n),$$

$$\Delta_{\text{ani}} = \Delta_0\gamma/\sqrt{1 + \gamma^2/2}.$$  

Note that the nematic order parameter $\Phi_k$ and anisotropic gap component $\Delta_{\text{ani}}$ are unrenormalized by disorder.

At $T_c$, the self-consistency expressions for the amplitude of the $d$-wave nematic order parameter $\Phi_0$ and the superconducting order parameter $\Delta_0$ are given by

$$\Phi_0 = -T \sum_{\omega_n k} V_{\text{imp}} d_k (i\bar{\omega}_n - \xi_k - \Phi_k) \over \hat{\Delta}_n^2 + (\xi_k + \Phi_k)^2,$$

where $V_{\text{imp}}$ is the interaction strength between the impurity and the electron, and $\xi_k$ is the single-particle energy. The self-energy $\Sigma_{\text{nem}}(\omega)$ is calculated as $\sum_k G(k', \omega_n)$, and $\hat{G}(k, \omega_n)$ is the Nambu Green’s function.
Figure 3 now shows the result of a numerical evaluation of equations (13) and (14). As expected, disorder gradually suppresses the nematic order as also found in [34]. From the inset in figure 2, we can anticipate that the $r < 0$ case, which shows no competition, should lead to a $T_c$ suppression with disorder, as indeed shown in figure 3. For a small suppression of $T_{nem}$, $T_c$ appears to increase when $r > 0$, i.e. when the gap minima are along the elongated direction of Fermi surface. However, as shown in figure 2, such a pairing state is a metastable state. Thus disorder-induced $T_c$ enhancement appears to be disfavored in this one band model.

3. Three-band model

We now investigate whether the basic notions which govern the effect of disorder on $T_c$, $T_{nem}$ in the one-band case continue to hold in a somewhat more realistic multiband framework appropriate for the FeSe system that motivated this study, and ask whether a disorder-driven $T_c$ enhancement is possible as a consequence of multiband physics. Unlike its monolayer and intercalate cousins, bulk FeSe has well-established Fermi surface hole pockets at $\Gamma$ and electron pockets at $X$ and $Y$, as modeled in figure 4(a) in the 1-Fe zone. Although many phenomenological assumptions for the forms of the interactions on these three bands are possible, we assume for simplicity the same Pomeranchuk harmonic for the nematic instability on all bands, leading to the distorted Fermi surface pockets also plotted in the figure. We further adopt various simple forms of the BCS pairing interaction on all three bands, including pairing anisotropy on one band or the other, as also illustrated in figures 4(b)–(f). Because we operate without a microscopic theory, we have considerable freedom to choose gap structures consistent with $C_2$ symmetry in the nematic phase. We therefore consider anisotropy on the hole and the electron pockets independently, although in reality all will distort simultaneously. Note that all order parameters on all bands are determined self-consistently. Our goal is simply to demonstrate that a $T_c$ enhancement with disorder due to competition with nematic order is possible, and deduce what qualitative conclusions we can from that novel situation.

3.1. Electronic structure and pairing interaction

The Hamiltonian for this three band model is

$$\mathcal{H} = \sum_{\mathbf{k},\mathbf{l},\sigma} \left[ (\xi_{\mathbf{k},\sigma} + \Phi_{\mathbf{k},\sigma}) c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma} + (\Delta_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{l},-\sigma} + \text{h.c.}) \right],$$

$$= \sum_{\mathbf{k}} |\Psi_\mathbf{k}\rangle H_\mathbf{k} |\Psi_\mathbf{k}\rangle,$$

where $c_{\mathbf{k},\sigma}^\dagger$, $c_{\mathbf{k},\sigma}$ creates (annihilates) a fermion with momentum $\mathbf{k}$ and spin $\sigma$ in the $i$th band. $\Psi$ is an extended Nambu basis for three bands, $\Psi = (e_{-k,1}^\dagger, e_{k,1}^\dagger, e_{-k,2}^\dagger, e_{k,2}^\dagger, e_{-k,3}^\dagger, e_{k,3}^\dagger)$. The fermionic dispersions in the $C_4$ symmetric phase are

$$\Delta_n = -7\sum_{\mathbf{k}} \frac{V^2}{\omega_n^2} \frac{1}{\Delta_n^2}(\xi^2 - \Phi^2) \Delta^2.$$
We assume a circular hole pocket and slightly elliptic electron pockets with $\varepsilon = 0.6$.

