Emergent defect states as a source of resistivity anisotropy in the nematic phase of iron pnictides

Maria N. Gastiasoro¹, I. Paul², Y. Wang³, P. J. Hirschfeld³, and Brian M. Andersen¹
¹Niels Bohr Institute, University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen, Denmark
²Laboratoire Matériaux et Phénomènes Quantiques (UMR 7162 CNRS), Université Paris Diderot-Paris 7, Bat. Condorcet, 75205 Paris Cedex 13, France
³Department of Physics, University of Florida, Gainesville, Florida 32611, USA
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We consider the role of potential scatterers in the nematic phase of Fe-based superconductors above the transition temperature to the (π,0) magnetic state but below the orthorhombic structural transition. The anisotropic spin fluctuations in this region can be frozen by disorder, to create elongated magnetic droplets whose anisotropy grows as the magnetic transition is approached. Such states act as strong anisotropic defect potentials which scatter with much higher probability perpendicular to their length than parallel, although the actual crystal symmetry breaking is tiny. We calculate the scattering potentials, relaxation rates, and conductivity in this region, and show that such emergent defect states are essential for the transport anisotropy observed in experiments.

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The origin of electronic nematic behavior, i.e. spontaneous breaking of discrete rotational symmetry preserving translational symmetry, is one of the most fascinating questions in the field of Fe-based superconductivity, involving the interplay of magnetic, orbital, and ionic fluctuations. Strong in-plane anisotropy has been reported in transport[1–7], angular resolved photoemission (ARPES)[8], neutron scattering[9], optical spectroscopy[10,11], Andreev point contact[12] and torque magnetometry[13] measurements. Since the various fluctuation channels in these multiband systems all couple to one another below the tetragonal to orthorhombic structural transition that occurs at T_s in many systems, all response functions become anisotropic and it is not easy to decide which fluctuations drive the ordering nematic phenomena observed. Theoretically, both spin nematic and orbital scenarios have been proposed.[14]

In systems with large spin nematic susceptibility, strong anisotropy is expected in the spin fluctuations in the orthorhombic phase below T_s, even if the structural anisotropy is small. Such anisotropy will certainly influence transport properties; this is the basis of theories of transport by several groups[15–17], arguing that at T_s, the magnetic correlation length becomes anisotropic and drives the anisotropy in the electronic inelastic scattering rate. Disorder is described entirely through a momentum-independent scattering rate and is required only to short-circuit “cold spots” on the Fermi surface.

In the present work, the transport anisotropy of the nematic phase is also explained via spin fluctuation anisotropy, but through the generation of strongly anisotropic impurity states. Our work is motivated by the observation by many STM experiments of C_4 symmetry breaking around point defects locally[18–24]; these experiments can exhibit effects that are missed by average bulk probes. In fact, in some systems evidence for nematic symmetry breaking in the form of highly anisotropic C_2 defect states is seen in the nominally tetragonal phase above T_s.[24] These responses are generally attributed to residual local strains which break C_4 symmetry locally, together with a large residual nematic susceptibility.[25] In the ordered stripe (π,0) magnetic phase below the Néel temperature T_N in many of the parent and underdoped materials, the C_4 symmetry is broken by the magnetism itself. Nevertheless the symmetry breaking of the electronic structure around local Co defects in lightly doped Ca122 was observed to be so enhanced that this result was cited as the first evidence for a strong nematic tendency in these systems[18]. In addition, it was suggested in Ref.[23] that such “nematogen” defects could be responsible for the transport anisotropy.

Recently, we examined the microscopic origin of nematic defect states in the ordered phase, and proposed that they result from the effect of a nonmagnetic impurity on the energy balance between two magnetic phases, the (π,0) stripe ground state and a nearby (π, π) competing Néel state[26]. The relative stability of the latter at hole doping leads to an elongated dimer-like structure in both charge distribution and low-energy local density of states (LDOS) in agreement with experiments[18,23]. C_4-broken impurity states were discussed earlier in the context of localized spin models[27] and pinned fluctuating orbital order[28], but in neither cases was the dimer-like structure seen in experiment reported.

