Quasi-one Dimensional Nanostructures as Signature of Nematicity in Iron Pnictides and Chalcogenides

Dheeraj Kumar Singh, Alirea Akbari, and Pinaki Majumdar

1Harish-Chandra Research Institute, HBNI, Chhatnag Road, Jhunsi, Allahabad 211019, India
2Asia Pacific Center for Theoretical Physics, Pohang, Gyeongbuk 790-784, Korea and
3Department of Physics, and Max Planck POSTECH Center for Complex Phase Materials, POSTECH, Pohang 790-784, Korea

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Impurity scattering is found to lead to quasi-one dimensional nanoscale modulation of the local density of states in the iron pnictides and chalcogenides. This ‘quasiparticle interference’ feature is remarkably similar across a wide variety of pnictide and chalcogenide phases, suggesting a common origin. We show that an unified understanding of the experiments can be obtained by simply invoking a four-fold symmetry breaking $d_{xz} - d_{yz}$ orbital splitting, of a magnitude already suggested by the experiments. This can explain the one-dimensional characteristics in the local density of states which corresponds to multiple parallel running peak structures observed in the orthorhombic nematic, tetragonal paramagnetic, as well as the spin-density wave and superconducting states in these materials.

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The anisotropic electronic properties of iron pnictides [1] are reflected in transport measurements [2–4], optical conductivity [5], angle-resolved photoemission spectroscopy (ARPES) [6], and scanning tunneling microscopy (STM) [7]. The anisotropy is intriguing. It is not unexpected in a state having a broken four-fold rotational symmetry such as the $(\pi,0)$ spin-density wave (SDW) state or the orthorhombic ‘spin nematic’ state, but the lattice anisotropy does not explain the splitting of $\approx 60$meV between the $d_{xz}$ and $d_{yz}$ orbitals [8, 9]. The orbital splitting (OS) actually persists into the high temperature tetragonal phase [9]. This suggests that the OS, rather than the orthorhombic symmetry or magnetic order, could be the key player in electronic anisotropy.

A similar OS exists in various phases [11–14] of the chalcogenide including the superconducting state. The energy scale of FeSe splitting, and its orbital character, has been contrasted with those of the pnictides, with some suggestions of a momentum dependent, i.e., non-uniform splitting. Unlike the pnictides where the degeneracy of bands dominated mainly by $d_{xz}$ and $d_{yz}$ orbitals at X (or Y) points is lifted at low temperature, the OS for chalcogenides may also exhibit sign reversal. Some have reported it to be of entirely different nature (OS, rather than the orthorhombic symmetry or magnetic order, could be the key player in electronic anisotropy).

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Valuable insight into electronic anisotropy can be obtained through the ‘quasiparticle interference’ (QPI) phenomena which basically probes the spatial variation of the local density of states (LDOS), due to impurities in the medium, using the spectroscopic imaging (SI) STM [17]. A remarkable characteristic of the momentum-space QPI (i.e., the Fourier transformed LDOS) common to the SDW state, the orthorhobic nematic phase, and the tetragonal paramagnetic phase, in the pnictides is the occurrence of quasi-one dimensional real-space LDOS modulation over a lengthscale $\sim 8a_{Fe-Fe}$, where $a_{Fe-Fe}$ is the nearest neighbor distance between iron atoms [7, 18, 19]. The observed structure corresponds to parallel running ridges in momentum space separated by $\sim \pi/4$, the exact separation being material dependent. The structures are aligned along a direction reciprocal to the ferromagnetic direction in the SDW state, or $b$-axis in the orthorhombic phase for pnictides. Similar momentum-space structures have been reported in chalcogenides, however, they may be aligned along either of the orthogonal directions. This suggests a common origin of the anisotropy in the electronic structure, rather than in specific ordering tendencies.

In the SDW state, the orbital occupancy difference that can result from the electronic reconstruction is $n_{xz} - n_{yz} \sim 0.1$ [20], which corresponds roughly to an energy splitting of 50meV. According to the experiments, the OS observed above Neel temperature $T_N$ can be as large as $\sim 60$meV [6], therefore it is natural to explore the consequences of this ‘orbital bias’ in studying the SDW state as well, ignored in earlier work [21–24]. Such a term should assume further importance, beyond magnetic anisotropy, in the electron-doped region of SDW state where the magnetic moments are small, and magnetic order induced band reconstruction is less pronounced.