The nematic and superconducting order parameters are taken to be $F = F_{nem}$ and $f_{D} = D \phi_{nem}$, respectively. The multiband self-consistency equations for the nematic and SC orders analogous to equations (13)–(14) are then obtained as

$$\xi_{\text{nem}} = \mu_{\text{h}} - \frac{k_{2}^{2}}{2m}, \quad \xi_{\text{c1}} = \frac{k_{2}^{2}}{2m(1 + \varepsilon)} + \frac{k_{y}^{2}}{2m(1 - \varepsilon)} - \mu_{c}, \quad \xi_{\text{c2}} = \frac{k_{2}^{2}}{2m(1 - \varepsilon)} + \frac{k_{y}^{2}}{2m(1 + \varepsilon)} - \mu_{c}.$$

We assume a circular hole pocket and slightly elliptic electron pockets with $\varepsilon = 0.6$.

The nematic and superconducting order parameters are taken to be $F_{\text{nem}} = \Phi_{i} d_{k_{i}}$ and $\Delta_{k_{i}} = \Delta_{i} \chi_{i}(\phi_{i})$, respectively. The multiband self-consistency equations for the nematic and SC orders analogous to equations (13)–(14) are then obtained as

$$\Phi_{i} = - T \sum_{\omega_{v}, k} V_{\text{nem}} d_{k_{i}} (\chi_{j} - \xi_{k_{i}} - \Phi_{k_{i}}), \quad \Delta_{k_{i}} = - T \sum_{\omega_{v}, k} \frac{V_{\text{sc}} \chi_{i}(\phi_{i}) \chi_{j}(\phi_{j}) D_{k_{i}}}{\omega_{v}^{2} + (\xi_{k_{i}} + \Phi_{k_{i}})^{2}}.$$

Here $\omega_{v}$ is the fermionic Matsubara frequency at temperature $T$, and $\chi_{i} = (1 + r_{i} \cos 2\phi_{i}) \sqrt{1 + r_{i}^{2}/2}$, where the parameter $r_{i}$ controls the anisotropy of the SC order.
Note that while \( f \) is always measured with respect to the positive \( x \) axis at each pocket, \( r_{ei} \) will now be assumed to have same sign on pockets \( e_1 \) and \( e_2 \), such that an overall \( C_2 \) state is realized. Two possible such choices are illustrated in figures 4(e) and (f).

We use a separable form of interactions for the nematic (V
\text{^nem}_{ij} d_k \cdot d_{k'}) and the SC order (V
\text{^sc}_{ij} \mathcal{Y}_1(\phi_i) \mathcal{Y}_2(\phi_j))

















where summation over the repeated indices is implied. In equation (21), disorder-renormalized quantities are given as multiband generalizations of equations (22)–(24)

\[
\hat{\Sigma}_{ij}^{\text{iso}} = \Delta_0^{\text{iso}} \sqrt{1 + \frac{\tau_i^2}{\tau_j^2}} + \Sigma_{ij}(\omega_n),
\]

\[
\Delta_{ij}^{\text{int}} = \Delta_0^{\text{int}} \sqrt{1 + \frac{\tau_i^2}{\tau_j^2}}.
\]

Note that the Nambu components of the disorder self-energy

\[
\Sigma_{0j}(\omega_n) = n_{\text{imp}} \sum_{j,k} |u_{ij}|^2 \mathcal{G}_{0j}(\mathbf{k}_j, \omega_n),
\]

\[
\Sigma_{ij}(\omega_n) = -n_{\text{imp}} \sum_{j,k} |u_{ij}|^2 \mathcal{G}_{ij}(\mathbf{k}_j, \omega_n),
\]

involve both intra- and interband scattering processes via the impurity scattering potential matrix in the band basis \( u_{ij} \), which is taken to have only two elements: \( \nu \) for intra- and \( \upsilon \) for interband scattering, for all band components, with \( \eta \equiv \upsilon/\nu \). Here \( \mathcal{G}_{0j}(\mathbf{k}_j, \omega_n) \) is the \( 0\text{th}(1\text{st}) \) component of the \( j \text{th} \) band’s Nambu Green’s function and \( \Delta_{ij}^{\text{iso}} \) is the isotropic component of the gap function for \( j \text{th} \) band. Note that we ignore the \( \tau_3 \) component of the impurity self-energy, which mainly renormalizes the chemical potential.

It is now relatively easy to arrange for nematic order and superconductivity to compete, without fine tuning of the interactions. Bulk FeSe itself is known to have an order parameter that is highly anisotropic, with nodes or near-nodes somewhere on the Fermi surface [2]. We therefore focus particularly on cases with large gap anisotropy, either on the hole pocket (figures 4(c) and (d)) or on the electron pockets (figures 4(e) and (f)).

Note we only consider \( s_\pm \) type pairing states, with overall sign change between electron and hole pockets. However, our conclusions are mostly qualitatively valid for \( s_+ \) states as well, since minimal pairbreaking is required to obtain a \( T_c \) enhancement in an \( s_\pm \) state, and we therefore are forced to assume relatively weak interband scattering, such that the sign difference does not play an essential role.

