Gap function of hexagonal pnictide superconductor SrPtAs from quasiparticle interference spectrum

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Abstract - The pnictide superconductor SrPtAs has a hexagonal layered structure containing inversion symmetry. It is formed by stacking two inequivalent PtAs layers separated by Sr layers. The former have no local (in-plane) inversion symmetry and, therefore, a (layer-)staggered Rashba spin orbit coupling appears which splits the three Kramers degenerate bands per layer into six quasi-2D bands. The symmetry of the superconducting state of SrPtAs is unknown. Three candidates, spin-singlet $A_{1g}$ and $E_g$ as well as triplet $A_{2u}$ states have been proposed. We predict the quasiparticle interference (QPI) spectrum for these gap functions in $t$-matrix Born approximation. We show that distinct differences in the pattern of characteristic QPI wave vectors appear. These results may be important to determine the gap symmetry of SrPtAs by STM-QPI method.

Transition metal pnictide superconductors (SC), in particular the Fe-based systems, are all of the tetragonal (orthorhombic) structure. The layered Pt-pnictide SrPtAs [1] is the first superconductor ($T_c = 2.4$ K) in that class with hexagonal structure composed of honeycomb PtAs layers spaced by Sr layers. It may be viewed as a MgB$_2$-type structure with Mg sites occupied by Sr and B sites in an ordered fashion such that PtAs alternate in the 2D honeycomb layers as well along the hexagonal c-axis. The resulting structure has an overall 3D inversion center whereas the individual layers lack 2D inversion symmetry which is not contained in the $C_{3v}$ layer point group.

Because the electronic states at the Fermi level are mostly of Pt(5d) type with strong spin orbit coupling this leads to a peculiar electronic band structure [2]. Firstly the two inequivalent PtAs layers have only small interlayer hopping which results in a quasi-2D band structure consisting of three hole bands and associated Fermi surface (FS) columns. Secondly an effective 2D Rashba spin orbit coupling term leads to a large splitting of the three bands which depends on $k_z$ in such a way that overall 3D inversion symmetry is restored.

This has consequences for the possible superconducting pair states. Due to essentially decoupled layers it is reasonable to assume only intra-layer pairing. Then one can expect features as in the non-centrosymmetric superconductors consisting of a mixture of spin-singlet and triplet pairing of the in-plane order parameter due to the lack of local 2D inversion symmetry. For the overall 3D superconducting state even or odd parity classification is restored due to the two inequivalent Sr-Pt layers. The momentum dependence of these unconventional pair states was investigated theoretically by Goryo et al. [3] and it was found that even $A_{1g}$, $E_g$ and odd $A_{2u}$ states are viable candidates. However, so far there is only few experimental evidence to discriminate between them [4].

One of the most powerful recent methods to determine the symmetry of the gap function is the STM quasiparticle interference (QPI) technique [5]. The Fourier transform of the differential conductance scans as a function of bias voltage gives a fingerprint of the Fermi surface in the normal state and, in addition, of the $k$-dependence of the gap function in the SC state. It has by now been successfully applied to a variety of cuprate [6–12], Fe-pnictides [13–19], and heavy-fermion unconventional superconductors [20–22]. There are no STM results yet for the hexagonal pnictide SC SrPtAs.

Therefore, in this work we propose the application of QPI to investigate the SrPtAs SC gap function. We will compare the predicted QPI spectra for the three main gap
candidates discussed so far to provide criteria for discriminating among them in future STM experiments.