In this letter, we suggest an unified explanation for the common QPI characteristics of different phases of iron-based superconducting systems. Our proposition is that an explicit OS term in the Hamiltonian is crucial irrespective of phases. Thus, our point of departure in the standard five-orbital Hamiltonian is the OS term: $H_{orb} = -\frac{\delta}{2} \sum_{\sigma} (d_{ixz\sigma} d_{ixz\sigma} - d_{iyz\sigma} d_{iyz\sigma})$. Here, $d_{ixz\sigma} (d_{iyz\sigma})$ is the creation (annihilation) operator for an electron in the orbital $d_{xz}$ with spin $\sigma$ at site $i$. The impurity scattering effects that generate the spatial LDOS modulations, i.e., QPI patterns, are handled via a $t$-matrix approach on the mean field states of this theory. Our key results are the following:

(i) We obtain nearly one-dimensional LDOS modulation, i.e., real-space QPI patterns, a feature observed universally across various phases. The corresponding momentum structure has multiple parallel and almost linear peak structures with correct orientation. (ii) For the five-orbital model used in this work, the wavelength of one-dimensional LDOS modulations is $\sim 8a_{Fe-Fe}$ and the parallel peak structures...
in the momentum space are separated by $\sim \pi/4$, in excellent agreement with STM measurements in the SDW state of Ca(Fe$_{1-x}$Co$_x$)$_2$As$_2$. (iii) We identify two large energy windows where the LDOS modulation is one dimensional. For the SDW state it is oriented along the FM direction for 60 meV $\gtrsim -\omega \gtrsim 0$ meV and along the AF direction for 120 meV $\gtrsim -\omega \gtrsim 60$ meV. This happens when the energy of the $d_{xz}$ orbital to be lower than that of $d_{yz}$. (iv) The key factor responsible for all the findings above is the OS term which leads to the upward or downward shift of either set of electron pockets located around (0, $\pm \pi$) or ($\pm \pi$, 0). Combined with a large spectral density due to nearby band extrema, it results in a strongly momentum dependent spectral density along the constant energy surfaces, yielding the anisotropic patterns.

**Superconductivity:** We start with the QPI in the superconducting (SC) phase. The mean field (MF) Hamiltonian written in the Nambu formalism is:

$$H_{sc} = \sum_{k} \Psi^\dagger(k) \hat{H}(k) \Psi(k)$$

$$= \sum_{k} \Psi^\dagger(k) \left( \begin{array}{c} \hat{\varepsilon}(k) \\ \hat{\Delta}(k) \\ \hat{\Delta}^\dagger(k) \\ -\hat{\varepsilon}(k) \end{array} \right) \Psi(k),$$

where the electron field operator is defined as $\Psi^\dagger_{k\mu\sigma} = (d^\dagger_{k1\uparrow}, d^\dagger_{k2\downarrow}, ..., d^\dagger_{-k1\downarrow}, d^\dagger_{-k2\uparrow})$ with subscript 1 to 5 denoting the five $d$ orbitals $d_{xz}$, $d_{yz}$, $d_{zx}$, $d_{xy}$, and $d_{yz}$ in the same order. $\hat{\varepsilon}(k)$ is a $5 \times 5$ hopping matrix [25]. $\hat{\Delta}(k)$ is a $5 \times 5$ pairing matrix. Effective pairing in the $s^\pm$-wave state is mediated by the antiferromagnetic fluctuations generated by the interplay of Fermi surface nesting and on site Coulomb interaction. For simplicity, we neglect interorbital pairing, which has been justified by a recent comparison with experimental data [26]. The diagonal elements of $\hat{\Delta}(k)$ are $\Delta^{\pm}(k) = \Delta_o \cos k_x \cos k_y$, where the gap parameter $\Delta_o$ is assumed same and isotropic (in general, the SC gap is also expected to be anisotropic [27]) for all the orbitals and is set to be 20 meV. The bandfilling $n$ is fixed at 6.1.

