Full t-matrix approach to quasiparticle interference in non-centrosymmetric superconductors

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Abstract. We develop the full t-matrix theory of quasiparticle interference (QPI) for non-centrosymmetric (NCS) superconductors with Rashba spin-orbit coupling. We give a closed solution for the QPI spectrum for arbitrary combination and strength of nonmagnetic ($V_c$) and magnetic ($V_m$) impurity scattering potentials in terms of integrated normal and anomalous Green’s functions. The theory is applied to a realistic 2D model of the Ce-based 131-type heavy fermion superconductors. We discuss the QPI dependence on frequency, composition and strength of scattering and compare with Born approximation results. We show that the QPI pattern is remarkably stable against changes in the scattering model and can therefore give reliable information on the properties of Rashba-split Fermi surface sheets and in particular on the accidental nodal position of the mixed singlet-triplet gap function in NCS superconductors.

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1 Introduction

The determination of gap symmetry and nodal positions is the most important problem in unconventional superconductors (SC). Various methods are available that give at least a partial knowledge on the gap properties. Particular useful methods for this purpose are angle-resolved photoemission spectroscopy (ARPES) experiments [1,2], specific heat and thermal transport measurements in a rotating field [3] which are based on the Doppler-shift effect. More recently STM-based quasiparticle interference technique (QPI) has been applied which utilizes the ripples in electronic density generated by random magnetic or non-magnetic surface impurities. In the normal state they are determined only by the shape of the Fermi surface sheets if the impurity scattering is isotropic. However, in the superconducting state the opening of an anisotropic gap introduces typical changes in the shape of the QPI spectrum from which information on the gap symmetry may be obtained. Experimentally this method has been used, e.g. in cuprates [4,5] and Fe-pnictides [6,7]. Theoretical investigations were given in [8–15] for the cuprates and [16–18] for the pnictide systems. In these high-T\textsubscript{c} superconductors, however, ARPES is also readily applicable for determination of gap anisotropy. Sofar this is not possible for heavy fermion unconventional superconductors where SC gaps are only in the range of 1 meV. In this case the former two methods are more powerful. QPI technique has recently been proposed as a way to discriminate between different d-wave pairing states in 115 systems [19] and was for the first time successfully demonstrated for CeCoIn\textsubscript{5} [20,21]. Before it was also used to investigate quasiparticle properties in the hidden order state of URu\textsubscript{2}Si\textsubscript{2} [22–24].

In the NCS superconductors with inversion symmetry breaking the nodal positions are accidental and not determined by symmetry. Examples are the tetragonal heavy fermion 131 and 113 compounds [25] like CePt\textsubscript{3}Si [26] and CeRhSi\textsubscript{3} [27]. QPI might provide a new way to determine their position and the singlet-triplet mixture of the order parameter in these compounds more precisely. No experimental results have been reported but the theory in weak scattering Born approximation was developed for NCS superconductors with Rashba spin orbit coupling [28]. It was shown that a number of unconventional QPI features are to be expected: Pronounced differences in the charge- and spin- QPI appear due to the effect of Rashba coherence factors. The latter exhibits Rashba - induced anisotropies even for isotropic exchange scattering. Furthermore a new kind of cross- QPI between charge and spin channel appears which is directly related to the non-zero Rashba vector.

It remained however unclear to which extent the conclusions on QPI pattern from Born approximation are stable with respect to the frequency dependence of the t-matrix that inevitably appears for stronger scattering, giving even the possibility of resonance formation. Therefore in this work we develop the full t-matrix QPI theory for NCS superconductors without posing any conditions on the absolute and relative strengths of nonmagnetic ($V_c$) and magnetic ($V_m$) impurity scattering. Unlike in most treatments we give the results of full t-matrix theory as...
Fig. 1. (Color online) a) 2D band structure along ΓXMΓ with $t_2 = 0.35t_1, g = 0.2t_1$, and $\mu = -2t_1$. The total band width is $W \approx 8t_1 \equiv T^* \approx 14$ K (exp. Kondo temperature [26]) $\equiv 1.2$ meV corresponding to reference energy scale $t_1 = 0.15$ meV. b) Normal state electron Fermi surface around M(\(\pi, \pi\)) point. Dashed lines indicate nodes of gap functions \(\Delta_{k \xi}\) with parameters: \(\epsilon_0 = 2t_1, \psi_1 = t_1, \) and \(\epsilon_0 = 0.66t_1\) (also in subsequent figures). Only \(\Delta_{k \xi}\) (blue) has nodes on the Fermi surface. c) Spectral function for the superconducting state around M point. Set of characteristic QPI wave vectors \(q_{1a} - q_{6b}\) correspond to those in the spectral functions given in Figs. 4-6. Momentum range in b) and c) is given by $-\pi \leq (q_{x,y} - \pi) \leq \pi$.