The one-body Hamiltonian for three SrPtAs hole bands of mixed As(4p)-Pt(5d) character close to the Fermi energy derived in ref. [2] and used in refs. [3,23] is given by

\[ H_0 = \sum_{k,l',s',b} c_{kl's'b}^b \epsilon_{kl's'b}^b + \sum_{k,l,s,b} \alpha_b \lambda_b \sigma b \epsilon_{kl's'b}^b, \tag{1} \]

where \( c_{kl's'b}^b \) creates conduction electrons with \( b = 1,2,3 \) denoting the (hole) band, \( l,l' = 1,2 \) the inequivalent PtAs layers and \( s = \pm \frac{1}{2} \) the (real) spin. Furthermore, \( \epsilon_{kl's'b}^b = \epsilon_{kl's'b}^0 - \mu_b \) (\( \mu \) = chemical potential) is the Fourier-transformed \( (l,k' = \text{layer}) \) hopping matrix and \( \alpha_b \lambda_b \) the Rashba-type spin orbit coupling matrix for the PtAs layers which lack inversion symmetry. They are given by

\[ \epsilon_{kl's'b}^0 = \begin{bmatrix} \epsilon_{kl's'b}^0 - \mu_b & \epsilon_{kl's'b}^b \\ \epsilon_{kl's'b}^b & - \mu_b \end{bmatrix}, \quad \lambda_b^s = \begin{bmatrix} \lambda_b^s & 0 \\ 0 & - \lambda_b^s \end{bmatrix}. \tag{2} \]

The intra-layer hopping is described by \( \epsilon_{kl's'b}^b \) and the interlayer hybridization by \( \epsilon_{kl's'b}^b \). Here \( \lambda_b^s \) has opposite signs for \( l = 1,2 \) to restore the global inversion symmetry. Its strength is given by the orbital (band) dependent Rashba coupling \( \alpha_b \). Explicitly [2,3],

\[ \epsilon_{kl's'b}^b = t_b \left[ \cos k_y a + 2 \cos \frac{\sqrt{3} k_x a}{2} \cos \frac{k_y a}{2} \right] + t_b' \cos k_z c, \]

\[ | \epsilon_{kl's'b}^b |^2 = t_b^2 \cos^2 \frac{k_z a}{2} \left[ 3 + 2 \cos k_y a + 4 \cos \frac{\sqrt{3} k_x a}{2} \cos \frac{k_y a}{2} \right], \]

\[ \lambda_b^s = \sin k_y a - 2 \cos \frac{\sqrt{3} k_x a}{2} \sin \frac{k_y a}{2}. \tag{3} \]

The hopping and Rashba parameters for realistic Fermi surface hole sheets [23] are given in fig. 1. From \( H_0 \) the normal state quasiparticle bands are

\[ \Omega_{b \pm}^k = (\epsilon_{kl's'b}^b - \mu_b) \pm \sqrt{| \epsilon_{kl's'b}^b |^2 + \alpha_b^2 \lambda_b^s}. \tag{4} \]

The Fermi surface cuts of the six bands \((b = 1-3, \pm)\) which are twofold Kramers (pseudo-spin) degenerate are shown in fig. 1 for the normal state. The difference between \( k_z = 0, \pi/c \) is due to the effect of interlayer hopping \( \epsilon_{kl's'b}^b \).

Possible superconducting gap functions were proposed in refs. [3,23–25]. The most likely candidates are the even singlet \( A_{1g} \) and \( E_g \) and the odd triplet \( A_{1u} \) representations. Their explicit \( k \)-dependence on the six bands is given by

\[ A_{1g}: \Delta_{b \pm}^k = \Delta_b^0 (1 + s_0 \epsilon_b + t_b h_b), \]

\[ A_{2u}: \Delta_{b \pm}^k = \Delta_b^0 (s_0 + s_b \epsilon_b + h_b), \]

\[ E_g: \Delta_{b \pm}^k = \sum_{s = \pm} \Delta_0 (s \epsilon_b + t_b h_b), \tag{5} \]

where \( s = \pm \) denotes the time-reversed chiral states of \( E_g \) with \( \epsilon_b^s = \epsilon_{b,k} \pm ie_{b,k} \) and \( h_b^s = h_{b,k} \pm ih_{b,k} \). We use [2] for \( b = 1 \): \((1.25, 0.1, 0.05, 0.5, 0.4)\); for \( b = 2 \): \((1.0, 0.1, 0.05, 2.5, 0.28)\); and for \( b = 3 \): \((-0.48, 0.075, -0.03, 0.6, 0.046)\). \( q'_b \) are characteristic QPI scattering vectors.