The complete Hamiltonian is given by $H_{orb} + H_{sc} + H_{imp}$,

where $H_{imp} = \sum_{\mu<\nu} V_{imp} d^\dagger_{\mu\sigma} d_{\nu\sigma}$ accounts for a non-magnetic delta like impurity scatterer present at site $i^*$. Only orbitally diagonal scattering is retained [28]. Then, the modulation caused in the LDOS by the impurity term is calculated within the $t$-matrix approximation.

**Spin density wave state:** The MF Hamiltonian is obtained after standard decoupling of the on-site terms:

$$H_{int} = U \sum_{\mu<\nu} n_{\mu\uparrow} n_{\nu\downarrow} + (U' - \frac{J}{2}) \sum_{\mu<\nu} n_{\mu\uparrow} n_{\nu\downarrow}$$

$$- 2J \sum_{\mu<\nu} \mathbf{S}_{\mu\uparrow} \cdot \mathbf{S}_{\nu\downarrow} + J \sum_{\mu<\nu,\sigma} d^\dagger_{\mu\sigma} d^\dagger_{\nu\sigma} d_{\nu\sigma} d_{\mu\sigma}.$$

Here, the respective terms represent intraorbital, interorbital density-density, Hund’s coupling and pair-hopping energy in

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**FIG. 1.** Results in the nematic state for orbital splitting $\delta_{orb} = 60$ meV. (a)-(c) show the behavior of CCEs for the quasiparticle energy $\omega = -100, -50, 0$ meV in the $(k_x, k_y)$-plane (units: $\pi/a$, range [-1, 1]). $q_1$ and $q_2$ are intrapocket scattering vectors associated with the electron pockets around (0, $\pm \pi$) and ($\pm \pi$, 0), respectively. Intrapocket scattering vectors for the hole pockets are not shown. $q_3$ and $q_4$ are the interpocket scattering vectors. (d)-(f) For most $\omega$ three parallel rod-like structures exist in the momentum space QPI, the outer peaks are positive the inner peak is negative. Middle: ($q_1$, $q_2$)-plane (units: $\pi/a$, range [1, 1]). Since the orientation of these rod-like structures also changes near $\omega \sim -60$ meV, 1d LDOS modulation ((g)-(i)) also changes its orientation from $x$ direction to $y$. LDOS modulation shown for $80 \times 80$ size with the impurity atom located at the center, calculation done for $300 \times 300$ lattice size. Bottom: ($x$, $y$)-plane (units: $a$, range [-40, 40])

**FIG. 2.** Plots of QPI along the high-symmetry directions in the nematic state. The bottom curve and top curve corresponds to energy $\omega = 0$ meV and $\omega = -120$ meV, respectively. The energy difference for the consecutive curves is 10 meV. The brown and red curves are guide to the eye for scattering vector $q_1$ and $q_2$. 

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[25] Reference 25

[26] Reference 26

[27] Reference 27

[28] Reference 28
the given order. Then, the MF Hamiltonian is

$$\mathcal{H}_{SDW} = \sum_{\mathbf{k}\sigma} \Psi_{\mathbf{k}\sigma}^\dagger \left[ \hat{\varepsilon}_\mathbf{k} + \hat{N} \begin{array}{c} \sgn \sigma \hat{\Delta} \\ \sgn \sigma \hat{\Delta} \end{array} \right] \Psi_{\mathbf{k}\sigma}, \quad (3)$$

where \( \Psi_{\mathbf{k}\sigma}^\dagger = (d_{\mathbf{k}1\sigma}^\dagger, ..., d_{\mathbf{k}5\sigma}^\dagger, d_{\mathbf{k}1\bar{\sigma}}^\dagger, ..., d_{\mathbf{k}5\bar{\sigma}}^\dagger) \) with \( \hat{N}' = d_{\mathbf{k}1\bar{\sigma}}^\dagger d_{\mathbf{k}1\sigma} \). \( Q = (\pi, 0) \) is the ordering wavevector. Matrices \( \hat{N} \) and \( \Delta \) are obtained in a self-consistent manner. The bandfilling in this case is \( n = 6.0 \). We chose intraorbital Coulomb interaction \( U = 0.96\text{eV} \) and Hund’s coupling \( J = 0.25U \) while pair-hopping interaction \( J' = J \) and interorbital density-density interaction parameter \( U' = U - 2J \) are determined by the standard relations. Our choice of \( U \) yields a net magnetization \( m = 0.3 \) consistent with the experiments.

