Quasiparticle scattering interference in (K,Tl)Fe$_x$Se$_2$ superconductors

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Abstract – We model the quasiparticle interference (QPI) pattern in the recently discovered (K,Tl)Fe$_x$Se$_2$ superconductors. We show in the superconducting state that, due to the absence of hole pockets at the Brillouin zone center, the quasiparticle scattering occurs around the momentum transfer $q = (0,0)$ and $(\pm \pi, \pm \pi)$ between electron pockets located at the zone boundary. More importantly, although both $d_{x^2-y^2}$-wave and $s$-wave pairing symmetries lead to nodeless quasiparticle excitations, distinct QPI features are predicted between both types of pairing symmetry. The so-called Z-map of the QPI exhibits strongest scattering with $q = (\pm \pi, \pm \pi)$ for the $d_{x^2-y^2}$-wave pairing symmetry, which is absent in the case of an isotropic $s$-wave pairing symmetry. The significant contrast in the QPI pattern between the $d_{x^2-y^2}$-wave and the isotropic $s$-wave pairing symmetry can be used to probe the pairing symmetry within the Fourier-transform STM technique.

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Introduction. – The very recent discovery of high-$T_c$ (above 30 K) superconductivity in AFe$_x$Se$_2$ (A = K, Tl, Cs) [1–3] has generated new excitement. Relative to other iron-based superconductors (such as LaOFeAs, BaFe$_2$As$_2$, FeSe etc.), the end members, TlFe$_2$Se$_2$ and KFe$_2$Se$_2$ (called as the “122” iron-selenides), are heavily electron doped (0.5 electron/Fe). Band structure calculations [4–8] on these end compounds show only electron pockets, primarily located around the M-point of the Brillouin zone (BZ) defined for a simple tetragonal structure. Angle-resolved photoemission spectroscopy (ARPES) measurements observed these electron-like Fermi surface pockets around the M-points, and showed either no hole-like pockets [9,10] or very weak electron-like pockets [11–13] near the zone center $\Gamma$. The strong Fe-deficient compound ($x \leq 1.6$) shows insulating behavior [3,14]. This is in contrast to other iron-based parent compounds, which are poor metals, raising the interest in the possibility of a Mott insulating state [15–18] induced by patterned Fe vacancies [19,20]. These observations add to the possibility that the pairing symmetry in the new compounds is unconventional. In particular, the absence of $\Gamma$-centered hole pockets would invalidate the popular $s_\pm$-type of pairing symmetry, which was proposed for earlier iron-based superconductors. Recent calculations have predicted that the superconducting state could have $d_{x^2-y^2}$-wave, [21–24] $s$-wave, [18] or $s_\pm$-wave [25] pairing symmetry. All these scenarios lead to nodeless superconducting gap structure, which is in agreement with the ARPES observations and other experiments. If the superconductivity arises solely around the electron pockets at the zone boundary in the “122” iron-selenides, phase-sensitive measurements [26] should be applicable to differentiate the pairing states. So far, this kind of measurements has not been reported yet.

Recently, one of the present authors and co-workers have proposed use of the existence or absence of intra-gap resonance states induced by a nonmagnetic impurity to probe the superconducting pairing symmetry. [27] It has been found that the impurity-induced resonance state can only exist for a $d_{x^2-y^2}$-wave pairing state. As mentioned above, since this $d_{x^2-y^2}$-wave pairing state does not introduce nodal quasiparticles, due to the unique Fermi surface topology, the impurity-induced resonance state is located near the superconducting gap edge and requires a strong potential scattering. An alternative technique, which can directly identify the sign change of the superconducting order parameter across various regions of the Fermi surface, is the quasiparticle interference (QPI) probe. This
technique has made a great advance in understanding low-energy quasiparticle properties and superconducting gap symmetry in high-$T_c$ cuprates [28–30]. The underlying principle for the QPI is that even a weak impurity scattering will mix two electronic states with two different momenta but on the same energy shell contour in the Brillouin zone, and the resultant momentum transfer (or scattering interference pattern) corresponds to the modulation in the local density of states, which can be measured by the Fourier-transform STM technique [31]. The analysis of QPI in the presence of impurity scattering has been theoretically proposed [32,33] to probe the pairing symmetry in earlier iron-based superconductors. Results of later QPI measurements [34] are consistent with the scenario of the order parameter having a sign reversal across the electron and hole pockets. Recently, the QPI signatures have also been discussed either for the whole phase diagram, including the metallic spin-density wave order [35], or in the presence of a magnetic field [36].