\[ E_g(1,1): \Delta_b^k = 2 \Delta_0 (\epsilon_{b,k} \pm t_b h_b). \tag{6} \]

The (real) layer gap matrices in spin space \((\uparrow, \downarrow)\) are then given by

\[ \Delta_{k_1}^b = \begin{bmatrix} 0 & p \Delta_{b \uparrow}^k \\ -p \Delta_{b \downarrow}^k & 0 \end{bmatrix}, \quad \Delta_{k_2}^b = \begin{bmatrix} 0 & \Delta_{b \downarrow}^k \\ -\Delta_{b \uparrow}^k & 0 \end{bmatrix}, \tag{7} \]

with \( p \) denoting the gap parity \( p = 1 \) for \( A_{1g}, E_g \) and \( p = -1 \) for \( A_{1u} \). The form factors in eqs. (5), (6), (7) are defined by

\[ \epsilon_b = \cos k_y a + 2 \cos \frac{\sqrt{3} k_x a}{2} \cos \frac{k_y a}{2}, \]

\[ h_b = \sin k_y a - 2 \cos \frac{\sqrt{3} k_x a}{2} \sin \frac{k_y a}{2}, \tag{8} \]

for the non-degenerate \((A_{1g}, E_g)\) case and for the twofold degenerate \( E_g \) gap function we have

\[ \epsilon_{b,1} = \frac{1}{2} \epsilon_b, \quad h_{b,1} = \frac{1}{2} h_b, \quad \epsilon_{b,2} = \frac{\sqrt{3}}{2} \left[ \cos k_y a - \cos \frac{\sqrt{3} k_x a}{2} \right], \quad h_{b,2} = \frac{\sqrt{3}}{2} \sin k_y a - \sin \frac{\sqrt{3} k_x a}{2}. \tag{9} \]

Due to even \( \epsilon_b \) and odd \( h_b \) form factors, the gap elements in eqs. (5), (7) fulfill the relation \( \Delta_{b \pm}^k = \Delta_{b \mp}^k \).
where we define $\tilde{\epsilon}_k^b = \epsilon_k^b - \mu_b$ for each band. Then $G_B^{-1}(k, i\omega_n)$ may be obtained by substituting $\tilde{\lambda}_k^b \rightarrow -\lambda_k^b$ and $\Delta_{k\pm} \rightarrow -\Delta_{k\mp}$ in the above equation. Note that the model gap functions $A_{1g}$ and $A_{2u}$ of eq. (5) and $E_g(1,1)$ of eq. (6) are chosen real, i.e., $\Delta_{k\pm} = \Delta_{k\mp}$.

After inversion $G(k, i\omega_n)$ may be used to calculate the QPI spectrum $\tilde{\Lambda}_0(q, i\omega_n)$ which is proportional to the spatial Fourier transform of the STM differential conductance [5]. We assume that only a $q$-independent non-magnetic impurity scattering $U_c$ is present. For weak scattering with $U_c N_b(\mu) \ll 1$ ($N_b$ is DOS of band $b$) we may restrict ourselves to the Born approximation. Even when this is not valid, the full $t$-matrix theory gives very similar results for the $q$-space structure of the QPI function [27]. Within the Born approximation [28,29] it is given by $\tilde{\Lambda}_0(q, i\omega_n) = U_c \Lambda_0(q, i\omega_n)$ with (summation over $b$ is implied)

$$\Lambda_0(q, i\omega_n) = \frac{1}{2N} \sum_k tr_{\sigma\tau\kappa} \left[ \frac{1 + \gamma_{\tau}}{2} \tilde{G}_k \gamma_{\tau} \sigma_0 \tilde{G}_{k-q} \right].$$

The trace is performed with respect to Nambu spin ($\tau$), real spin ($\sigma$) and layer index ($\kappa$) where $\gamma_{\tau}$ is a Pauli matrix and $\sigma_0$, $\kappa_0$ are unit matrices.