The emergent nematogen defect states found in Ref.[26] become C_4 symmetric above T_N in the tetragonal phase. Yet transport anisotropy experiments in Ba122 exhibit significant anisotropy also in the “nematic phase” T_N < T < T_s where there is no long-range magnetic stripe order, or in the tetragonal phase in the presence
It is not clear, however, whether nematogens can form around point-like impurities in this phase, i.e. whether the anisotropic spin fluctuations in a spin-nematic scenario can condense around a defect to give a similar transport anisotropy in this case.

There are several key aspects of the transport experiments\cite{11,17} above \(T_N\) that any theory needs to account for: 1) the counterintuitive sign of the resistivity anisotropy on the electron-doped side, where \(\rho_0 > \rho_a\) although \(b < a\); 2) the possible sign change but also significant decrease of the anisotropy on the hole-doped side\cite{5}; 3) the decrease of the anisotropy upon annealing\cite{6}; 4) the pronounced increase in \(\rho\) on the hole-doped side\cite{5}; and 5) the decrease in \(\rho\) for the impurities alone are able to account for only some of these salient features, and that including the role of emergent defect states in these correlated systems provides a more natural explanation for the observations.

In this work, we discuss first the growth of anisotropic spin fluctuations in the nematic phase as \(T_N\) is approached from above. We extend the theory of impurity-induced emergent defect states into the nematic phase with an unbiased microscopic calculation of the local electronic structure near a point-like nonmagnetic impurity potential in a situation where the \(C_4\) symmetry of the host bands has been broken very slightly below \(T\). This gives rise to the same anisotropic spin fluctuations considered as the source of transport anisotropy by the authors of Refs.\cite{14,17}, but impurities play a very different and essential role. We find that the impurity state in the nematic phase is strongly anisotropic due to the enhanced background nematic response arising from electronic correlations.\cite{24} Specifically, we calculate the momentum-dependent effective impurity potential, scattering rate, and conductivity in the nematic phase.

The Hamiltonian is given by

\[
\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{oo} + \mathcal{H}_{int} + \mathcal{H}_{imp},
\]

where \(\mathcal{H}_0\) denotes the kinetic energy

\[
\mathcal{H}_0 = \sum_{ij, \mu, \sigma} t_{ij}^{\mu \nu} c_{i\mu \sigma}^\dagger c_{j\nu \sigma} - \mu_0 \sum_{i} n_{i\sigma},
\]

with tight-binding parameters adopted from Ref.\cite{30} Here, \(i\) and \(j\) denote lattice sites, \(\sigma\) the spin, and \(\mu_0\) is the chemical potential that sets the doping level \(x = 0\). The indices \(\mu\) and \(\nu\) are the five iron \(d\) orbitals. \(\mathcal{H}_{oo}\) is mimics the orthorhombicity of the band below \(T_{N^0}\), for a non-zero \(\delta\) orbital order parameter. We have also studied \(C_2\) symmetric bands arising from hopping anisotropy and found similar results to those reported below. The third term in Eq.\cite{1} describes the Hubbard-Hund interaction

\[
\mathcal{H}_{int} = U \sum_{i, \mu} n_{i\mu \uparrow} n_{i\mu \downarrow} + (U' - J/2) \sum_{i, \mu < \nu, \sigma} n_{i\mu \sigma} n_{i\nu \sigma},
\]

\[
-2J \sum_{i, \mu < \nu} \hat{S}_{i\mu} \cdot \hat{S}_{i\nu} + J' \sum_{i, \mu < \nu} c_{i\mu \sigma}^\dagger c_{i\nu \sigma} c_{i\nu \sigma},
\]

including the intraorbital (interorbital) on-site repulsion \(U (U')\), the Hund’s coupling \(J\) and the pair hopping energy \(J'\). We assume \(U' = U - 2J\) and \(J' = J\) and fix \(U = 1.0\) eV and \(J = U/4\). Finally, \(\mathcal{H}_{imp} = V_{imp} \sum_{\mu} c_{i\mu \sigma}^\dagger c_{i\mu \sigma}^\dagger c_{i\mu \sigma} c_{i\mu \sigma}\) is the impurity potential, adding a potential \(V_{imp} = 1.5\) eV at the impurity site \(i^*\). We neglect the orbital dependence of the impurity potential for simplicity. After mean-field decoupling of Eq.\cite{3} we solve the following eigenvalue problem \(\sum_{\nu} H_{\nu\sigma} n_{i\nu \sigma} = E_{n\sigma} n_{i\mu \sigma}\), where

