Quasiparticle interference in the spin-density wave phase of iron-based superconductors

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(Dated: May 3, 2010)

We propose an explanation for the electronic nematic state observed recently in parent iron-based superconductors [T.-M. Chuang et al., Science \textbf{327}, 181 (2010)]. We argue that the quasi-one-dimensional nanostructure identified in the quasiparticle interference (QPI) is a consequence of the interplay of the magnetic \((\pi, 0)\) spin-density wave (SDW) order with the underlying electronic structure. We show that the evolution of the QPI peaks largely reflects quasiparticle scattering between electronic bands involved in the SDW formation. Because of the ellipticity of the electron pocket and the fact that only one of the electron pockets is involved in the SDW, the resulting QPI has a pronounced one-dimensional structure. We further predict that the QPI crosses over to two-dimensionality on an energy scale, set by the SDW gap, which we estimate from neutron scattering data to be around 90 meV.

PACS numbers: 74.70.Xa, 75.10.Lp, 75.30.Fv

Introduction. One of the key challenges in condensed matter physics is to understand the nature of the many-body states which manifest themselves in experimentally observable anomalous properties. Such states may exhibit subtle, or even entirely novel, forms of static or fluctuating order. One of the most recent examples is the nematic electronic structure observed by means of spectroscopic imaging-scanning tunneling microscopy (SI-STM) experiments in \(\text{Ca}(\text{Fe}_{1-x}\text{Co}_x)\text{As}_2\), parent material of iron-based superconductors\cite{1}. Given a certain similarity between the phase diagrams of iron-based and cuprate superconductors\cite{2} – both contain an antiferromagnetic phase at small, and a superconducting phase at larger, dopings – and in view of the checkerboard electronic pattern observed earlier in the cuprates\cite{3}, this experiment also refocuses attention on a possible role of quasi-one-dimensional physics. Indeed, the possibility of nematic order arising from orbital physics in such quasi-two-dimensional electronic systems has already been discussed in Ref.\cite{4}.

Despite such similarities, there are considerable differences in the normal state electronic structure of the respective parent compounds. The iron-based compound exhibits two circular hole pockets of unequal size, centered around the \(\Gamma\) point \((0, 0)\), and two elliptic electron pockets centered at the \((0, \pm \pi)\) and \((\pm \pi, 0)\) points of the unfolded Brillouin zone (UBZ, based on the \(\text{Fe}-\text{lattice})\). Electron and hole bands are significantly scattered around the \(\Gamma\) point \((0, 0)\). As nesting enhances SDW instabilities, several researchers have argued for an itinerant description of the magnetism in these compounds based at least partly on nesting\cite{5}. Also, in this picture the specific selection of a \((0, \pi)\) or \((\pi, 0)\) magnetic order, as well as the anisotropy of the spin wave spectra\cite{6}, were attributed to the ellipticity of the electronic pockets\cite{7,8}.

Here, we analyze signatures of this SDW order in SI-STM measurements like those reported in Ref.\cite{1}. We do so within the framework of QPI developed in the context of the cuprates\cite{9,10}. We show that the evolution of the QPI peaks is largely due to quasiparticle scattering between the electronic bands involved in the SDW formation. Because of the ellipticity of the electron pockets, and due to the fact that only one of the electron pockets is involved in the SDW, the resulting QPI pattern has a pronounced one-dimensional structure. This is in good agreement with the abovementioned experiments\cite{1}. Our theory predicts a crossover to two-dimensionality in the QPI to occur at a scale set by (twice) the SDW gap, \(2\Delta_1\), which we estimate to be around 90 meV. The exact value, however, depends on the size of the magnetic moments which can vary from compound to compound.

This paper is organized as follows. We set the stage by introducing model, notation and parameters to describe the underlying electronic structure. We next provide a qualitative account of the gross features of SI-STM measurements based on the electronic structure of the SDW phase. This we then back up with a detailed calculation of the relevant Green functions within the T-matrix formalism. We close with the discussion of the interplay of inter- and intra-band impurity scattering.

The model. We employ an effective mean-field four-band model with two circular hole pockets at \((0, 0)\) \((\alpha\)-bands\) and two elliptic electron pockets at \(Q_1\) and \(Q_2\) \((\beta\)-bands\)\cite{10}:

\[
H_c = \sum_{k, \sigma, i=1, 2, \alpha, \beta_1, \beta_2} \varepsilon_k^\alpha \hat{c}_{i k \sigma}^\dagger \hat{c}_{i k \sigma} + \sum_{k \sigma} \Delta_1 \sigma \left[ \hat{c}_{\alpha 1 k \sigma}^\dagger \hat{c}_{\beta 1 k + Q_1}^\dagger \hat{c}_{\beta 1 k + Q_1 \sigma} + H.c. \right]
\]

We set the dispersions to \(\varepsilon_k^\alpha = t_\alpha (\cos p_x + \cos p_y) - \mu_i\) and \(\varepsilon_k^\beta = \varepsilon_0 + t_\beta (1 + \varepsilon \cos(p_x + \pi) + (1 - \varepsilon) \cos(p_y)) - \mu_i\).
note the characteristic scattering wave vectors which appear.