### 3.2. Results

We first focus on the effect of disorder on the pure nematic state. Both interband and intraband scattering suppress the nematic order in the current model, as shown in the inset to figure 5, which displays the variation of \( T_{\text{nem}} \) with increasing impurity concentration. As the interband scattering increases, nematicity goes down rapidly; since interband scattering connects Fermi surfaces with different signs of \( \Phi_k \), this is equivalent to the effect seen for the one-band case in [34].

The relative effects of interband impurity scattering obviously depends on the gap structure, i.e. whether a sign changing state is realized. Evidence for sign changing gap behavior in this system is limited, and

![Figure 5. Suppression of nematic order by disorder in 3-band model.](image-url)
reviewed in [2]. The most significant is probably the recent experiment by Wang et al [36], who observed a \( q = (\pi, 0) \) low-energy inelastic neutron scattering resonance very similar to that generally taken as strong evidence for the \( s_\pm \) state in other Fe-based superconductors [37]. Earlier, STM [38] and some thermal conductivity and penetration depth measurements [39] had reported a gap with nodes. More recently, and possibly on slightly different samples, a gap with very deep minima has been suggested to be consistent with STM [40], penetration depth [21, 41], and low temperature thermal conductivity measurements [42] as well. For our purposes, such tiny differences in gap structure are probably irrelevant, assuming that the nodes are accidental.

The superconducting transition temperature \( T_c \) in the presence of disorder and nematicity is now determined by solving the multiband linearized gap equation, (21), which contains the nematic order parameter \( \Phi_n \), itself determined by equation (20). We first examine the simplest case, \( r_h = 0 \) on all bands, i.e. an isotropic gap in the presence of the nematically distorted Fermi surfaces. The isotropic state in the presence of a single nematic pocket was not a stable solution for the nematic distortion chosen. However, in the presence of the electron pockets and an interband interaction, an isotropic state in the presence of nematic order can be lower in energy than the pure nematic one, as seen in figure 6(a). The competition of the two order parameters is shown explicitly in figure 6(b) and in fact is seen to lead to a modest \( T_c \) enhancement with disorder as seen in figures 6(c) and (d). This effect may now be enhanced somewhat by considering nonzero \( \eta_n \). Note that these effects, while roughly consistent in magnitude with the \( T_c \) enhancement effect seen in experiment, will be suppressed in an \( s_\pm \) state by any additional source of pairbreaking, e.g. as when the interband scattering rate is increased (figure 6(d)).

Note that within the current model the ability of the hole band gap anisotropy to enhance \( T_c \) further is limited by the narrow range of stability of this state (see figures 6(a)–(c)). It is interesting therefore to explore the role of gap anisotropy on the electron pockets, which we illustrate in figure 7. In panels (a) and (c), the range of stability of a state which enhances \( T_c \) with disorder is found to be much wider than in the hole pocket case. In addition, this range is asymmetric with respect to the anisotropy parameter \( r_h \), indicating that it is more likely to observe \( T_c \) enhancement if \( r_h > 0 \), i.e. if the gap minima on the most nematically distorted pockets are aligned with the pocket elongation axis (figure 4).

4. Discussion

The motivation for this study has been a recent low-energy electron irradiation experiment by Teknowijoyo et al [21], which found a surprising enhancement of \( T_c \) with increasing disorder in FeSe, a system with no long-range magnetic order but strong nematic order below the structural transition. It is worth noting that until now, all
other Fe-based superconductors similarly irradiated have had their critical temperatures strongly suppressed by this type of disorder, which should create nearly ideal pointlike potential scatterers. This striking result raises several questions about the interplay of superconductivity and nematicity, and may provide an important clue to the physics of the mysterious FeSe material.

The experimental situation with regard to competition of superconductivity and nematic order, required for our scenario, is currently unclear. In several situations, including hydrostatic pressure \cite{5, 6} and doping by sulfur or field gating \cite{43, 44}, $T_n$ decreases while $T_c$ increases, implying competition of the two orders. However, Böhmer et al reported seeing no direct effect of the onset of superconductivity on the orthorhombic order parameter in FeSe crystals \cite{12}, and recently, Wang et al \cite{45} presented clear evidence that the orthorhombic distortion was enhanced by the occurrence of superconductivity in S-doped FeSe crystals. This suggests that the interplay between the two orders may be more subtle than assumed here. If our approach is qualitatively correct, however, it implies that disorder-induced $T_c$ enhancement of the type reported in \cite{21} and discussed here should disappear in the S-doped systems.