For all QPI calculations, the strength of the impurity potential \( V_0 \) is set to be 200meV. A mesh size of 300 \( \times \) 300 in the momentum space is used. Real-space QPI or LDOS modulation is obtained using the property of Fourier transform. The OS is set to be \( \delta = 60\text{meV} \) unless stated otherwise.

**Nematic Phase:** QPI in the nematic phase is calculated by setting the order parameters to zero (bandfilling \( n = 6.0 \)).

To understand QPI patterns in the orthorhombic nematic or tetragonal paramagnetic phase as shown in Fig. 1(d)-(i), we first examine the quasiparticle spectral functions (Fig. 1(a)-(c)). An important consequence of a non zero OS \( \delta \) is the difference in size of the two sets of pockets around \((\pi, 0)\) and \((0, \pm \pi)\) with large but non-uniform spectral density along both of them (Fig. 1(a)). Note that the pockets are on the verge of disappearance in case the quasiparticle energy is increased further from \( \omega \sim -100\text{meV} \). The spectral density is larger along these pockets because of the nearby extrema. As a result, \( \mathbf{q}_1 \) and \( \mathbf{q}_2 \) are the important scattering vectors. Among various \( \mathbf{q}_1 \) and \( \mathbf{q}_2 \) those aligned parallel to either of \( k_x \) and \( k_y \) are the most prominent ones, as they connect the regions dominated by the same orbital. This follows straight from the fact that only intraorbital scattering is allowed. The main consequence to be described below is the orientation of LDOS modulation along either \( x \) or \( y \).

For \( \omega \sim -100\text{meV} \), \( \mathbf{q}_1 \) associated with the electron pockets around \((0, \pm \pi)\) should be the most important scattering vector despite the fact that \( \mathbf{q}_2 \) does also connect the pockets having larger spectral density. That is because of the availability of a larger phase space as the electron pockets are bigger in contrast with those around \((\pi, 0)\). In particular, \( \mathbf{q}_1 \)’s which are parallel to \( k_x \) should dominate the QPI patterns as they connect the region dominated by same orbitals.

When energy increases through \( \omega \sim -60\text{meV} \), CCEs move away from the band extrema, and the smaller pocket around \((\pm \pi, 0)\) becomes bigger while the bigger ones around \((\pm \pi, 0)\) do not show much change. However, the spectral density along the pockets around \((\pm \pi, 0)\) remains larger in comparison to that along the pocket around \((0, \pm \pi)\). Thus, \( \mathbf{q}_2 \) instead of \( \mathbf{q}_1 \) becomes the dominant scattering vector. CCEs move further away from the band extrema, when \( \omega \) increases and decreases after crossing \( \sim 0\text{meV} \) again. Then, the QPI patterns are expected to become nearly isotropic and featureless.

As anticipated, a larger spectral-density along the sides parallel to the major axis of elliptical CCEs around \((\pm \pi, 0)\) and \((0, \pm \pi)\) results in the dominance of \( \mathbf{q}_1 \) or \( \mathbf{q}_2 \) in the

