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Testing the sign-changing superconducting gap in iron-based superconductors with quasiparticle interference and neutron scattering

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Abstract

We present a phenomenological calculation of the quasiparticle interference (QPI) pattern and inelastic neutron scattering (INS) spectra in iron-pnictide and layered iron-selenide compounds by using material specific band structure and superconducting (SC) gap properties. As both the QPI and the INS spectra arise due to scattering of the Bogolyubov quasiparticles, they exhibit a one-to-one correspondence of the scattering vectors and the energy scales. We show that these two spectroscopies complement each other in such a way that a comparative study allows one to extract quantitative and unambiguous information about the underlying pairing structure and the phase of the SC gap. Due to the nodeless and isotropic nature of the SC gaps, both the QPI and INS maps are concentrated at only two energies in pnictide (two SC gaps) and one energy in iron-selenide, while the associated scattering vectors \( q \) for scattering of sign-changing and same sign of the SC gaps change between these spectroscopies. The results presented, particularly for the newly discovered iron-selenide compounds, can be used to test the nodeless d-wave pairing in this class of high temperature superconductor.

(Some figures may appear in colour only in the online journal)

1. Introduction

The most crucial information for unraveling the mechanism of pairing is the structure of the superconducting (SC) gap function, a measure of the amplitude and the phase of electron pairs. Although the SC gap function of conventional phonon-mediated (attractive pairing interaction) superconductors has the same sign all over the \( k \)-space (s-wave symmetry), that of spin-fluctuation-mediated (repulsive pairing interaction) superconductors has the same sign all over the \( k \)-space and the phase of electron pairs. Although the SC gap function of conventional phonon-mediated (attractive pairing interaction) superconductors has the same sign all over the \( k \)-space (s-wave symmetry), that of spin-fluctuation-mediated (repulsive pairing interaction) superconductors has the same sign all over the \( k \)-space.

Fermi momenta connected by the characteristic ‘hot-spot’ wavevector \( \mathbf{Q} \) of spin-fluctuations [2, 3]. As a consequence of the sign reversal, nodal planes in which the SC gap vanishes should exist in \( k \)-space. If such nodal planes intersect the Fermi surface (FS), as in d-wave cuprate, nodal quasiparticle states emerge in the low-energy spectra. However, if the FS consists of small pockets and does not touch the nodal line, s± pairing in iron-pnictide and single layer iron-chalcogenides [4] or d-wave pairing in double layered iron-selenide (\( \text{Fe}_2\text{Se}_2 \)) [5–8] develops despite a sign symmetry and the Fermi surface topology remain the same. See, for example, [1].

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reversal of the pairing. Therefore, to precisely establish an unconventional pairing symmetry and separate it from a conventional s-wave, the relative sign of the SC gap on the FS must be established.

The magnetic resonance mode develops in the SC state and was shown theoretically to arise from the sign-flip of the SC gap at the ‘hot-spot’ [7, 9–12]. However, there are other theories which also reproduce the resonance mode without the requirement of sign change of the SC gap [13–15]. Alternative and important new spectroscopy comes from the quasiparticle interference (QPI) pattern, measured by scanning tunneling microscopy (STM), which in principle visualizes all possible elastic scattering vectors. It therefore can distinguish the sign-changing ‘hot-spot’ vectors by studying their evolution with varying magnetic field [16–19].

A magnetic field breaks the time-reversal symmetry of the SC quasiparticles and thus illuminate those scattering vectors which scatter quasiparticles of the same pairing phase, thanks to the remarkable properties of the Bogolyubov coherence factors [20]. These observations can be questioned based on at least two arguments: (1) magnetic field induced vortex states drastically redistribute the spectral weight across the ‘bright-spots’ on the constant energy surface, making this procedure complicated; (2) a magnetic impurity always carries a scalar potential which allows simultaneous scattering of quasiparticles of opposite pairing phase [18, 19]. We show in this paper that the INS and QPI maps complement each other and allow determination of the relative phase. Thus, we propose that a comparative study between the inelastic neutron scattering (INS) spectra and the QPI pattern, taken together, can be a viable tool to quantitatively and unambiguously determine the relative sign of the SC gap.

Our approach is based on a very simple observation: both the INS and the QPI patterns arise from similar scattering of the Bogoliubov quasiparticles, forming Cooper pairs (inelastic and elastic scatterings, respectively) and thus their observed dispersions, \( \Omega(q) \), must have an one-to-one relationship in these two spectroscopies. In an INS spectrum, a scattering \( q \) vector will be observed if it connects two quasiparticle states at \( k_i \) and \( k_f \) at which \( \text{sgn}[\Delta_{k_i}] \neq \text{sgn}[\Delta_{k_f}] \) and thus its energy scale will be determined by \( |\Delta_{k_f}| + |\Delta_{k_i}| \). The same vector will only appear in the QPI spectrum if \( |\Delta_{k_f}| = |\Delta_{k_i}| \), because QPI probes elastic scattering. The comparison between the INS and the QPI maps can therefore emphasize the regions of momentum space with opposite sign of the gap function, connected by scattering momenta. This emphasis can be further facilitated by studying the magnetic field dependence of the QPI map. Such a comparative study has proven to give valuable information about the pairing symmetry in cuprates [21].