First we discuss the purely 2D model for SrPtAs neglecting the dispersion along $k_z$ setting $\epsilon_k^b \equiv 0$. Then the Fermi surface cut for each $k_z$ is equivalent to that of fig. 1(b) ($k_z = \pi/c$) where $\epsilon_k^b \equiv 0$ vanishes even for the 3D case with finite interlayer hybridization. In the 2D model the Green’s function can be obtained easily by inverting eq. (11) due to $\epsilon_k^b \neq 0$. To perform the traces in eq. (12) it is convenient to transform $\tilde{G}(k, i\omega_n)$ to reordered spinor basis ($c_{k11}^\uparrow, c_{k11}^\downarrow, c_{k21}^\uparrow, c_{k21}^\downarrow$) for $A$ and ($c_{-k11}^\uparrow, c_{-k11}^\downarrow, c_{-k21}^\uparrow, c_{-k21}^\downarrow$) for $B$ we have

$$\tilde{\Lambda}_0(q, i\omega_n) = \frac{1}{2N} \sum_{k \xi} \frac{(i\omega_n + \epsilon_k^b)(i\omega_n + \epsilon_{k-q\xi}^b) - \Delta_k^b \Delta_{k-q\xi}^b}{[(i\omega_n)^2 - E_k^2][i\omega_n^2 - E_{k-q\xi}^2]}.$$
by a suitable definition of the Rashba split bands as in eq. (14) they do not appear explicitly in eq. (13). For the same reason the latter also describes the QPI spectrum for magnetic scattering in the Born approximation.

For the numerical calculation we use the general 3D QPI by including the interlayer hopping and its resulting $k_z$ dispersion. When $\epsilon_{c, k}$ is nonzero the quasiparticle excitation spectrum is obtained by the zeros of the determinant $D_b(k, \omega_n) = 0$ which is given by

$$D_b(k, \omega_n) = \left[ (\omega_n)^2 - E^{b_{2+}}_{k_+} \right] \left[ (\omega_n)^2 - E^{b_{2-}}_{k_-} \right] + |\epsilon_{c, k}|^4 - 2|\epsilon_{c, k}|^2 \left[ (\omega_n)^2 + (\tilde{\epsilon}_{b_{2+}} + \tilde{\epsilon}_{b_{2-}} - p\Delta^b_{k_+} - \Delta^b_{k_-}) \right].$$

The 3D quasiparticle energies $\Omega^b_{k_{\pm}}$, including the effect of interlayer hopping $\epsilon_{c, k}$ with dispersion along $k_z$, are obtained as

$$\Omega^b_{k_{\pm}} = \frac{1}{2}(E^{b_{2+}}_{k_+} + E^{b_{2-}}_{k_-}) + |\epsilon_{c, k}|^2 \pm \left[ \frac{1}{4}(E^{b_{2+}}_{k_+} - E^{b_{2-}}_{k_-})^2 \right] \times$$

$$\times \left[ (\tilde{\epsilon}_{b_{2+}} + \tilde{\epsilon}_{b_{2-}})^2 + (\Delta^b_{k_+} - p\Delta^b_{k_-})^2 \right]^\frac{1}{2}.$$ (16)

Here $\tilde{\epsilon}_{b_{2+}} + \tilde{\epsilon}_{b_{2-}} = 2\tilde{\epsilon}^b_{b_0, k}$. For $\Delta^b_{k_{\pm}} = 0$ we recover the quasiparticle bands $\Omega^b_{k_{\pm}}$ of the normal state in eq. (4). Obviously, for $\epsilon_{c, k} = 0$, the $\Omega^b_{k_{\pm}}$ reduce to the $\tilde{E}^b_{k_{\pm}}$ of eq. (14).