\[
H_{\nu\sigma} = t_{ij}^{\mu \nu} + \delta_{ij} \mu_{\nu} - \mu_0 + \delta(\delta_{\mu \nu \sigma} - \delta_{\mu \sigma \nu}) + \delta_{i\nu} V_{imp}
+ U(n_{i\mu \sigma}) + \sum_{\mu' \neq \mu} (U'(n_{i\mu' \sigma}) + (U' - J)(n_{i\mu' \sigma})),
\]

on a \(30 \times 30\) lattice with self-consistently obtained densities \(\langle n_{i\mu \sigma} \rangle = \sum_{n} \left| u_{i\mu \sigma}^n \right|^2 f(E_{n\sigma})\) for each site and orbital.

In the homogeneous orthorhombic “nematic” phase above \(T_N\), the important effect of the \(xz-yz\) orbital splitting is to enhance (diminish) the spin susceptibility at \(Q_1 \equiv (\pi, 0)\) (\(Q_2 \equiv (0, \pi)\)) as shown in Fig.\cite{1} for two cases with \(\delta_1 = 16\) meV (\(T_{N^0}^1\)) and \(\delta_2 = 80\) meV (\(T_{N^0}^2\)). The enhanced susceptibility at \(Q_1 \equiv (\pi, 0)\) pushes \(T_N\)

![FIG. 1. (Color online) Real part of the homogeneous RPA spin susceptibility \(\chi_{RPA}(q, 0)\) at \(Q_1 \equiv (\pi, 0)\) (red curves) and \(Q_2 \equiv (0, \pi)\) (blue curves) as a function of \(T\) normalized to the Neél temperature \(T_N^0\) of the tetragonal band (\(4 = 0\)). Open (solid) symbols refer to the degree of orbital order, \(\delta_1 = 16\) meV (\(\delta_2 = 80\) meV), and the dashed green (dashed orange) vertical lines indicate the corresponding relevant \(T_N\).](image-url)
up. As seen explicitly from Fig. 1 even a small orbital splitting $\delta$ leads eventually to an arbitrarily large spin anisotropy upon approaching the instability.

How does the electronic structure near the impurities reflect the spin anisotropy of the nematic phase? In Fig. 2 we show local magnetization $m(r)$ nucleated by an impurity in the nematic state as a function of $T$. As seen, the emergent defect objects pins the order locally\cite{31,32} and therefore incorporates the growing spin fluctuation anisotropy in the host upon approaching the magnetic instability. The growing $x$-$y$ anisotropy is clearly evident in the Fourier images in the lower row of Fig. 2. These impurity nematogens are the nematic phase equivalents of the nematogens studied in the SDW phase of Ref. \cite{20}.

In order to determine the transport properties of the nematic defect states, we calculate first the scattering rate in the Born approximation

\[ \frac{1}{\tau_{\text{imp}}} = \frac{2\pi}{h} V \sum_{\mathbf{k}'\beta} \left| \text{tr} \left( \hat{\sigma}_l \hat{V}_{\mathbf{imp}}^{\text{imp}}(\mathbf{k} \alpha, \mathbf{k}' \beta) \right) \right|^2 \times \delta(\epsilon_{\mathbf{k} \alpha} - \epsilon_{\mathbf{k}' \beta}) \left( 1 - \frac{\mathbf{v}_F^\mathbf{k}(\mathbf{k}) \cdot \mathbf{v}_F^\mathbf{k}(\mathbf{k}')}{|\mathbf{v}_F^\mathbf{k}(\mathbf{k})||\mathbf{v}_F^\mathbf{k}(\mathbf{k}')|} \right), \tag{5} \]