**Iron-pnictide.** In the case of iron-pnictide superconductors, however, the presence of multiple bands at the Fermi level (\( E_F \)) and multiple SC gap amplitudes at each band make the aforementioned analysis much more complicated and exotic. In these compounds, the FS consists of two disconnected concentric hole pockets (namely, \( \alpha \) and \( \beta \) pockets) and one electron pocket (\( \gamma \) pocket) centered at the \( \Gamma \) and M points, respectively. Prominent nesting between the hole pockets and the electron pocket has been shown theoretically to lead to an \( s^\pm \)-pairing in this family of superconductors [4]. Within this pairing, all the FS pockets possess nodeless and isotropic SC gaps, but the sign of the gaps is reversed between the hole pockets and the electron pocket. To complicate the story, the two hole pockets acquire very different magnitudes of the SC gaps [12, 22, 23]. Therefore, macroscopic geometrical separation of the two phases, as in the cuprate corner-junction experiment, cannot be performed in these systems to test the pairing symmetry [24].

In our earlier study, we have theoretically shown that because of the two values of the SC gap in the two hole pockets, the INS spectrum is split into two energy scales [12]. Furthermore, as the two hole pockets have very different areas as a function of doping, the corresponding \( q \) vectors are also different at these two resonances. Here, we show that these INS scattering vectors also appear in two different energy scales of the QPI patterns. Additional scattering vectors between the states of same sign of the SC gaps, which are prohibited in INS, appear in QPI. These results are consistent with STM data on electron doped Ba(Fe\(_{1−x}\)Co\(_x\))\(_2\)As\(_2\) as a function of doping [25]. Furthermore, the evolution of the QPI pattern as a function of magnetic field is also consistent with STM studies in single layer Fe(Se, Te) superconductors [17].

**\( \text{Fe}_2\text{Se}_2 \) superconductors.** The recent discovery of high-\( T_c \) superconductivity in double layered \( \text{Fe}_2\text{Se}_2 \) based superconductors makes the above story even more interesting and exotic [26–28]. The FS in this family of superconductors only hosts electron pockets at the M point (no hole pocket is present here as in iron-pnictide discussed above). Therefore, the leading nesting vector occurs between the two electron pockets which leads to a d-wave pairing (\( d_{xy} \) in 1 Fe unit cell and \( d_{xy} \) in 2 Fe unit cell notation) [12]. Unlike the d-wave pairing in cuprates, here it gives rise to a nodeless and isotropic SC gap on the FS, in consistency with experiments [29–32], but the gap function changes sign between the two electron pockets. We and others [5–7] have shown earlier that such a d-wave pairing leads to a magnetic resonance mode at \( Q \) which is observed later by INS measurements [33].

Here we show that this INS scattering vector \( Q \) will also show up in the QPI vector at the bias energy equal to the SC gap magnitude. Furthermore, we phenomenologically demonstrate that with the application of a magnetic field, other QPI scattering vectors at which the SC gap does not change sign can be illuminated. The relative evolution of the QPI map as a function of magnetic field will provide a valuable test for the relative phase of the SC state on the FS in this family of superconductors.

The paper is organized as follows. In section 2, we provide the formalism for both QPI and INS spectra. We extract out very simple equations for these two spectroscopies which can be used with experimental inputs to reconcile them. In section 3, we present the results for iron-pnictide, while the results for layered iron-selenide are given in section 4.
The magnetic field dependence of the QPI map is computed for a layered iron-selenide system in section 4.1. Finally, we conclude in section 5.

2. Formalism

A direct correlation between the INS and the QPI spectra can only be made within the bare level in which the same Green’s functions are involved. This correspondence therefore would at least qualitatively be correct for dressed Green’s functions. In fact, one can again evaluate the Green’s functions for the filled state from the ARPES spectral weight A, which is exact for a single band case, but averaged over orbital indices in a multiband system. In a multiband superconductor, the Green’s functions for the normal and anomalous parts can be written in the eigenbasis as

\[ G_v(k, i\omega_n) = \frac{\alpha_v^2(k)}{i\omega_n - E_v(k)} + \frac{\beta_v^2(k)}{i\omega_n + E_v(k)}, \]

\[ F_v(k, i\omega_n) = \alpha_v(k)\beta_v(k) \]

\[ \times \left( \frac{1}{i\omega_n - E_v(k)} - \frac{1}{i\omega_n + E_v(k)} \right), \]