closed analytical expressions where only the momentum integration of Green’s functions has to be performed numerically. We show that in full t-matrix theory beyond Born approximation two new aspects appear: i) The QPI functions are the sum of diagonal (non-spin flip) and anti-diagonal (spin flip) part. The latter are present only in the superconducting phase and correspond to Andreev scattering terms that change particles into holes and vice versa. ii) Due to the imaginary part of the full t-matrix a new integration kernel appears in the diagonal part which is not present in Born approximation. We will show that nevertheless the momentum-space pattern of QPI function is remarkably stable under the change of potential model or whether Born approximation of full t-matrix theory is used. Therefore our results strengthen confidence that QPI investigation could give reliable results on the accidental node positions in NCS Rashba superconductors, just as it was able to identify the symmetry-determined node positions of the \(d_{x^2-y^2}\) singlet superconducting CeCoIn$_5$ [20].

2 Model of electronic states in non-centrosymmetric compounds

The BCS model for non-centrosymmetric superconductors is given by [29–31]

\[
H_{SC} = \sum_{k\sigma\sigma'} \left( \epsilon_k - \mu \right) \sigma_0 + g_{k} \cdot \sigma \right) \xi_{k\sigma'}^{+} \xi_{k\sigma}, \\
+ \frac{1}{2} \sum_{k\sigma,\sigma'} \left( \Delta_{k\xi\sigma'\sigma}^{\dagger} \xi_{-k\sigma'}^{+} \xi_{k\sigma} + H.c. \right),
\]

where \(\epsilon_k\) is the band energy \(\mu\) the chemical potential. Furthermore \(g_k = -g_{-k}\) defines the antisymmetric Rashba spin orbit coupling term due to broken inversion symmetry [32]. Therefore the superconducting 2 \(\times\) 2 gap matrix \(\Delta_k = [\psi_k \sigma_0 + d_k \cdot \sigma] \xi_{k\sigma}\) has even singlet \((\psi_k)\) as well as odd triplet \((d_k)\) components. The latter must be parallel to the Rashba vector \(d_k = \phi_k \xi\) to avoid detrimental effects by pairbreaking [33]. Here the fully symmetric \(\phi_k \equiv \phi_k\) is set to a constant. Furthermore \(\sigma = (\sigma_x, \sigma_y, \sigma_z)\) denotes the Pauli matrices. After diagonalization of the model we obtain an effective two band superconductor on the Rashba split \((\xi = \pm 1)\) bands given by \(\epsilon_{k\xi} = \epsilon_k - \mu + \xi |g_k|\). They correspond to split Fermi surface (FS) sheets \((\epsilon_{k\xi} = 0)\) with opposite helical spin polarizations and two different superconducting gaps \(\Delta_{k\xi} = \psi_k + \xi |d_k|\).

We will investigate in detail a 2D model for Ce-based 131 systems [34,35]. The possible effects of magnetic order in these compounds [36] are not treated here. For the kinetic energy we consider only in-plane dispersion given by \(\epsilon_k = 2t_1 (\cos k_x + \cos k_y) + 4t_2 \cos k_x \cos k_y\), where \(t_1\) and \(t_2\) are nearest and next nearest neighbor hopping, respectively. Furthermore we choose \(g_k = g (\sin k_y x - \sin k_x y) = g (\sin k_y, -\sin k_x, 0)\), (2) in the tetragonal plane [33]. The resulting Rashba-split bands are shown in Fig. 1a and the electron-type Fermi surface around the M(\(\pi, \pi\)) points in Fig. 1b. The split constant-energy surfaces \((\omega > 0)\) for the superconducting state are presented in Fig. 1c. It is known from thermal conductivity [37] that the superconducting gap has line nodes (in 3D). To achieve nodes on the M-point Fermi surface we use an extended s-wave [33] form for \(\psi_k\) with \(A_{1g}\) (full symmetry) and as before \(d_k = \phi_k \xi\). The latter belongs to the nontrivial \(A_{2u}\) triplet representation of \(C_{4v}\) symmetry group that transforms like the \(k_y x - k_x y\) basis function: It is invariant under \(2C_2\) and \(C_4\) rotations but changes sign under \(2\sigma_x\) and \(2\sigma_y\) reflections from mirror planes parallel to the tetragonal axes and diagonals, respectively [38,39]. For the quasiparticle states of \(H_{SC}\) this leads to the two distinct gaps \((\xi = \pm 1)\)