Then, after the inversion of eq. (11) and performing the trace in eq. (12), we obtain the general 3D QPI function as

See eq. (17) above

where $\xi = \pm$ and $\tilde{\xi} = -\xi$. The denominator in eq. (17) is equal to the product $D_b(k, \omega_n)D_b(k - q, \omega_n)$. The above expression for $A_0(q, \omega_n)$ reduces to the 2D expression in eq. (13) for $\epsilon_{c, k} = 0$. In contrast to eq. (13) the momentum integral also includes the $k_z$-direction in eq. (17). In the above expressions for $A_0(q, \omega_n)$ we have neglected terms $\sim |\epsilon_{c, k}|^2|\frac{\partial}{\partial k_z}|^4$ in the numerators since they influence only the amplitude.

Now we discuss the numerical results for the expected QPI spectrum calculated with eq. (17). It turns out that the influence of the $c$-axis dispersion in the bands is of little importance due to the smallness of $t^b_{k_x}$ in the present case of SrPtAs. Although small differences in the 3D QPI contribution of each individual $k_z$ slice are present, the integration along $k_z$ smoothes the differences to the simple 2D case described by eq. (13).

We first consider the normal state whose two cuts of spectral functions (2D) are shown in fig. 1. Particularly, in fig. 1(b) the Fermi surface is plotted for $k_z = \pi/c$ with the typical characteristic wave vectors denoted by $q^b_i$ ($i = 1$–6). The normal state DOS at the Fermi level is 74% of band-3 character [2]. The QPI should therefore be dominated by this band. Indeed this is found when considering the individual $b = 1$–3 contributions in eqs. (13), (17). The two main features in fig. 3(a) are a large central ring and touching arcs around the zone boundary (K) points. The ring is due to $q_6$ and $q_4$ scattering (fig. 1(b)) inside and between band-3 sheets (the dashed arrows are folded back into the first BZ). The arcs are due to $q_1$-type scattering between different band-3 sheets. When the voltage increases, the ring shrinks due to the hole-type bands. In addition, linear features perpendicular to the hexagonal sides appear. They are due to a continuum of $q_3''$-$q_6$ scattering with the result of the averaging over the different $k_z$ cuts.

The superconducting candidate states have very different nodal structure (fig. 2(a)–(c)) and, therefore, also different quasiparticle equal energy surfaces and associated characteristic scattering wave vectors $q_i$ ($i = 1$–8) (fig. 2(d)–(f)). This leads to three distinct QPI spectra for the gap candidates shown in fig. 4. They also exhibit a considerably different behavior as a function of bias voltage or frequency. A few characteristic wave vectors $q_i$ associated with the equal energy surfaces in (fig. 2(d)–(f)) can clearly be seen in the QPI spectrum of fig. 4 for low frequencies. In particular, the faint rings with $q_{1,2}$ due to the small $b = 2$ band are now visible in fig. 4(a,a) and (b,a) because the contribution of the $b = 3$ band is mostly gapped out for $A_{1g}$ and $A_{2u}$. For $E_q$ in fig. 4(c,a), however, the different node structure leads to particular scattering wave vectors ($q_{4-5}$), on $b = 1$ sheets. In principle, $q_{1,2}$ resemble the normal state $q_{1,2}$. For larger $\omega$ they also appear for $A_{2u}$ in fig. 4(b,b), (b,c). At still larger $\omega = 0.075$ some features of the normal state QPI at $q_{4,5}$ reappear in fig. 4(a,c)–(c,c). Also the scattering between different $b = 3$ sheets perpendicular to hexagonal BZ directions appears in the $E_q$ QPI of fig. 4(c,c).

To summarize we have presented the QPI theory in the Born approximation for a hexagonal pnictide.
superconductor SrPtAs. Its main hole band can be clearly identified in the normal state QPI. In the superconducting state the three candidate gap functions proposed in ref. [3] show different types of equal energy quasiparticle sheets leading to three distinct QPI pattern and bias voltage dependencies. Therefore, a detailed experimental investigation of QPI in SrPtAs should be able to discriminate between the theoretically proposed gap symmetries. This is particularly desirable because recent NMR and NQR experiments [4] suggest a fully gapped spin singlet state.

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