respectively. \( n \) is the Matsubara frequency. Here \( E_v(k) = \pm \sqrt{\xi_v^2(k) + \Delta_v^2(k)} \) is the \( v \)th Bogolyubov quasiparticle band. \( \xi_v^2(k) \) is the non-interaction band modeled by tight-binding parametrization to the material specific LDA bands, as discussed later. \( \Delta_v(k) = \Delta_0^v g(k) \) is the momentum-dependent SC gap with \( \Delta_0^v \) the band specific SC gap magnitude. \( g(k) \) is the structure factor for the pairing symmetry which is taken to be same for all bands in a given system. \( \alpha_v(k)(\beta_v(k)) = \sqrt{\frac{1}{2}(1 \pm \frac{\xi_v(k)}{E_v(k)})} \) are the Bogolyubov coherence factors for the quasiparticle states \( \pm E_v(k) \), respectively. The above Green’s functions can be projected to the orbital basis as \( G_{\nu\nu}(k, i\omega_n) = \langle \phi_{\nu}^\ast(k) G_v(k, i\omega_n) \phi_{\nu}^\ast(k) \rangle \) and similarly for \( F_{\nu\nu}(k, i\omega_n) \) represent the eigenvectors of the \( v \)th band onto the \( \nu \)th orbital.

QPI profile. STM measures the local density of states (LDOS) of quasiparticles which arrive at the tip after going through multiple intrinsic elastic scattering (due to magnetic and non-magnetic scatterers [18, 19, 34]) in the system. Such scattering vectors can be visualized by Fourier transforming the LDOS into the \( q \) space to obtain [18, 19, 34–37]

\[ B_{\text{rstu}}(q, i\Omega_m) = \text{Im} \sum_{k, v, \nu, \nu'} M^{\nu\nu'}_{\text{rstu}}(k, q) \times [G^{\nu\nu'}(k, i\omega_n) G^{\nu\nu'}(k + q, i\omega_n) \\
- F^{\nu\nu'}(k, i\omega_n) F^{\nu\nu'}(k - q, -i\omega_n)]. \] (3)

Here \( M \) is the orbital to band matrix element made up of the eigenvectors as \( M^{\nu\nu'}_{\text{rstu}}(k, q) = \phi_{\nu}^\ast(k + q) \phi_{\nu'}^\ast(k) \phi_{\nu}^\ast(k) \phi_{\nu'}^\ast(k + q) \). The matrix element can be important for shaping the spectral weight distributions for the multiband case. Nevertheless, the relative intensities of the scattering vectors are determined by the nesting conditions and the SC gap amplitude for elastic scattering. In addition, a scattering matrix element, \( C(k, q) \), appears due to the coherence factors, \( \alpha_v(k) \) and \( \beta_v(k) \), of the Bogolyubov quasiparticles which is sensitive to the momentum-dependent phase of the SC order parameter and the symmetry of the scattering potential, \( V_q \) [16, 20]. The Green’s function is expressed in terms of the spectral weight as \( G^{\nu\nu'}(k, i\Omega_m) = -\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A^{\nu\nu'}(k, \omega')(i\Omega_m - \omega') \).

If no many-body broadening is included then the spectral weight can be presented by a delta function. Taking these facts into account, we simplify equation (3) to calculate the total QPI map as [16]

\[ B(q, \Omega_{QPI}) \approx |V_q| \sum_{k, \nu, \nu'} C^{\nu\nu'}(k, q) \times \delta(\Omega_{QPI} - E_v(k)) \delta(\Omega_{QPI} - E_v(k + q)). \] (4)

(Here we assumed \( M = 1 \) for simplicity [37] and took analytical continuation, \( i\Omega_m \to \Omega_{QPI} + i\eta \) (\( \eta \) is a small broadening).) The explicit form of the scattering matrix element as given in [16, 17] is \( C^{\nu\nu'}(k, q) = (\text{sgn}[\Delta_v(k)] \text{sgn}[\Delta_v(k + q)] \alpha_v(k) \alpha_v(k + q) \mp \beta_v(k) \beta_v(k + q))^2 \), where the negative and positive signs represent scattering through a scalar (even under time reversal) and a magnetic (odd under time reversal) potential, respectively. Furthermore, scattering from disorder that converts electrons into holes as they are scattered gives rise to the coherence factor \( C_{\nu\nu'}(k, q) = (\text{sgn}[\Delta_v(k)] \alpha_v(k) \alpha_v(k + q) \mp \beta_v(k) \beta_v(k + q))^2 \). At \( E_F \) the two delta functions in equation (4) give \( \Omega_{\text{QPI}}^{\nu\nu'}(q) = |\Delta_v(k_F)| = |\Delta_v(k_F + q)| \). Imposing this constraint, we obtain \( \alpha_v(k_F) = \alpha_v(k_F + q) \) and \( \beta_v(k_F) = \beta_v(k_F + q) \) at \( E_F \) (by substituting \( \xi_k = 0 \) in the equations for \( \alpha, \beta \) given above). This leads to a systematic selection rule for \( q \) vectors which depends on the nature of the scatterer. In the case of weak scalar potential scattering, \( C \sim 0 \) for those \( q \) at which \( \text{sgn}[\Delta_v(k_F)] = \text{sgn}[\Delta_v(k_F + q)] \), while for QPI scattering off magnetic impurities or gap inhomogeneities, \( C \sim 0 \) for those \( q \) at which \( \text{sgn}[\Delta_v(k_F)] \neq \text{sgn}[\Delta_v(k_F + q)] \). By contrast, for scattering off magnetic impurities or gap inhomogeneities, \( C \sim 0 \) for those \( q \) at which \( \text{sgn}[\Delta_v(k_F)] \neq \text{sgn}[\Delta_v(k_F + q)] \). Therefore, focusing on the low-energy region where \( \Omega_{QPI} \leq \Delta \), we can write the conditions to obtain a non-vanishing QPI vector as