\[
\Delta_{k\xi} = \psi_0 + \psi_1 (\cos k_x + \cos k_y) + \xi \phi_0 g \sqrt{\sin^2 k_x + \sin^2 k_y},
\]

(3)

on the Rashba-split Fermi surfaces \(\epsilon_{k\xi} = 0\). The corresponding quasiparticle energies are given by \(E_{k\xi} = \{|g_k^2 + \Delta_{k\xi}^2|^2\}^{1/2}\). The gap zeroes of the hybrid gap function are accidental and their existence requires the fine-tuning of singlet and triplet amplitudes \(\psi_1\) and \(\phi_0\) in Eq. (3) (see caption of Fig. 1). For positive parameters the nodes (node lines in 3D) appear only for the \(E_{k\xi}\) quasiparticle sheet but not for \(E_{k+}\) and are shown as dashed lines in Fig. 1b. The evolution of constant energy surfaces in the SC state is shown in Fig. 1c. A few wave vectors \(q_i\) connecting high curvature points close to nodal positions that will appear prominently in QPI spectra for small \(\omega\) are indicated by arrows. For larger \(\omega\) FS sheets are reconnected. For the calculation of the QPI pattern we use the normal and anomalous 2 \(\times\) 2 spin-space matrix Green’s functions of the unperturbed system

\[
G(k, i\omega_n) = G_+(k, i\omega_n) \sigma_0 + G_-(k, i\omega_n) (g_k \cdot \sigma), \\
F(k, i\omega_n) = [F_+(k, i\omega_n) \sigma_0 + F_-(k, i\omega_n) (g_k \cdot \sigma)] i\sigma_y,
\]

(4)
where the unit Rashba vector is defined by $\hat{g}_k = g_k / |g_k|$. The scalar bare Green’s functions are given by

$$G_+(k, i\omega_n) = \frac{1}{2} \sum_\xi \frac{i\omega_n + \epsilon_k}{(i\omega_n)^2 - E^2_k},$$

$$G_-(k, i\omega_n) = \frac{1}{2} \sum_\xi \frac{i\omega_n + \epsilon_k}{(i\omega_n)^2 - E^2_k},$$

(5)

$$F_+(k, i\omega_n) = \frac{1}{2} \sum_\xi \frac{\Delta_k}{(i\omega_n)^2 - E^2_k},$$

$$F_-(k, i\omega_n) = \frac{1}{2} \sum_\xi \frac{\Delta_k}{(i\omega_n)^2 - E^2_k}.$$

### 3 Scattering potential

The QPI density oscillations are obtained from the full Green’s function that is determined by the effect of scattering from random charge and spin impurities at the surface. We treat both cases and express the total scattering Hamiltonian containing nonmagnetic potential and isotropic exchange scattering in compact form as

$$H_{imp} = \sum_{k,q} V_0 (q) S_\alpha S_{\alpha'} \rho_{\alpha} \Psi_{\alpha k+q},$$

(6)