![FIG. 3. Results in the superconducting state. (a) Quasiparticle spectral function in \((k_x, k_y)\)-plane (units: \(\pi/a\), range \([1, 1]\)). (b) Momentum space QPI in \((q_x, q_y)\)-plane (units: \(\pi/a\), range \([1, 1]\)). (c) Real-space QPI is shown for \(80 \times 80\) lattice size with impurity atom at the center. SC order parameter \(\Delta_+ = 20\text{meV} \) in the \(s^+\) SC state, and quasiparticle energy \(\omega = -88\text{meV} \). In the presence of orbital splitting \(\delta = 60\text{meV} \), CCE pockets at \((\pm \pi, 0)\) are very small with a highly anisotropic spectral density distribution along them. The intrapocket scattering vector \(\mathbf{q}_2\) is mainly responsible for the features observed near \((0, 0)\) in the momentum-space QPI pattern. These consist of three parallel rod-like structures, the outer ones with positive peak and inner one with negative peak. Real-space QPI consists of three bright spots separated by a distance of \(10a_{\mathbf{x} - \mathbf{y}}\) as observed in the experiments.](image)

![FIG. 4. Panels (a)-(c) show the quasiparticle spectral function for \(-100\text{meV}\) in the \((\pi, 0)\) SDW state for various temperatures. Total magnetization is \(m_{\text{tot}} = 0.3\). The resulting momentum-space pattern with three parallel rod-like structures is along a direction reciprocal to ferromagnetic chain and LDOS modulation with wavelength \(\sim 8a\) is very robust against the change in temperature. Range for all the quantities are as in Fig. 1.](image)
momentum-space QPI patterns, which is shown in Fig. 1(d)-(f). When $\omega < -60\text{meV}$, $q_1$ leads to a nearly parallel rod-like positive peak structures at $(\pm \pi/5, 0)$ running parallel to $q_x = \pm \pi/5$. A negative peak structure along $q_x = 0$ is also seen. When $\omega$ decreases and crosses $-60\text{meV}$, $q_2$ instead of $q_1$ becomes relevant and the patterns are rotated by 90°. Near $\omega = 0$, QPI is featureless. A recent SI-STM on FeSe$_{1-x}$S$_x$ does also report an isotropic QPI patterns for positive $\omega$.

Figure 1(g)-(i) shows the real-space QPI in the immediate vicinity of the impurity atom on a $80 \times 80$ lattice size for better visibility though the calculation was done for 300 $\times$ 300 lattice size. Nearly 1d LDOS modulation is obtained over a wide energy window of $\sim$ $100\text{meV}$ centered around $\omega = -60 \text{meV}$. As expected, modulating directions are orthogonal to each other i.e. along $x$ and $y$ for $\omega \lesssim -60\text{meV}$ and $\gtrsim -60\text{meV}$, respectively. The wavelength of modulation for $\omega = -100\text{meV}$ is $\lambda_n \approx 10\Delta_{\text{Fe-Fe}}$, which is close to $\sim 13\Delta_{\text{Fe-Fe}}$, observed in the nematic state of NaFeAs [19]. Note that QPI dispersion shows an almost linear dependence for consecutive rod-like structures in the momentum-space QPI patterns is $\approx 0.25\pi/a_{\text{Fe-Fe}}$ and $0.15\pi/a_{\text{Fe-Fe}}$, which translate to wavelength $\approx 8\Delta_{\text{Fe-Fe}}$ and $\approx 13\Delta_{\text{Fe-Fe}}$ of LDOS modulation, respectively for the two pnictides. The structure size in the reciprocal spaces is comparable with $0.2\pi/a_{\text{Fe-Fe}}$ and $10\Delta_{\text{Fe-Fe}}$ obtained within the five-orbital of Ikeda et al. considered in this work.

**Conclusions:** The occurrence of parallel rod-like structures in the momentum space QPI or 1d spatial modulation of the LDOS in various phases of pnictides and chalcogenides is an indication of common factor at play. We identify this as a symmetry breaking term involving non-degenerate $d_{zx}$ and $d_{yz}$ orbitals. Incorporating such a term while considering different phases, we have obtained all the essential features of QPI patterns and particularly the 1d LDOS modulations. In addition, we find it crucial that the energy of $d_{zx}$ orbital be lower so that the orientation of anisotropic structures is robust against the change in quasiparticle energy. It is also illustrated how the non-uniform spectral-density distribution along the constant energy contours, because of the nearby band extremum, leads to highly anisotropic impurity scattering.