\[ \Omega_{\text{QPI}}^{\nu\nu'}(q) = |\Delta_v(k_F)| = |\Delta_v(k_F + q)|, \]

\[ \text{sgn}[\Delta_v(k_F)] \neq \text{sgn}[\Delta_v(k_F + q)] \quad \text{for scalar imp.}, \]

\[ \text{sgn}[\Delta_v(k_F)] \neq \text{sgn}[\Delta_v(k_F + q)] \quad \text{for mag. imp.}. \]

Note that as a magnetic impurity is always associated with a scalar potential, it, in principle, involves QPI scattering which satisfies equation (6) as well but its intensity will depend on the relative strength of the potential. We take \( V(q) \) as a constant potential.

INS spectra. The calculation of the INS spectrum follows similarly with the exception that the latter is an inelastic scattering of the quasiparticle spectrum. INS probes the imaginary part of the susceptibility which can be written in the orbital basis as [12, 38]

\[ \chi_{\text{rstu}}(q, i\Omega_m) = -\frac{1}{2} \sum_{k, n, \nu, \nu'} M^{\nu\nu'}_{\text{rstu}}(k, q) \times [G^{\nu\nu'}(k, i\omega_n) G^{\nu\nu'}(k + q, i\omega_n + i\Omega_m) \\
+ F^{\nu\nu'}(k, i\omega_n) F^{\nu\nu'}(k - q, -i\omega_n - i\Omega_m)]. \] (8)
We have shown earlier in [12] that in many cases the difference between a realistic matrix element and a matrix element assumed to be a smooth function of energy and momentum is thus not important in calculating the magnetic scattering structure. The INS dispersion is mostly governed by the locus of the discontinuous jumps in $\chi_0$ and due to the Kramers–Kronig relationship, the corresponding $\chi''_0$ attains a peak at the same location (within the random-phase approximation (RPA), the peak position shifts slightly to a lower energy). Similarly to equation (4) above, we absorb the INS matrix element term in $C_{\nu'\nu}(k, q)$ and performing the Matsubara summation in equation (8) we obtain the total SC $\chi_0$ as

$$\chi_0(q, \Omega_{\text{INS}}) \approx \sum_{k, \nu, \nu'} C_{\nu'\nu}(k, q) \times \delta (\Omega_{\text{INS}} - E_\nu(k) - E_\nu(k + q)).$$

(9)

Here, the explicit form of $C$ is $C_{\nu'\nu}(k, q) = \beta_\nu(k) \alpha_{\nu'}(k + q) |\delta_{\nu'\nu}(k)| + \beta_\nu(k) \alpha_{\nu'}(k + q) = (1 - \text{sgn}[\Delta_\nu(k)]) \text{sgn}[\Delta_\nu(k + q)]$ at $E_F$. This implies that the magnetic structure in the SC $\chi_0$ below $\Omega_{\text{INS}} \leq 2\Delta$ is entirely governed by two conditions [7, 9–12]:

$$\Omega_{\text{INS}}^{\nu'\nu}(q) = |\Delta_\nu(k_F)| + |\Delta_{\nu'}(k_F + q)|,$$

(10)

$$\Delta_{\nu'}(k_F(q)) \neq \Delta_\nu(k_F + q).$$

(11)

We will use QPI equations (5)–(7) and INS equations (10) and (11) to perform a comparative analysis of the two sets of spectroscopic data in iron-pnictide and iron-selenide superconductors.

3. Results on iron-pnictide

Fermi surfaces in pnictide. The low-energy Hamiltonian of the iron-pnictide system is dominated by five d-orbitals of the Fe atoms. We take the tight-binding model from [38] where the parameters are fitted to the corresponding first-principles dispersion. The doping is evaluated within the rigid-band shift approximation. At $x = -0.1$, the computed FS consists of two concentric hole pockets at the $\Gamma$ points which are called $\alpha$- (inner pocket as depicted by the red line in figure 1(a)) and $\beta$-pockets (blue line) and one electron pocket at the M point (green line). All the results in this paper are presented in the unfolded BZ coming from 1 Fe unit cell.