Here we use the Nambu 4-component spinor representation $\Psi = (\psi_{\uparrow}, \psi_{\downarrow}, c_{-\uparrow}, c_{-\downarrow})$. In the Nambu space the $4 \times 4$ matrices $\rho_\alpha$ ($\alpha = (0, i) = (0, x, y, z)$) are given by [40] $\{\rho_\alpha\} = \{\hat{\rho}_0, \rho\}$ are given by $\tau_3\sigma_0, \tau_3\sigma_y, \tau_3\sigma_z$. Here the $\tau_\alpha$- and $\sigma_\alpha$- Pauli matrices (with $\tau_0 = \sigma_0 \equiv 1$) act on Nambu and spin indices, respectively. Furthermore we define $\{S_\alpha\} = (1, S)$. The first index $\alpha = 0$ corresponds to nonmagnetic impurity scattering $V_0(q)$ and entries $i = x, y, z$ to isotropic magnetic exchange scattering $V_\alpha(q) = V_{xx}(q)$ from impurity spins $S$. The spin components $S_i$ are assumed as frozen, i.e. polarized in a given direction by a small magnetic field. An important consequence of the Rashba coupling is that spin and charge channels for impurity scattering are not decoupled as in the case of centrosymmetric metals where $g_k = 0$. This has also been shown for spin and charge response functions [34]. The $q$-dependence of the scattering is due to two effects [9, 12], the finite extension of the potential at the impurity site and the (random) distribution of the impurities. The former tends to cut off the QPI spectrum at large momenta and the latter causes its blurring. These are side effects which will not be considered further, therefore in the following we will restrict to momentum independent $V_\alpha$.

### 4 T-matrix theory

The t-matrix describing the repeated scattering of conduction electrons at an impurity site is given by the Lippmann-Schwinger equation in Nambu space according to

$$\hat{t}_{kk'}(i\omega_n) = \hat{V}_{kk'} + \sum_{k''} \hat{V}_{kk''} \hat{G}_{kk''}(i\omega_n) \hat{t}_{kk''}(i\omega_n).$$

(7)

Where $\hat{V}_{kk'} = \hat{V}(q)$ with momentum transfer $q = k - k'$ is the impurity scattering potential given in Eq. (6). The above equation can only be solved in closed form under the assumption that $\hat{V}(q)$ is independent of the momentum transfer. This corresponds to on-site impurity scattering potentials only. We restrict to the case that the impurity spin is polarized in z-direction (up or down) by a small external field. Then

$$\hat{V} = V_0 \hat{\rho}_0 + V_z \hat{\rho}_z = V_c \tau_3 \sigma_0 + V_m \tau_0 \sigma_z,$$

(8)

with $V_c = V_0$ and $V_m = S_c V_0$ giving the strength of nonmagnetic (charge) and magnetic (spin exchange) scattering, respectively. Then the momentum independent t-matrix is given by

$$\hat{t}(i\omega_n) = [1 - \hat{\hat{G}}(i\omega_n)]^{-1} \hat{V}.$$  

(9)

Here $\hat{\hat{G}}(i\omega_n) = (1/N) \sum_k \hat{\hat{G}}(k, i\omega_n)$ is the momentum integral over the $4 \times 4$ Green’s function matrix

$$\hat{\hat{G}}(k, i\omega_n) = \left[ G(k, i\omega_n) \ F(k, i\omega_n) \ F^+(k, -i\omega_n) \ G(-k, -i\omega_n) \right],$$  

(10)
whose entries are the $2 \times 2$ normal and and anomalous Green’s functions in spin space according to Eq. (4). Because $G_{\ell}(\mathbf{k}, i\omega_n)$ and $F_{\ell}(\mathbf{k}, i\omega_n)$ are symmetric and the Rashba vector $\hat{g}_{\mathbf{k}}$ is antisymmetric under inversion $\mathbf{k} \rightarrow -\mathbf{k}$ one always has

$$\frac{1}{N} \sum_{\mathbf{k}} G_{\ell}(\mathbf{k}, i\omega_n) \hat{g}_{\mathbf{k}} = 0,$$

and

$$\frac{1}{N} \sum_{\mathbf{k}} F_{\ell}(\mathbf{k}, i\omega_n) \hat{g}_{\mathbf{k}} = 0.$$

This simplifies our analysis considerably because then only two integrated scalar Green’s functions

$$g(i\omega_n) \equiv g_{+}(i\omega_n) = \frac{1}{N} \sum_{\mathbf{k}} G_{+}(\mathbf{k}, i\omega_n),$$

and

$$f(i\omega_n) \equiv f_{+}(i\omega_n) = \frac{1}{N} \sum_{\mathbf{k}} F_{+}(\mathbf{k}, i\omega_n)$$

remain. Explicitly we have

$$g(i\omega_n) = \frac{1}{2N} \sum_{\mathbf{k}\xi} \frac{(i\omega_n + \epsilon_{k\xi})}{(i\omega_n)^2 - E_{k\xi}^2},$$

$$f(i\omega_n) = \frac{1}{2N} \sum_{\mathbf{k}\xi} \frac{\Delta_{k\xi}}{(i\omega_n)^2 - E_{k\xi}^2}. \quad (11)$$