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SUPPLEMENTARY MATERIAL

QPI in the superconducting state

Modulation in the DOS due to an impurity atom is given by

$$\delta \rho(q, \omega) = \frac{i}{2\pi} \sum_k g(k, q, \omega),$$

where $g(k, q, \omega)$ in terms of the change in the Green’s function is

$$g(k, q, \omega) = \sum_{i=1}^{S} (\delta G^{ii}(k, k', \omega) - \delta G^{i*}(k', k, \omega)).$$

Here, $k - k' = q$.

The change in the Green’s function matrix due to a single non-magnetic impurity is

$$\delta \hat{G}(k, k', \omega) = \hat{G}^0(k, \omega) \hat{T}(\omega) \hat{G}^0(k', \omega).$$

The meanfield Green’s function $\hat{G}^0(k, \omega) = ((\omega + i\eta)\hat{I} - \hat{H}(k))^{-1}$. $\hat{I}$ is a $10 \times 10$ identity matrix. Matrix

$$\hat{T}(\omega) = (\hat{I} - \hat{V} \hat{G}(\omega))^{-1} \hat{V},$$

with

$$\hat{G}(\omega) = \frac{1}{N} \sum_k \hat{G}^0(k, \omega).$$

Also,

$$\hat{V} = V_{\text{imp}} \left( \begin{array} {cc} \hat{I} & \hat{O} \\ \hat{O} & -\hat{I} \end{array} \right).$$

$\hat{I}$ and $\hat{O}$ are $5 \times 5$ identity matrix and null matrices, respectively. LDOS modulation or QPI in real space $(\delta \rho(r, \omega))$ can be obtained by Fourier transform of $\delta \rho(q, \omega)$.

QPI in the SDW state

Matrix elements of matrices $\hat{\Delta}$ and $\hat{\Delta}$ in Eq. (1) are

$$2\Delta_{\mu\mu} = U m_{\mu\mu} + J \sum_{\nu \neq \mu} m_{\nu\nu},$$

and

$$2\Delta_{\mu\nu} = J m_{\mu\nu} + (U - 2J) m_{\nu\mu}$$

where charge densities and magnetizations are given by

$$n_{\mu\nu} = \sum_{k\sigma} \langle d_{k\mu\sigma}^\dagger d_{k\nu\sigma} \rangle, \quad m_{\mu\nu} = \sum_{k\sigma} \langle d_{k\mu\sigma}^\dagger d_{k\nu\sigma} \rangle.$$
Note that $d_{k^\mu\sigma}^\dagger = d_{k^\mu+Q\sigma}^\dagger$ with bar over orbital indices indicates shifting of momentum by $Q = (\pi, 0)$. Summation over $k$ is in the first Brillouin zone.

The expressions remains similar to the case of SC state. However, there are several differences as well. Impurity matrix is now

$$
\tilde{V} = V_{\text{imp}} \begin{pmatrix} \hat{1} & \hat{1} \\ \hat{1} & \hat{1} \end{pmatrix}.
$$

(13)

The change in the DOS is given by $\delta \rho_\alpha(q, \omega)$

$$
\delta \rho_\alpha(q, \omega) = \frac{i}{2\pi} \sum_k g_\alpha(k, q, \omega)
$$

(14)

with

$$
g_0(k, q, \omega) = \text{Tr}\delta\tilde{G}(k, k', \omega) - \text{Tr}\delta\tilde{G}^*(k', k, \omega)
$$

$$
g_1(k, q, \omega) = \sum_{\mu \leq 5} \delta G_{\mu,\mu+5}(k, k', \omega) - \delta G_{\mu,\mu+5}^*(k', k, \omega)
$$

$$
g_2(k, q, \omega) = \sum_{\mu \leq 5} \delta G_{\mu+5,\mu}(k, k', \omega) - \delta G_{\mu+5,\mu}^*(k', k, \omega)
$$

(15)

and corresponding LDOS modulation is obtained as

$$
\delta \rho(r, \omega) = \frac{1}{N} \sum_q (\delta \rho_0(q, \omega)e^{i q \cdot r} + \delta \rho_1(q, \omega)e^{i(q - Q) \cdot r} + \delta \rho_2(q, \omega)e^{i(q + Q) \cdot r}).
$$

(16)