SC gap properties. From the shapes of the FS pockets, at least four inter-pocket scattering channels exist in the pnictide which span along various high-symmetry $q$ directions as shown by arrows of different colors in figure 1(a). Among the four vectors, Mazin et al [4] have shown theoretically that the nestings for $q_1$ and $q_2$ are the strongest and lead to a sign-changing $s^\pm$-pairing symmetry in this class of superconductor. This phase symmetry of the SC gap is consistent with the spin-fluctuation mechanism of electron pairing. The pairing and SC gap amplitudes have three essential properties which are relevant to our present study: (1) the SC gap changes sign between the electron and hole pockets (the black to white background colors in figure 1(a) reflect the $s^\pm$-pairing symmetry), (2) the SC gap magnitude on all FS pockets is nodeless and isotropic, and (3) evidence from ARPES [22], STM [25] and numerous bulk probes [23] indicates that

$$|\Delta_\nu| \approx |\Delta_{\nu'}| \approx 2|\Delta_B|$$

(12)

at all dopings and for both electron and hole dopings.

Sketch of the QPI and INS maps. All the aforementioned FS and SC gap properties lead to very different QPI and INS properties in pnictide from the ones obtained in single band cuprates [16, 36].

(i) The nodeless and isotropic nature of the SC gaps makes all the QPI and INS maps concentrate at only two energy scales, instead of the characteristic dispersion seen in the nodal and anisotropic d-wave gaps in cuprates. The QPI maps will be prominent only at $\Omega_{\text{QPI}}^{1} = |\Delta_B|$ and $\Omega_{\text{QPI}}^{2} = |\Delta_B| \approx |\Delta_{\nu'}|$, obeying equation (5), while the INS maps will show up only at $\Omega_{\text{INS}}^{1} = |\Delta_B| + |\Delta_{\nu'}|$ and $\Omega_{\text{INS}}^{2} = |\Delta_B| + |\Delta_{\nu'}|$, according to equation (10).

(ii) At $\Omega_{\text{QPI}}^{1} = |\Delta_B|$ no interband elastic scattering is allowed as $|\Delta_{\nu'}| < |\Delta_{\alpha\gamma'}|$. Therefore, the QPI map in figure 1(b1) only shows intra-$\beta$-FS scattering which concentrates near $q = 0$. As the SC gap does not change sign on each pocket, some finite magnetic field will be necessary to illuminate these small $q$ vectors. Of course, in real material, finite broadening can introduce some quasiparticle states of the $\alpha$ and $\gamma$ bands near $\Omega_{\text{QPI}} = |\Delta_B|$ to visualize a weak intensity at $q_2$ (at zero magnetic field).

(iii) At $\Omega_{\text{INS}}^{2} = |\Delta_B| + |\Delta_{\nu'}|$ the interband scattering vector $q_1$ and intraband scattering vectors $q_3$ and $q_4$ appear in figure 1(b2). $q_3$ and $q_4$ become illuminated at zero magnetic field while $q_2$ will gain more intensity at finite magnetic field, in consistency with the data from [17].

(iv) At $\Omega_{\text{INS}}^{1} = |\Delta_B| + |\Delta_{\nu'}|$ the $q_1$ vector can be observed through INS study in figure 1(c1). Note that, among the four maps shown in figure 1, this is the only place where $q_2$ can be determined precisely.

(v) Similarly, at $\Omega_{\text{INS}}^{2} = |\Delta_B| + |\Delta_{\nu'}|$, the $q_1$ vector will be observed as sketched in figure 1(c2). At zero magnetic field this INS spectrum will match exactly with the QPI pattern shown in figure 1(b2).

(vi) The doping dependence of the $q$ vectors and their energy scales (not studied here) can also be used to gain confidence in the FS topology and the location of the sign reversal of the pairing symmetry. The INS energy scales, $\Omega_{\text{INS}}^{1,2}$, obtain dome-like behavior with doping in accord with the dome-like behavior of the SC gaps as calculated in [12]. By implication, the same doping dependence is expected in $\Omega_{\text{QPI}}^{1,2}$. Even in a multi SC gaps pnictide system, such one-to-one correspondence is possible as all gaps show similar dome-like doping dependence [22, 23, 25]. The areas of the hole pockets increase with hole doping; simultaneously the area of the electron pocket decreases. This doping dependence is reversed for electron doping. Therefore, all $q$ vectors
Figure 1. (a) Computed FS for iron-pnictide within the five band tight-binding model at a representative electron doping of $x = 0.1$. The BZ is chosen for 1 Fe unit cell notation. The black to white background depicts the $s^{\pm}$-pairing symmetry which takes the form of $2 \cos(k_x a) \cos(k_y a)$ in the 1 Fe unit cell. The arrows give different interband scattering channels which constitute QPI and INS maps. (b1) According to equation (5), the QPI map at $|\Delta_\beta| < |\Delta_\alpha| \approx |\Delta_\gamma|$ only reveals the intraband scattering (schematic) within the $\beta$-FS pocket. (b2) All possible interband scatterings from $\alpha \rightarrow \gamma$-FS ($q_1$) and from $\gamma \rightarrow \gamma$-FS ($q_{3,4}$), but not from $\beta \rightarrow \gamma$-FS ($q_2$), become turned on at $\Omega_{\text{QPI}}$. (c1) Due to the inelastic scattering process in INS, only the scattering between $\alpha$- or $\beta$- and $\gamma$-FSs is allowed which changes the sign of the SC gap, according to equation (11). $q_4$ for the $\beta \rightarrow \gamma$-FS appears at $\Omega_{\text{INS}} = |\Delta_\beta| + |\Delta_\gamma|$ in (c1). $q_3$ for the $\alpha \rightarrow \gamma$-FS appears at $\Omega_{\text{INS}} = |\Delta_\alpha| + |\Delta_\gamma|$ in (c2). As $|\Delta_\alpha| \approx |\Delta_\gamma|$, the INS spectrum in (c2) will resemble the QPI map in (b2) at zero magnetic field. Note that in the INS calculation, we have not included the Umklapp scattering which will symmetrize the INS spectrum with respect to the Umklapp vector $Q$. This is done to facilitate the direct comparison with QPI maps which are not calculated using Umklapp scattering to mimic the experimental procedure.