These function have the symmetry properties $g(i\omega_n)^* = g(-i\omega_n)$ and $f(i\omega_n)^* = f(i\omega_n) = f(-i\omega_n)$. Then the integrated $4 \times 4$ - matrix Green’s function can be written as

$$\hat{g}(i\omega_n) = \left[ \begin{array}{cc} g(i\omega_n)\sigma_0 & f(i\omega_n)(i\sigma_y) \\ f(i\omega_n)^*(i\sigma_y)^{\dagger} & -g(i\omega_n)^*\sigma_0 \end{array} \right]. \quad (12)$$

Using this result and the expression for the scattering potential in Eq. (8) we obtain the final result for the $4 \times 4$ t- matrix by inversion as

$$\hat{t}(i\omega_n) = \left[ \begin{array}{cc} t_{+}(i\omega_n)^{\dagger}\sigma_0 + \hat{t}_{+}(i\omega_n)\sigma_{z} & -\hat{t}_{-}(i\omega_n)\sigma_{z} - t_{-}(i\omega_n)(i\sigma_y)^{\dagger} \\ -\hat{t}_{-}(i\omega_n)\sigma_{z} - t_{+}(i\omega_n)(i\sigma_y) & t_{+}(i\omega_n)^{\dagger}\sigma_0 + \hat{t}_{+}(i\omega_n)\sigma_{z} \end{array} \right]. \quad (13)$$

The diagonal (d) and antidiagonal (a) t-matrix elements are explicitly given by

$$t_d(i\omega_n) = \frac{1}{2} \sum_{\nu = \pm} \frac{V_{\nu}[1 - V_{\nu}g(i\omega_n)]}{1 - V_{\nu}g(i\omega_n)^2 + V_{\nu}^2 f(i\omega_n)^2},$$

$$\hat{t}_d(i\omega_n) = \frac{1}{2} \sum_{\nu = \pm} \nu \frac{V_{\nu}[1 - V_{\nu}g(i\omega_n)]}{1 - V_{\nu}g(i\omega_n)^2 + V_{\nu}^2 f(i\omega_n)^2},$$

$$t_a(i\omega_n) = \frac{1}{2} \sum_{\nu = \pm} \frac{V_{\nu}^2 f(i\omega_n)}{1 - V_{\nu}g(i\omega_n)^2 + V_{\nu}^2 f(i\omega_n)^2},$$

$$\hat{t}_a(i\omega_n) = \frac{1}{2} \sum_{\nu = \pm} \nu \frac{V_{\nu}^2 f(i\omega_n)}{1 - V_{\nu}g(i\omega_n)^2 + V_{\nu}^2 f(i\omega_n)^2}. \quad (14)$$

Here $t_d(i\omega_n)^* = t_d(-i\omega_n)$, $\hat{t}_d(i\omega_n)^* = \hat{t}_d(-i\omega_n)$, $t_a(i\omega_n)^* = t_a(i\omega_n)$, and $t_a(i\omega_n)^* = t_a(i\omega_n)$. Furthermore we defined $\nu = \pm$ and $V_{\pm} = V_\nu \pm V_m$ as the sum or difference of normal and magnetic scattering. In the special case of only nonmagnetic scattering ($V_m = 0, V_\nu = V_\nu$) the matrix elements simplify to

$$t_d(i\omega_n) = \frac{V_\nu[1 - V_\nu g(i\omega_n)]}{1 - V_\nu g(i\omega_n)^2 + V_\nu^2 f(i\omega_n)^2},$$

$$t_a(i\omega_n) = \frac{V_\nu^2 f(i\omega_n)}{1 - V_\nu g(i\omega_n)^2 + V_\nu^2 f(i\omega_n)^2}. \quad (15)$$
and \( \tilde{t}_g(i\omega_n) = \tilde{t}_a(i\omega_n) = 0 \). In this case the t-matrix reduces to

\[
\tilde{t}(i\omega_n) = \begin{bmatrix}
t^a_x(i\omega_n)\sigma_0 & -t_a(i\omega_n)(i\sigma_y) \\
-t_a(i\omega_n)(i\sigma_y) & -t_d(i\omega_n)\sigma_0
\end{bmatrix},
\]

(16)

which has the same spin-space structure as \( \tilde{g}(i\omega_n) \) in Eq. (12) due to the scalar scattering potential \( V_c \).