Motivated by this recent success, here we perform a detailed analysis of QPI in the newly discovered “122” iron-selenide superconductors. Both nonmagnetic and magnetic impurity scatterings are considered. We demonstrate a pronounced difference in the QPI characteristic of a simple $s$-wave and $d_{x^2-y^2}$-wave pairing symmetry. Because the Fermi surfaces of the new (K,Tl)Fe$_2$Se$_2$ compounds comprise small pockets of only one type of carrier, this kind of study will also provide an opportunity to identify the unique role of Fermi surface topology on the QPI pattern even for the same pairing symmetry.

**QPI methodology.**—As we have mentioned above, in the superconducting “122” iron selenides, there is either no hole pocket or faint features of electron pocket at the zone center. For the case of electron pocket at the zone center, because of the faint feature (that is, weak spectral intensity), its existence will at most yield some additional QPI pattern with weak intensity. Therefore, we consider here a simplified single-band model, which enables us to obtain a full understanding of the QPI pattern due to the different Fermi surface topology and pairing symmetry. Recently, similar simplified single-band models (Hubbard model and $t$-$J$-type model) were also used to discuss the magnetism and superconductivity in “122” iron selenides [37,38]. The model Hamiltonian is defined on a two-dimensional (2D) square lattice and consists of the pristine and impurity scattering parts, $H = H_0 + H_{imp}$. The pristine part $H_0$ is

$$H = \sum_{k,\sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_k [\Delta_k c_{k\uparrow}^\dagger c_{k\downarrow} + H.c.].$$

(1)

Here the operators $c_{k\sigma}$ ($c_{k\sigma}^\dagger$) create (annihilate) an electron with momentum $k$ and spin $\sigma$. The quantity $\xi_k$ denotes the energy dispersion. We consider only the singlet pairing and the superconducting gap function is described by $\Delta_k$. The impurity scattering part is given by

$$H_{imp} = \sum_{\sigma} [U_s + \sigma U_m] c_{0\sigma}^\dagger c_{0\sigma},$$

(2)

where the first term represents the zero-range normal potential scattering from a nonmagnetic impurity located at the origin of the lattice (for mathematical convenience) and the scattering strength is denoted as $U_s$, while the second term describes the scattering from a magnetic impurity with strength $U_m$.

For our purpose here, we calculate the Green’s function in the presence of either a nonmagnetic impurity or pair potential impurity scattering, which is defined as

$$\hat{G}(ij;\tau) = -\langle T_\tau [\hat{\Psi}(\tau)\hat{\Psi}^\dagger] \rangle$$

with $\hat{\Psi} = (c_{i\uparrow}, c_{i\downarrow})$ as a two-component operator in the Nambu space. Within the $T$-matrix method, the Green’s function is obtained as

$$\hat{G}(i,j;\omega_n) = \hat{G}_0(i,j;\omega_n) + \hat{G}_0(i,0;\omega_n) \hat{T}(\omega_n) \hat{G}_0(0,j;\omega_n),$$

(3)

where $\omega_n = (2n + 1)\pi T$ is the Matsubara frequency with $n$ an integer and $T$ the electronic temperature, and $\hat{G}_0(i,j;\omega_n)$ is the real-space Green’s function for the pristine system. The $T$-matrix is given by

$$\hat{T}(\omega_n) = \hat{V} \hat{G}_0(0,0;\omega_n) \hat{V}^{-1},$$

(4)

where $\hat{V} = U_s \tau_3 + U_m \tau_0$ with $\tau_0$ and $\tau_3$ are the components of Pauli matrices in Nambu space.