where $l = 0$ ($l = 3$) corresponds to the charge (magnetic) scattering rate and $1/\tau_{\text{imp}} = 1/\tau_{\text{imp}}^0 + 1/\tau_{\text{imp}}^3$ is the total scattering rate on band $\alpha$. The term $V_{\sigma\sigma'}^{\text{imp}}(\mathbf{k} \alpha, \mathbf{k}' \beta) = \langle \mathbf{k}' \beta' | \hat{V}_{\mathbf{imp}} | \mathbf{k} \sigma \rangle \equiv \langle \mathbf{k}' \beta' | \mathcal{H} - \mathcal{H}(V_{\mathbf{imp}} = 0) | \mathbf{k} \sigma \rangle$ is the matrix element of the impurity Hamiltonian for the fully converged self-consistent eigenvalue problem

\[ \hat{V}_{\sigma\sigma'}^{\text{imp}}(\mathbf{k} \alpha, \mathbf{k}' \beta) = \sum_{\mu\nu} a^\alpha_{\mathbf{k} \mu} \omega_{\mathbf{k} \sigma \mu}^{\mathbf{k} \alpha} a^\beta_{\mathbf{k}' \nu} - \epsilon_{\mathbf{k} \alpha} \delta_{\mathbf{k} \mathbf{k}'} \delta_{\alpha \beta}. \tag{6} \]

Here $\omega_{\mathbf{k} \sigma \mu}^{\mathbf{k} \alpha} = 1/N \sum_{\mathbf{k}''} \sum_{\nu} \omega_{\mathbf{k}'' \sigma \nu}^{\mathbf{k} \alpha} a^{\mu}_{\mathbf{k}'' \nu} E_{\mathbf{k}''} e^{-i \mathbf{k}' \mathbf{r}_{\mathbf{e}}^{\mathbf{k} \mathbf{k}''} \epsilon_{\mathbf{k}''}}$, and $a^\alpha_{\mathbf{k} \mu}$ are the matrix elements of the unitary transformation from orbitals to bands. Finally, $v_F^\mathbf{k}(\mathbf{k})$ denotes the Fermi velocity of band $\alpha$, and the last term in parentheses in Eq. (5) is an approximation to the vertex corrections in the full Kubo formula by Ziman\cite{33} that has proven accurate for anisotropic scatterers\cite{34}.

In Fig. 3, we show the effect of local freezing of the spin fluctuations on the scattering rate anisotropy by plotting $1/\tau_{\text{imp}}$ explicitly, first for a point-like scatterer of potential $V_{\text{imp}}$ with no self-consistency in \[\text{Fig.} \text{3(a)}\). It is seen that the distribution of scattering weight reflects the small orbital ordering that has created a slightly orthorhombic Fermi surface. Since $V_{\text{imp}}$ is momentum independent, the variation reflects primarily the band-orbital matrix elements for this model. Figure \[\text{3(b)}\) now shows how the nematogen scattering rate reflects the intrinsic spin fluctuations in the system. The localized object in real space couples fluctuations at all $\mathbf{q}$ but these include important contributions from those scattering processes that dominate the fluctuations in the homogeneous system, i.e. the scattering between like orbitals on hole and electron pockets as seen in \[\text{3(b)}\). The point-like scatterer leads to a scattering rate that is nearly $T$-independent, while the nematogen scattering rate grows as the magnetic tran-
sition is approached, as shown in Fig. 3(c). For the nematogen scattering, the charge scattering rate is also nearly $T$-independent. It is the magnetic scattering rate that provides both the strong $T$-dependence and the enhanced anisotropy.

Turning finally to the conductivity obtained from

$$\sigma_{ij} = e^2 \frac{1}{V} \sum_{k\alpha} v_i^{\alpha}(k)v_j^{\alpha}(k)\tau(\epsilon_{k\alpha}) \left(-\frac{\partial f}{\partial \epsilon_{k\alpha}}\right), \quad (7)$$

we show in Fig. 4 the resistivity anisotropy $\Delta \rho = (\rho_b - \rho_a)/\rho_0$ as a function of $T$ with $\rho_0 = (\rho_a + \rho_b)/2$. As expected from Fig. 3, the anisotropy in the case of point-like scatterers is essentially $T$-independent and caused only by the band. On the other hand, for the nematogens $\Delta \rho$ rises rapidly upon approaching the magnetic instability, in agreement with experiments. As $T_N$ is approached, the divergence of the spin fluctuation scattering rate is cut off eventually: in our simulation by the system size, in the real sample by the inter-nematogen distance.