Clearly one aspect of the simple model presented here is unphysical, namely that the pairing interaction assumed is ‘rigid’, in the sense that as the Fermi surface deformed as $T_c$ is lowered, our model does not capture the concomitant evolution of the pairing interaction before $T_c$ is reached (it does treat the anisotropy of the gap in the presence of a distorted Fermi surface self-consistently). It seems therefore possible that our model overestimates competition of superconductivity, and nematicity and therefore artificially favors $T_c$ enhancement when nematicity is suppressed. A more complete microscopic treatment of the effect of nematic order on pairing is outside the scope of present manuscript and will be treated elsewhere.

5. Conclusions

In summary, we have studied the interplay between nematicity and superconductivity for a system with one band and three bands, modeling the the nematic instability with a mean field treatment of a $d$-wave Pomeranchuk transition. We have shown that in several physically plausible circumstances, nematic order competes with superconductivity, and may allow $T_c$ to rise, as observed in \cite{21}, when disorder suppresses nematicity. Indeed, such an enhancement appears rather natural in the presence of sufficiently strong

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**Figure 7.** Results for 3-band model with anisotropy on electron band only, $\Delta \sim (1 + r_c \cos 2\phi)$. (a) Free energy of nematic superconductor relative to pure nematic state versus $r_c$. (b) Order parameter (green, red line) for $r_d = 0$, $r_c = 0.5$ plotted over nematically distorted Fermi surface. (c) $T_c$ normalized to $T_{c,0}$ for pure system versus anisotropy parameter $r_d$ for two different disorder concentrations, corresponding to suppressions of $T_{c,0}$ by 5 and 10%. Blue shaded region in panels (a) and (c) indicates region of thermodynamic stability of coexistence phase. (d) $T_c/T_{c,0}$ versus disorder scattering rate $\Gamma$ for $r_d = 0.5$ with gap for inter/intraband scattering potential ratio $\eta = u/v = 0, 0.1$. 

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nematicity. We note that the effect is qualitatively different from a $T_c$ enhancement resulting from the competition between superconductivity and antiferromagnetism discussed by earlier authors.

We have further discussed how the $T_c$ enhancement effect is sensitive to the degree and orientation of the gap anisotropy with respect to the deformed Fermi surface. In particular, we showed that superconducting gaps with minima along the stretched axis of the deformed Fermi surface are easily suppressed by nematic order. Upon introduction of disorder, which rapidly destroys nematic order, such states show significant $T_c$ enhancement. In the one-band case, these states do not appear to be thermodynamically stable, but they are stabilized by the addition of additional pockets, as in the three-band model studied here. In contrast, SC states with gap maxima along the stretched direction of Fermi surface, do not compete strongly with nematic order, so $T_c$ of an $s_\pm$ state is suppressed as usual by disorder.

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Appendix. Free energy

Here we calculate the free energy of our system including mean field treatments of nematic and superconducting order. In general, the free energy is given by

$$\mathcal{F} = \langle \mathcal{H} \rangle - TS,$$

where the entropy $S$ is

$$S = -2 \sum_k \left[ f(E_k) \log E_k + (1 - f(E_k)) \log (1 - f(E_k)) \right].$$

Here $E_k = \sqrt{(\xi_k + \Phi_k)^2 + \Delta_k^2}$, $f$ is the Fermi function. The first term in equation (A1) is the expectation value of the mean field Hamiltonian, which can be evaluated using coherence factors

$$u_k^2 = \frac{1}{2} \left[ 1 + \frac{\xi_k + \Phi_k}{E_k} \right],$$

$$v_k^2 = \frac{1}{2} \left[ 1 - \frac{\xi_k + \Phi_k}{E_k} \right].$$

For the one band case, the expectation value of the kinetic energy may be written as

$$\langle \mathcal{H}_{\text{kin}} \rangle = \left\langle \sum_{k,\sigma} \tilde{\xi}_k \sigma^+_{k,\sigma} \sigma_{k,\sigma} \right\rangle$$

$$= \sum_{k,\sigma} \left( 1 - \tanh \left( \frac{E_k}{2T} \right) \right) \tilde{\xi}_k \sigma,$$

where $\tilde{\xi}_k = \xi_k + \Phi_k$. The potential energy term for the one band case is

$$\langle \mathcal{H}_{\text{pot}} \rangle = -\frac{\Phi_k^2}{V_{\text{nem}}} - \frac{\Delta_0^2}{|V_{\text{cl}}|},$$

and for three bands

$$\langle \mathcal{H}_{\text{pot}} \rangle = -\frac{2\phi_h (\Phi_{\text{cl}} + \Phi_{\text{tl}})}{V_{\text{nem}}} + \frac{\Delta_0 (\Delta_{\text{cl}} + \Delta_{\text{tl}})}{|V_{\text{cl}}|}.$$
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