From now on, we will term the usual nonmagnetic impurity scattering $\tau_3$-scattering and the scattering off a pair potential impurity $\tau_1$-scattering. We emphasize again that the latter type of scattering is more relevant to the STM measurements of samples in the presence of vortices. The QPI is characterized by the Fourier-transform of the local density of states (LDOS), that is

$$\hat{T}(\omega_n) = \hat{V} \hat{G}_0(0,0;\omega_n) \hat{V}^{-1},$$

where $\hat{V} = U_s \tau_3 + U_m \tau_0$ with $\tau_0$ and $\tau_3$ are the components of Pauli matrices in Nambu space.

The LDOS is given by

$$\rho_{\gamma} (\omega) = \frac{1}{N \tau} \sum_k \rho_k (\omega) e^{-\frac{\omega}{\tau}},$$

Here the LDOS is given by

$$\rho_k (\omega) = \frac{1}{N \tau} \sum_{\gamma} \rho_{\gamma} (\omega) e^{-\frac{\omega}{\tau}},$$

with $\rho_{\gamma}$ being the site-diagonal normal (electron) component of the matrix Green’s function. Note that we have measured the LDOS in the presence of the impurity scattering by removing the uniform background. In the weak scattering limit, a little algebra yields [39]

$$\rho_k (\omega) = \frac{U_0}{N \tau} \sum_k \left[ [A_k (\omega) B_{k+q} (\omega) + B_k (\omega) A_{k+q} (\omega)] - [J_k (\omega) K_{k+q} (\omega) + K_k (\omega) J_{k+q} (\omega)] \right],$$

(5)

where the functions $A$, $B$, $J$, and $K$ are defined as

$$A(J) = -\langle 2/\pi \rangle \text{Im} [\hat{G}_{0,11}(\omega_k; \omega)]$$

and $B(K) = \text{Re} [\hat{G}_{0,11}(\omega_k; \omega)]$. Note that in the first-order approximation, there is no contribution from the magnetic potential scattering. Equation (5) shows that the QPI pattern is determined by the convolution of the bare Green’s functions in momentum space, which occurs between either normal Green’s functions or anomalous
ones (with a negative sign). These bare Green’s functions are given by

\( G_{0,11}(k; E) = \frac{u_k^2}{E - E_k} + \frac{v_k^2}{E + E_k}, \) \hspace{1cm} (6)

\( G_{0,12}(k; E) = u_k v_k \left[ \frac{1}{E - E_k} - \frac{1}{E + E_k} \right] , \) \hspace{1cm} (7)

where the quasiparticle energy \( E_k = \sqrt{\xi_k^2 + \Delta_k^2} \), and \( u_k = \sqrt{(1 + \xi_k/E_k)/2} \) and \( v_k = \text{sign} (\Delta_k) \sqrt{(1 - \xi_k/E_k)/2} \) are the electron and hole parts of the Bogoliubov wave function amplitude, respectively. Therefore, for a given momentum \( k \), the contribution to the Fourier amplitude \( \rho_0(E) \) is sensitive to the sign of \( v_k u_k \), which holds the key to revealing the uniqueness of a superconducting pairing symmetry in the QPI measurements.