3.1. Computed QPI maps of iron-pnictide

We compute the QPI maps for pnictide using equation (4) for the FSs given in figure 1(a). All the results presented in figure 2 scale linearly with the SC gap magnitude as the relationship given in equation (12) is maintained always.
Figure 2. (a1) Computed QPI map at $\Omega_{\text{QPI}} = |\Delta_\beta|$. As sketched in figure 1(b1), at this energy the $\mathbf{q}$ vectors come from intraband scattering within the $\beta$-FS which is concentrated near $\mathbf{q} = 0$. The weak intensity at $\mathbf{q}_2$ comes from finite broadening of the quasiparticle states at the $\gamma$-pocket which allows some spectral weight of this band to appear around $\Omega_{\text{QPI}} = |\Delta_\gamma|$. (a2) Same as (a1) but at $\Omega_{\text{QPI}} = |\Delta_\alpha| \approx |\Delta_\gamma|$. The results agree qualitatively with earlier ones [37], even after neglecting the orbital matrix element term in our case. However, we do not see the QPI pattern as being present apart from these two energy scales, unless a large lifetime broadening is used in the calculation to smear out the quasiparticle states. (b1), (b2) Corresponding experimental QPI data at these two energy scales for electron doped pnictide at $x = 0.06$ taken from [25]. The experimental data show all four $\mathbf{q}$ vectors depicted in figure 1 at the two energies, although their relative intensities are representative of our calculations in (a1) and (a2), respectively, due to the low experimental resolution. As our phenomenological calculation did not capture the actual intensities of the QPI maps, we normalize all QPI maps to their maxima. (c1), (c2) Experimental data [40] for a 111 compound LiFeAs at two bias energies, $\Omega_{\text{QPI}} = -1.9$ meV in (c1), and $\Omega_{\text{QPI}} = -11.7$ meV in (c2). Despite the differences in the FS topology for this 111 and our 122 system, we see that both results are in qualitative agreement. The experimental value of $\Delta$ for LiFeAs is 10 meV, which makes the result (c2) slightly above the SC region [40].

We will not include the scattering matrix element $C$ (i.e., equations (6) and (7)) in this case to theoretically study the behavior of all $\mathbf{q}$ vectors as a function of energy. The computed results follow a similar behavior to that sketched in figure 1, demonstrating that most of the evolution of the QPI maps can be understood from the simple energy and momentum conservation rules derived in equations (5)–(7).

All the intraband scattering vectors lie so close to the strong elastic peak at $\mathbf{q} = 0$ that it is often difficult to distinguish. We have taken the broadening to be $\eta = 1$ meV which is sufficient for the quasiparticle states at $\omega = |\Delta_\gamma|$ to extend up to $\omega = |\Delta_\beta|$, allowing some elastic scattering at $\mathbf{q}_2$ in figure 2(a1) (although it is prohibited in a clean limit). But our small broadening does not create visible intensity at
Figure 3. (a) Computed INS map at $\Omega_{\text{INS}}^1 = |\Delta_\alpha| + |\Delta_\gamma|$ in 1 Fe unit cell notation. The intensity peak shifts away from $\left(\pi, 0\right)$, implying that the corresponding resonance peak is incommensurate due to the shapes of the FSs. (b) The same as (a) but at $\Omega_{\text{INS}}^2 = |\Delta_\alpha| + |\Delta_\gamma|$. The $q_1$ peak is closer to the commensurate vector than $q_2$ in (a) as the $\alpha$-FS pocket is smaller than the $\beta$-one. The $q$ values are strongly dependent on the FS areas, and hence on the doping. The results are consistent with the calculated spin-excitation dispersion plot presented in [12] in the 2 Fe unit cell. Both the incommensurate and the commensurate resonance peaks are observed in INS experiments [42, 43].