The anti-diagonal \((a)\) blocks in the t-matrices Eqs. (13,16) which change the Nambu pseudo-spin \( \tau_\alpha \) appear only in the superconducting state where \( f(i\omega_n) \neq 0 \). They correspond to an Andreev-type scattering process where the holes scatter to electron states and vice versa due to the presence of the condensate. They are absent in Born approximation where no intermediate anomalous Green’s function \( F(\mathbf{k}, i\omega_n) \) appears in the scattering. Since the Bogoliubov quasiparticle states in the presence of the condensate are superpositions of up-spin electrons and down-spin holes the Andreev-type scattering will also lead to a spin-flip as seen from the general case in Eq. (13), even for the case of a pure scalar scattering potential in Eq. (16). Using the above closed analytical solution for the t-matrix we can now calculate the QPI spectrum.

5 QPI conductance

We calculate the change in STM tunneling conductance in charge or spin channel \( \alpha(0, x, y, z) \) due to impurity scattering in charge or spin channel \( \beta(0, x, y, z) \). For a magnetic impurity the scattering channel \( \beta \) is fixed by applying a small field \( H \ll H_{c2} \) along the \( x, y, z \) axis. The conductance channel \( \alpha \) is selected by using either a nonmagnetic \((\alpha = 0)\) or a half-metallic (fully spin polarized) tunneling tip with moment polarized along \( \alpha = x, y, z \) and an exchange splitting larger than the heavy fermion quasiparticle band width. Such configuration would allow in principle to determine all elements of the QPI differential conductance tensor. It is given by [8]

\[
\frac{d\delta I_\alpha(r,V)}{dV} \sim -\frac{1}{\pi} \text{Im} \left[ \text{Tr}_\sigma \left[ \tilde{\rho}_\alpha \delta \tilde{G}_\beta(r, r, \omega = V) \right] \right]_{11} \equiv \delta N_{\alpha\beta}(r, \omega).
\]

(17)

Here \( \delta \tilde{G}_\beta \) is the change of the \( 4 \times 4 \) matrix Green’s function in combined Nambu and spin space (each with dimension 2) which is due to impurity scattering in charge or spin channel \( \beta(0, x, y, z) \). Furthermore matrix index \((11)\) refers to the Nambu space which results from the trace with respect to \( r \) including the projector \( \frac{1}{2}(1+\tau_z) \). The remaining trace refers to spin space only.

In t-matrix theory the correction to the real-space Green’s function due to impurity scattering is given by

\[
\delta \tilde{G}(r, i\omega_n) = \tilde{G}_0(r, i\omega_n)\tilde{t}(i\omega_n)\tilde{G}_0(r, i\omega_n).
\]

(18)

Fig. 4. (Color online) a-c) Total charge- QPI (\( \delta \tilde{I}_c(\mathbf{q}, \omega) \)) in the normal state for different \( \omega < 0 \) (\( t_1 \) units) and scattering from non-magnetic impurities. d-f) The same quantity for the superconducting state. g-i) represent the anti-diagonal contributions (\( \delta \tilde{I}_d(\mathbf{q}, \omega) \)) of the total charge- QPI for the superconducting state. The frequency \( \omega = V \) satisfies \( \omega < |\Delta_{k\ell}| \simeq t_1 \ll W = T_r = St_1 \). Here \( V_r = t_1 \) and \( V_m = 0 \). The momentum range in each panel is given by \( -\pi \leq \mathbf{q}_{x,y,z} \leq \pi \). This applies also to all following figures.