Quasiparticle density of states and momentum-dependence of spectral functions. – Before we present the numerical results on the QPI, we point out that, for unconventional pairing symmetry, the quasiparticle energy is very sensitive to the Fermi surface topology. To illustrate this point, we consider the normal-state energy dispersion:

\[ \xi_k = -2t (\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu, \] \hspace{1cm} (8)

where \( t \) and \( t' \) are the nearest-neighbor and next-nearest-neighbor hopping integrals and \( \mu \) is the chemical potential. If, as is relevant to high-\( T_c \) cuprates, we take \( t = 1 \), \( t' = -0.3 \), and \( \mu = -1.0 \), the Fermi pockets are centered around the \((\pi, \pi)\) and equivalents in the BZ, as shown in fig. 1(a1). These pockets are cut by the zone diagonals, which makes the quasiparticle excitations gapless in the \( d_{x^2-y^2} \)-wave pairing symmetry, \( \Delta_k = (\Delta_0/2)(\cos k_x - \cos k_y)/2 \), and yields a \( V \)-shaped profile of quasiparticle density of states around the Fermi energy (see fig. 1(a2)). This enables the analysis of QPI in cuprates to provide a detailed band structure and \( d_{x^2-y^2} \)-wave gap structure [28–30]. However, if we take \( t = 0 \), \( t' = -1 \), and \( \mu = -3 \), as a simplified model of the band structure in the “122” iron selenides, the Fermi pockets are centered around the \((\pi, 0)\) point and equivalents in the BZ (see fig. 1(b1)). Due to the low density of electrons, these Fermi pockets are small in cross-section and, as revealed experimentally [9], are nearly isotropic. In this situation, the quasiparticle excitations are fully gapped and a well-shaped density of states profile is obtained (see fig. 1(b2)). For the isotropic \( s \)-wave pairing symmetry, the quasiparticle excitations are always fully gapped, irrespective of the detailed Fermi surface topology (see fig. 1(a2), (b2)). This explains why both \( d_{x^2-y^2} \)-wave and isotropic \( s \)-wave pairing symmetry scenarios are competing candidates for the photoemission spectroscopy measurements in “122” iron selenides. To further clarify the distinct feature of nodeless \( d \)-wave pairing symmetry as compared with its \( s \)-wave counterpart, we plot in figs. 2 and 3 both the imaginary and real parts of momentum-dependent Green’s functions

\( G_{0,11} \) and \( G_{0,12} \) for an energy near the coherent peak position. Again one can see that \( G_{0,11} \) does not show a sign reversal when the wave vector crosses between two electron pockets for both the nodeless \( d_{x^2-y^2} \)-wave and the isotropic \( s \)-wave pairing symmetry; while the \( G_{0,12} \) exhibits a sign change for only the nodeless \( d_{x^2-y^2} \)-wave pairing symmetry. Because the anomalous Green’s
The QPI would be a powerful technique to clarify the pairing symmetry. The QPI pattern exhibits a ring-like structure around the Fermi surface pockets just as in the normal state. Interestingly, the maximum intensity occurs at \( q = (\pm \pi, \pm \pi) \), regardless of whether the quasiparticle scattering is nonmagnetic or magnetic. For the s-wave pairing symmetry, as shown in fig. 5, the QPI pattern also shows a ring-like structure, reinforcing the suggestion that this part of the QPI pattern is due to the scattering between normal-state Fermi surface pockets. However, the maximum intensity at \( q = (\pm \pi, \pm \pi) \) only occurs in the presence of magnetic potential scattering.

To place our study into the context of STM experiments, we consider the so-called Z-map of the QPI pattern. In STM experiments, the differential tunneling conductance at a location \( r \) and voltage \( V \) is usually the product of the local tunneling matrix element and the local density of states. To filter out the spatial variation in the tunneling matrix element, it is now a common practice to measure the conductance ratio,

\[
Z_i(E) = \frac{\rho_i(E)}{\rho_i(-E)} - \frac{\rho_0(E)}{\rho_0(-E)}.
\]

Here \( \rho_0(\pm E) \) describe the sample-averaged local density of states and in our study the density of states for the pristine system. This serves to remove the background intensity, which is peaked at \( q = 0 \) in the momentum transfer space.
For the nonmagnetic (a) and magnetic (b) impurity scattering at energy $E = 0.1$ with nodeless $d_{x^2-y^2}$-wave pairing symmetry.