Note that the QPI maps shown in figures 2(a1) and (a2) will match exactly with (a) and (b), respectively, if a strong magnetic field is applied in the former case to eliminate the scattering of the same sign of the SC gaps. (c), (d) Experimental data for LiFeAs are presented at $\Omega_{\text{INS}}^1 = 5$ meV and $\Omega_{\text{INS}}^2 = 10$ meV from [44]. The data are rotated by 45° as they are available in the 2 Fe unit cell notation, while the present calculation is performed in the 1 Fe unit cell notation.

all other interband vectors, although the experimental data at the corresponding energy show some finite intensity at them, compare figure 2(a1) with the corresponding experimental data in figure 2(b1).

At $\Omega_{\text{QPI}}^2 = |\Delta_\alpha| \approx |\Delta_\gamma|$ all interband scattering vectors between the $\alpha$ and $\gamma$ FS appear on the QPI map as shown in figure 2(a2). As at $\Omega_{\text{QPI}}^1$, the $q_2$ vector can only show up at $\Omega_{\text{QPI}}^2$ due to residual broadening of the $\beta$ states up to the $\gamma$-pocket. The separation between $q_1$ and $q_3$ can be studied more clearly in the overdoped region of the hole doped side where the areas of the $\alpha$ and $\beta$ bands are distinguishably different.

The experimental data in figure 2(b2) also show all the calculated $q$ vectors. Subtle discrepancies in the relative intensities of each $q$ vector are expected, because we have not included any matrix element $M$ or the scattering coherence factor $C$ in this calculation. Furthermore, the magnitude of each $q$ vector does not match quantitatively with our calculation as the calculation is carried out at a different doping from the experimental data, although in both cases all three FS pockets are present. As both QPI and INS data are available as a function of momentum and energy for 111 family LiFeAs, we also compare our theory with these data. As shown in figures 2(c1) and (c2), the experimental data [40] qualitatively agree with the QPI vectors presented in the top panel. In performing such a comparison, we have to pay attention to the difference in FS topology and SC gap symmetries between the 122 and 111 families.

Once a magnetic field is applied, the relative intensity of $q_1$ with respect to that of $q_3, 4$ evolves with the strength of the field. This has been observed in Fe(Se, Te) compounds, in accord with our calculations [17–19].

The proximity of $q_4$ to the reciprocal vector $(\pi, 0)$ and its equivalent directions, which has been observed both in pnictide [25] and in iron-chalcogenide [17], has been argued theoretically to arise from the Bragg peak, instead of QPI scattering [41]. Comparing the evolution of the intensity of $q_4$ at two energies, $\Omega_{\text{QPI}}^2$ in figure 2(a1) and $\Omega_{\text{QPI}}^2$ in figure 2(a2), we can deduce that it is not associated with the Bragg peak as the latter does not have any energy dependence while $q_4$ has.
Figure 4. (a) Computed FS for a layered iron-selenide $K_xFe_2Se_2$ system within the two band tight-binding model in a representative 1 Fe unit cell notation. The black to white background depicts the $d_{x^2−y^2}$-pairing symmetry which takes the form of $\cos(k_x a) − \cos(k_y a)$ in the 1 Fe unit cell and a $d_{xy}$-wave in the 2 Fe unit cell (not shown) [7, 8]. The arrows give two interband scattering channels that survive in this class of material, compared to iron-pnictide in figure 1(a). (b1) Sketch of the QPI map according to equation (5) (the associated scattering matrix element which determines the sign of the SC state of the initial and final states is ignored here). (b2) The computed QPI map shows all the $q$-vectors predicted in (b1). The small differences in the magnitudes of the $q$-vectors from the two concentric electron pockets are not distinguishable due to finite broadening. (c1) In the INS spectrum, $q_1$ does not show up as it connects the quasiparticle state of same sign of the SC gap. (c2) The corresponding computational result of the INS spectrum at $Q_{INS} = 2Q_{QPI}$. The resonance spectrum is commensurate at $(\pi, \pi)$, while the inclusion of the orbital matrix element $M$ shifts it to be slightly incommensurate at a critical value of the interaction $U$ [7]. Our prediction agrees with recent INS measurements in this class of material [33].

3.2. Computed INS maps of iron-pnictide

The INS spectrum, a direct measure of $\chi''$, is calculated using equation (9) and the results are shown in figures 3(a) and (b) at two energies where the INS spectrum is finite. The present phenomenological approach does not include the overlap matrix element $M$ or the RPA correction. We have shown earlier in [12] that they do not change the essential features of the INS for these systems, except, of course, the intensity. $q_2$ and $q_1$ appear at $Q_{INS}^1$ and $Q_{INS}^2$, respectively, as expected, because they involve sign change of the SC gaps.
Figure 5. (a) Computed QPI result of K$_x$Fe$_{2−x}$Se$_2$ using equations (5) and (6) which mimics the zero magnetic field ($B$) condition. In this case, the QPI vectors which correspond to the scattering of states having opposite sign of the SC gaps become active [16]. (b) The same as (a) but using equations (5) and (7). This means that only scatterings of the same sign of the quasiparticle states which mimic a finite applied magnetic field condition are included. In principle, a magnetic impurity has a scalar component which will allow some scattering for the $q_1$ vector as well but of relatively weak intensity. (c) The differences between (a) and (b). The positions of the maxima and minima correspond to $q_1$ and $q_2$, respectively. This is an unambiguous method to find out which scattering channel involves sign change of the SC gap, a test which will confirm the presence of a d-wave gap in these materials.

between the initial and final states, $q_2$, being smaller than $q_1$, will lead to an incommensurate resonance while the latter is close to the commensurate one (both are doping dependent as described above). Both the commensurate [42] and the incommensurate [43] resonances have been detected by INS measurements, although the simultaneous presence of the two modes is yet to be detected in future measurements with better experimental resolution. The experimental data [44] for LiFeAs in figures 3(c) and (d) are consistent with the energy dependence of the $q_2$ and $q_1$ vectors.