With the above results in hand, we can explain the key properties 1)-5) of the transport experiments discussed in the introduction. Our picture assumes that the Ba122 system, in particular, contains a great deal of disorder away from the FeAs plane which determines the large values of the resistivity near $T_N$. This is consistent with the large constant $\rho(T_N)$ and small $T^2$ coefficient in the parent and lightly doped materials. These scatterers are weak, do not pin low-energy spin fluctuations, and cannot contribute to the resistivity anisotropy. In the parent compound even after annealing, a few vacancies in the FeAs plane create stronger scatterers remain, and give rise to a small peak in the $b$-axis resistivity above $T_N$ due to nematogen formation. Upon doping with Co, however, the concentration of nematogens rises quasi-linearly and enhances the resistivity anisotropy and peaks in $\rho_b$, as seen in experiment, until the critical doping where $T_N$ goes to zero and the magnetic fluctuations which drive the anisotropy weaken. Hole doping with K, on the other hand, introduces much weaker out-of-plane scatterers that cannot induce nematogens; the anisotropy is then essentially zero, with the exception of that driven by few residual vacancies.

We emphasize again that the physics of resistivity anisotropy in our view arises ultimately from the same anisotropy in the spin fluctuation spectrum invoked by the authors of Refs. 15-17. Nevertheless, the importance of these fluctuations in the current picture is that they condense into an emergent defect state above $T_N$ whose anisotropy grows in response to the small orthorhombic symmetry breaking below $T_c$, which then scatters electrons anisotropically. We have shown that a tiny Fermi surface asymmetry, reflected in a very weak anisotropy of the Drude weight[35], is dramatically enhanced by spin fluctuations near $T_N$ such that scattering rate anisotropies of order 100% are possible.

Strong evidence in favor of this picture comes from the annealing experiments of Ishida et al.[6], who show that when strong disorder is removed the anisotropy drops, and attribute the remaining anisotropy to Co atoms, as we do here. While a reduction in anisotropy with decreasing disorder is also possible in the inelastic scattering models, as pointed out e.g. by Breitkreitz et al.[17], it occurs in a parameter regime where spin fluctuation scattering dominates elastic scattering, in contrast to the situation in experiments.

While these theories seem to account for the dramatic reduction of anisotropy on the hole-doped side, this agreement depends on the ellipticity of the 2D electron bands assumed. In the Ba122 system, however, the electron pockets have an ellipticity that changes sign with $k_z$, leading to a near-cancellation of band structure contributions to the anisotropy. The scattering rate anisotropy due to the nematogens, on the other hand, depends uniquely on the orthorhombicity, rather than special features of the band. We note that the nematic susceptibility measured in this material is quite electron-hole symmetric.[36]

Recently, Kuo and Fisher[7] criticized the idea of an extrinsic source of the anisotropy, since samples with very different RRRs have similar resistivity anisotropies, and different chemical substituents corresponding to the same doping exhibit similar anisotropies as well. Neither of these observations contradicts our analysis, how-

![Fig. 4. (Color online) Resistivity anisotropy $\Delta \rho$ versus $T$ for non-selfconsistent point-like (empty diamonds) and self-consistent nematogen (filled diamonds) impurity scatterers. Inset shows the $T$-dependence of $\rho_a/\rho_0$ (circles) and $\rho_b/\rho_0$ (squares) for the nematogen case.](attachment:fig4.png)
ever, since first, the large differences in sample quality and RRR are caused largely by out-of-plane disorder that does not create nematogens. Second, for potentials strong enough to create nematogens, the anisotropy in the scattering rate arises from the spin fluctuations themselves; the strength of the potential for different impurities affects mainly the magnitude of the average resistivity and much less its anisotropy.

In summary, we have discussed an impurity-driven scenario for the remarkable transport anisotropy in Fe-based superconductors that explains all essential features of these measurements, and argues for an increased focus on the unusual role played by impurities in these systems with strong spin fluctuations near a magnetic transition.

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