Fig. 7: (Color online) The renormalized QPI maps, $|Z_{q}(E)|$, for the nonmagnetic (a) and magnetic (b) impurity scattering with isotropic $s$-wave pairing symmetry at energy $E = 0.1$.

We have also calculated the local density of states at the negative energy $-E$. With the given real-space $Z_{q}(E)$, we perform the Fourier transform to obtain the $Z$-map of QPI, as defined as $|Z_{q}(E)|$.

Figures 6 and 7 show the $Z$-maps of QPI patterns in the presence of either nonmagnetic or magnetic potential scattering for the nodeless $d_{x^2-y^2}$-wave and isotropic $s$-wave pairing symmetries. As shown in fig. 6, for the nodeless $d_{x^2-y^2}$-wave pairing symmetry, the $Z$-map exhibits a ring-like structure with significantly weak intensity but strongly enhanced intensity at $q = (\pm \pi, \pm \pi)$, regardless of the potential scattering being nonmagnetic or magnetic. However, for the isotropic $s$-wave pairing symmetry, opposite to the case of $d_{x^2-y^2}$-wave pairing symmetry, the $Z$-map of the QPI exhibits the ring-structure with a dramatically enhanced intensity but has a completely suppressed intensity at $q = (\pm \pi, \pm \pi)$. This sharp contrast of the $Z$-map between the $d_{x^2-y^2}$-wave and isotropic $s$-wave pairing symmetries provides a unique opportunity for the application of STM to reveal the superconducting pairing symmetry in “122” iron selenide superconductors.

Summary and concluding remarks. – We have studied the quasiparticle interference pattern due to both nonmagnetic and magnetic impurity scattering in the recently discovered “122” iron selenide superconductors. We have shown in the superconducting state that, although both $d_{x^2-y^2}$-wave and $s$-wave pairing symmetries lead to nodeless quasiparticle excitations, they have quite different consequence in the QPI maps. In particular, it has been found that the $Z$-map of the QPI patterns exhibits the strongest scattering with momentum transfer $q = (\pm \pi, \pm \pi)$ for the $d_{x^2-y^2}$-wave pairing symmetry, which is absent for the $s$-wave pairing symmetry. The significant contrast in the QPI patterns between the $d_{x^2-y^2}$-wave and the isotropic $s$-wave pairing symmetries in the presence of the same type of impurity scattering can be very efficient for probing the pairing symmetry in the “122” iron selenide superconductors within the Fourier-transform STM technique.

Note that our study is based on a simplified single-band model for the “122” iron selenide superconductors. On the one hand, this captures the essence of having only electron Fermi surface pockets at the zone boundary; and the choice of the simplified model has the advantage of bringing high-$T_c$ cuprates into contrast even if “122” iron selenide superconductors share the same pairing symmetry. On the other hand, we have also performed calculations of the QPI maps based on a model with a more realistic band structure [24,27], and confirmed the robustness of the QPI contrast between the nodeless $d_{x^2-y^2}$-wave and isotropic $s$-wave pairing symmetries.

We further note that the QPI analysis for the earlier iron pnictide superconductors with $s_{\pm}$-wave pairing symmetry [32,33,35] shows the most pronounced scattering at $q = (\pm \pi, 0) \pm (0, \pm \pi)$, which is between the electron (at the $M$-point in the BZ) and hole (at the $\Gamma$-point in the BZ) pockets. For the “122” iron selenide superconductors, due to the absence of the hole pockets at the BZ center, the quasiparticle scattering can only occur between the electron pockets and the QPI pattern shows pronounced structure around $q = (0,0) \pm (\pm \pi, \pm \pi)$ for either $d_{x^2-y^2}$-wave or isotropic $s$-wave pairing symmetry.

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