We introduce the experimentally observed (0, π) SDW order parameter, within a standard mean-field approximation: \( \Delta_1 \propto \sum_{\mathbf{p}} e_{\mathbf{p}}(\epsilon_{\alpha_{\mathbf{p}}})^2 \beta_{\mathbf{p}} \), where \( \epsilon_{\mathbf{p}} \) is the Fermi velocity and size of the Fermi pockets based on Refs. [3], namely \( t_{\alpha} = 0.85 eV \) and \( n_{\alpha} = -0.68 eV \). For these values, the Fermi velocities are 0.5eV for the \( \alpha \)-band, and the Fe-Fe lattice spacing, and \( n_{\alpha} = 0.8 eV \) and \( v_y = 0.49 eV \) along \( x \)- and \( y \)-directions for the \( \beta \)-band, and vice versa for \( \beta_2 \). We use \( a_x = a_y = a = 1 \).

We introduce the experimentally observed \((\pi, 0)\) SDW order parameter, within a standard mean-field approximation: \( \Delta_1 \propto \sum_{\mathbf{p}} e_{\mathbf{p}}(\epsilon_{\alpha_{\mathbf{p}}})^2 \beta_{\mathbf{p}} \). In this state, one of the \( \alpha \) fermions couples with only one band of \( \beta \) fermions, leaving the other hole and electron bands – and hence their electron and hole FSs – unaffected by the SDW. Without loss of generality we direct \( \Delta_1 \) along the \( z \)-quantization axis.

Results. In the following we focus on the discussion of the QPI in the SDW state at energies below twice the SDW gap. Throughout the paper we set \( \Delta_1 \approx 45 meV \), from a previous analysis of the experimental data [10].

The simplest way to understand QPI qualitatively is to consider the evolution of the spectral function in the SDW state in the fashion pioneered for the cuprates[12].
where $\otimes$ is the direct product of matrices and
\[
\tilde{\epsilon}^\sigma_k = \begin{bmatrix}
\epsilon_{12}^\sigma & 0 & 0 & 0 \\
0 & \epsilon_{12}^\sigma & \sigma \Delta_1 & 0 \\
0 & \sigma \Delta_1 & \epsilon_{22}^\sigma & 0 \\
0 & 0 & 0 & \epsilon_{22}^\sigma
\end{bmatrix}, \quad \hat{t}_{kk'} = \begin{bmatrix}
u_0 & u_Q & u_Q \\
u_0 & u_Q & u_Q \\
u_0 & u_Q & u_0 \\
u_0 & u_Q & u_0 \end{bmatrix}
\]

Here, we assume that the intraband impurity scattering, $u_0$, is bigger than the interband scattering between the bands separated by a large $Q$, $u_Q$, and set $u_Q = 0.2 u_0$. The Green function matrix is obtained via $G_{kk'}(\tau) = -\langle \tilde{T}_k(\tau) \tilde{T}_{k'}(0) \rangle$, whence
\[
G_{kk'}(\omega_n) = G_{kk'}^{0}(\omega_n) \delta_{kk'} + \hat{t}_{kk'}(\omega_n) G_{kk'}^{0}(\omega_n),
\]

where $G_{kk'}^{0}(\omega_n) = (i \omega_n - \tilde{\epsilon}_k^\sigma)^{-1}$ is the bare Green’s function of the conduction electrons. Solving the Dyson equation for the T-matrix $t_{kk'}(\omega_n) = \hat{U}_{kk'} + \sum_{kk''} \hat{G}_{kk''}(\omega_n) t_{kk''} G_{kk''}(\omega_n)$, the LDOS is obtained via analytic continuation $i \omega_n \rightarrow E + i 0^+$ according to $N(E, r) = -\frac{1}{\pi} \text{Im} \text{Tr} [ G(r, r, \omega_n) ]_{\omega_n \rightarrow E + i 0^+}$. Note that interference between the two partial waves give rise to spatial modulation of the amplitude of the total wave which is then reflected in the local density of states (LDOS). We now assume the Born approximation holds and set $u_0 = 0.1 t_{\alpha}$.

We show the absolute value of the resulting QPI for positive energies in Fig.2(b), (e), (h) for a non-magnetic impurity ($\gamma = 1$, $\gamma' = 0$) and in Fig.2(c), (f), (i) for a magnetic impurity ($\gamma = 0$, $\gamma' = 1$), respectively. Overall the QPI map resembles well the structure anticipated from the spectral density maps. In particular, we find the overall $C_2$ symmetry of the QPI maps whose structures are determined by scattering at momenta shown on the left panel. In particular, at 10meV the QPI shows peaks at $q_2$ and $q_3$ which refer to intra-pocket scattering, as well as $q_1$ which denote the inter-pocket scattering originating from the edges of the boomerangs. Overall, the QPI shown in Fig.2(b), (e) and Fig.2 resembles the one found experimentally in Ref. [1]. In particular, we find that as a result of SDW induced electronic structure reconstruction, the scattering interference modulations are strongly unidirectional and show $C_2$ symmetry with $q_1$ and $q_3$ induced structure along the AF $q_x$ axis. In the ferromagnetic $q_y$ axis modulations with wave vector $q_2$ are also found. As in the electronic structure, this persists only up to a scale set by the size the SDW gap.