As mentioned earlier, the INS maps will correspond to the QPI maps if the latter are performed at zero magnetic field. For the experimental data on LiFeAs, such a comparison between figures 2(c1) and (c2) for the QPI patterns and figures 3(c) and (d) for INS reveals good agreement.

4. Layered iron-selenide

**FS properties.** We turn next to the layered K$_x$Fe$_{2−x}$Se$_2$ based systems. These materials host only electron pockets at the M point with no hole pockets [45]. To model such electronic structure, we employ a two band tight-binding calculation of the t$_{2g}$ orbitals of the Fe d bands and the parameters are obtained by fitting to the material specific LDA dispersion [7]. The resulting FSs are shown by green lines in figure 4(a), and match well with ARPES FSs [45].

**SC gap properties.** The absence of hole pockets results in strong nesting between the electron pockets along $q_3$. We have shown earlier that such nesting leads to nodeless and isotropic d$_{x^2−y^2}$-pairing symmetry (in the 2 Fe unit cell the pairing symmetry becomes d$_{xy}$ [8]) and a spin resonance near the commensurate vector $q_3$ [7]. The spin resonance has recently been found experimentally in this class of material by Park et al [33].

**QPI and INS spectra.** Due to one SC gap and one FS (concentric electron pockets), both the QPI and INS maps appear only at one energy scale. The QPI map in this material as shown in figure 4(b1) resembles the QPI map for pnictide in figure 2(b2), with the exception that the electron–hole scattering $q_2$ is absent here. On the other hand, the INS spectrum (figure 4(c)) is rotated by 45° in comparison with the same plot for pnictide in figure 3(b) as the ‘hot-spot’ for sign-reversal of the SC gap is now aligned along $q_3$. It is interesting to note that although $q_3$ scattering is also present in pnictide as seen in the QPI maps, the leading nesting shifts along $q_1$, giving a very different pairing symmetry. This observation leads us to conclude that subtle differences between the nesting and the scattering which can carry rich physical insight can be untangled more clearly by comparing the QPI and INS spectra.

4.1. Magnetic field-dependent QPI maps

As mentioned before, another way to distinguish the scattering and nesting vectors in the QPI map is to study its magnetic field dependence at fixed energy. At zero magnetic field, the scattering matrix element $C$ only allows scattering of quasiparticle states of opposite phase of the SC gap, see equation (6). Therefore, the resulting QPI map at $\Omega_{QPI}$ will resemble the INS spectrum at $\Omega_{INS} = 2\Omega_{QPI}$, although the $q = 0$ elastic peak will be difficult to remove in the former case.

At finite magnetic field, the other scattering channel, $q_4$, at which the scattering from states of same sign of the SC gap becomes turned on is shown in figure 5(b). In practice, a magnetic impurity is always associated with a scalar component (not considered in the present calculation for simplicity), therefore $q_3$ should also be present. The relative intensity can be monitored by tuning the strength of the magnetic field [16, 17]. On the other hand, the difference between the QPI maps in figures 5(a) and (b), as shown in figure 5(c), can also be used to identify the sign-changing ‘hot-spot’ vector. The positions of the maxima and minima correspond to $q_3$ and $q_4$, respectively. The experimental detection of the maxima and minima can be tested to confirm the presence of a d-wave gap in these materials.
5. Conclusions

We have developed a phenomenological approach that allows one to connect the INS and QPI maps. We point out that the INS and QPI maps arise due to the inelastic and elastic scattering of the Bogoliubov quasiparticles, respectively, and bear a one-to-one correspondence as a function of scattering vector and energy. In fact, inelastic and elastic scattering complements these two spectroscopies to quantitatively and unambiguously identify the nature of the pairing symmetry in unconventional superconductors. By applying our model in iron-pnictide and layered iron-selenide compounds, we show that the QPI maps at zero magnetic field correspond exactly to the INS spectra at their representative energy (the $q = 0$ elastic scattering and other spurious effects in the QPI maps can be ignored because of ‘contamination from Bragg peaks’). We also show that upon applying a magnetic field, the QPI scattering of the same sign of the SC gaps can be illuminated in layered iron-selenides and produce detectable changes in the QPI. We point out that evolution of the QPI maps can be implemented experimentally to test the possible nodeless d-wave pairing in this class of material.

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