To analyze the energy dispersion of the QPI interference we show in Fig.2 its evolution along $q_x$ and $q_y$-directions for energies between -50 and 50 meV. The peaks associated with $q_2$ along the ferromagnetic $q_x$ direction and $q_1$ and $q_3$ along the AF $q_y$ direction are dispersive and their velocities are in direct correspondence with the quasiparticle group velocities of the bands involved in the SDW formation.

Finally, in Fig.3 we show a real space image of the QPI away from the impurity position and at -7meV. We observe that the QPI modulation is reflected in periodic structures seen along the $x$ and $y$ directions. In the AF $y$ direction with $q_1$ structure, we find a weak ’stripe’ pattern with a periodicity of the order of $\approx 7a$. In addition, we also find a stronger modulation of 10 – 15a along the FM $x$ direction, consistent with the structure described as nematic in Ref. [1]. The $x - y$ asymmetry of the structure is again a consequence of the SDW with $(0, \pi)$ magnetic order. We also stress that these extra modulations arise purely due to scattering between the bands involved in the SDW – no extra folding of the bands occurs.

One natural question to ask is: How stable is the observed QPI and the resulting real space ’stripe’ structure?
terband and intraband scattering is more subtle although
site. In addition, the change of the ratio between the in-

First, the QPI is sensitive to the size of the SDW gap. For large enough $\Delta_1$ the FSs of the bands involved in the SDW are completely gapped and the same is also true for the spectral densities at low energies. In this case, QPI will be determined by the bands which are not involved in the SDW, and, therefore, its structure will not show strong quasi-1D character. This may explain why the pure AF SDW state does not show any $C_2$-symmetric structure in the parent compounds where the magnetic moment (and the corresponding SDW gap) is quite large. 

Only when it is reduced upon doping, the bands involved in the SDW are located close to the FS and the QPI structure, described above, becomes visible. Note that the SDW gap used in our calculations corresponds to $\mu \approx 0.4\mu_B$. An additional factor why doping might be crucial for an observation of the superstructure is that the impurities act as pinning centers and the interference is more pronounced once disorder is increased. We also note that as soon as SDW forms due to the nesting of electron and hole bands, the main role of the underlying orbital structure is to modify the absolute intensities of the QPI as this depends on the underlying orbital matrix elements. However, it is unlikely that these factors would restore the four-fold symmetry in the QPI. Instead, it is expected that the corresponding QPI will be the same as in our Fig. 1 but with extra intensity modulation due to orbital matrix elements [15].

We note in passing that an increase of the intraband impurity scattering, $u_0$, does not change the results significantly in any way except that at large enough values of $u_0$, one finds local resonances around the impurity site. In addition, the change of the ratio between the interband and intraband scattering is more subtle although the resulting QPI still shows the $C_2$ anisotropy even up to $u_0 = u_0$. However, there is still another interesting effect that we find upon changing the energy from positive to negative values. In particular, in Fig. 1 we show the spectral density and the corresponding QPI from $-10 \text{meV}$ to $-60 \text{meV}$. At low negative energies, i.e., above $-20 \text{meV}$, the structure remains the same as for $+1 \text{meV}$. However, for $-30 \text{meV}$ we find a rotation of the QPI by 90 degrees. This occurs due to particle-hole asymmetry of the bands contributing to the SDW. In the SDW state, new energies $E^{c,d}_{\pm} = \frac{1}{2}(\varepsilon^c_{\pm} + \varepsilon^d_{\pm} + 4\Delta)^2$, which are pronounced for positive energies; $E^d$ yields pockets along the $y$ (FM) direction visible at relatively large negative energies. As a consequence, the QPI rotates 90 degrees at energies lower than $-30 \text{meV}$. This prediction would be interesting to check experimentally.

In summary, we have presented a theory for SI-STM measurements in the iron-based superconductor parent compounds in the presence of $(0, \pi)$ SDW magnetic order. We find that QPI introduced by scalar non-magnetic, as well as magnetic, impurities gives rise to a periodic modulation of the real space LDOS. Because of the ellipticity of the electron pockets, and the fact that only one of the electron pockets is involved in the SDW, the resulting QPI has a pronounced quasi-one-dimensional structure in good agreement with recent SI-STM experiments [1]. We further predict that the QPI becomes two-dimensional at energies larger than twice the SDW gap, $2\Delta_1$, which as we argue from the analysis of the neutron scattering data should be $\sim 90 \text{meV}$.

We are thankful to Igor Mazin for sharing with us his results prior to publication and useful comments. I.E. acknowledges the support from the RMES Program (Contract No. N 2.1.1/2985), and NSF (Grant DMR-0456669).

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