The Fourier transform of differential conductances is then obtained from the QPI functions \((\mathbf{k}' = \mathbf{k} - \mathbf{q})\)

\[
\delta N_\alpha(\mathbf{q}, \omega) = -\frac{1}{\pi} \text{Im} \left[ \tilde{\rho}_\alpha \delta \tilde{G}(\mathbf{k}, \mathbf{q}, \omega) \right]_{i\omega_n \rightarrow \omega + i\delta},
\]

(19)

\[
\tilde{\rho}_\alpha(\mathbf{k}, i\omega_n) = \frac{1}{N} \sum_{\mathbf{k}} \text{Tr}_\sigma \left[ \tilde{\rho}_\alpha \tilde{G}(\mathbf{k}, i\omega_n) \tilde{t}(i\omega_n) \tilde{G}(\mathbf{k}', i\omega_n) \right]_{11},
\]

with \( N = L^2 \) denoting the number of grid points. We assume here that the tunneling happens out of the coherent heavy quasiparticle states. This is justified for tempera-
t temperature $T^*$ [23] which is of the order 14 K for CePt$_3$Si [26]. We therefore restrict to frequencies (Figs. 4-6) of the order of the SC gap and we do not intend to describe the Fano resonance shape [23] that appears for higher frequencies of the order of the effective quasiparticle bandwidth $T^*$.

5.1 QPI pattern in Born-approximation

Here we focus on the spatial oscillations or momentum dependence by weak scattering and ignore the frequency dependence of the t-matrix which has to be included in the strong scattering limit [41]. In the Born approximation [28] we may calculate a general density $\delta N_{\alpha\beta}(q, \omega)$ in charge-spin channel $\alpha$ due to impurity scattering in arbitrary but fixed channel $\beta$ given by the frequency independent t-matrix

$$\tilde{t}(q, i\omega_n) = V_3(q)\tilde{\rho}_\beta \beta.$$

Using Eq. (20) leads to a density modulation determined by the QPI functions $\tilde{A}_{\alpha}(q, i\omega_n) = V_3(q)\tilde{A}_{\alpha\beta}(q, i\omega_n)$ according to

$$\frac{\delta N_{\alpha\beta}(q, \omega)}{\delta N_{\alpha\beta}(q, \omega)} = -\frac{1}{\pi} V_3(q)\text{Im} \left[ A_{\alpha\beta}(q, i\omega)_n \right] \left. \right|_{i\omega_n \rightarrow i\omega + i\delta},$$

$$A_{\alpha\beta}(q, i\omega_n) = \frac{1}{N} \sum_k \text{Tr}_{\sigma} \left[ \tilde{\rho}_\alpha \hat{G}(k, i\omega_n)\tilde{\rho}_\beta \hat{G}(k', i\omega_n) \right]_{11}.$$

This expression is evaluated by using Eq. (4) and performing the remaining $\sigma$-trace we finally get, using the scalar Green’s functions in Eq. (5):

$$A_{\alpha0}^q(i\omega_n) = \frac{1}{4N} \sum_{k\xi\xi'} \left[ 1 + \xi\xi' (\hat{g}_k \cdot \hat{g}_{k'}) \right] K_{kq}^\xi(q, i\omega_n),$$

$$A_{\alpha}^q(i\omega_n) = \frac{1}{4N} \sum_{k\xi\xi'} \left[ 1 - \xi\xi' (\hat{g}_k \cdot \hat{g}_{k'} - 2\hat{g}_k \cdot \hat{g}_{k'}) \right] K_{kq}^\xi(q, i\omega_n),$$

$$A_{\alpha}^q(i\omega_n) = \frac{1}{2N} \sum_{k\xi\xi'} \xi\xi' K_{kq}^\xi(q, i\omega_n),$$

where the integration kernel for intra-band ($\xi = \xi'$) and inter-band ($\xi \neq \xi'$) processes is given by

$$K_{\xi\xi'}(i\omega_n) = \frac{(i\omega_n + \Delta_{\xi\xi'}) (i\omega_n + \Delta_{\xi'\xi'}) - \Delta_{\xi\xi'} \Delta_{\xi'\xi'}}{[(i\omega_n)^2 - E_{k_{\xi\xi'}}^2][(i\omega_n)^2 - E_{k_{\xi'\xi'}}^2]}.$$

In addition the Rashba term leads to nondiagonal elements in the spin- QPI density, in the tetragonal case with $g_k = 0$ to $A_{\alpha\alpha}^q(i\omega_n) = A_{\alpha\alpha}^q(i\omega_n)$ which is evaluated as

$$A_{\alpha\alpha}^q(i\omega_n) = \frac{1}{4N} \sum_{k\xi\xi'} \xi\xi' (\hat{g}_k \cdot \hat{g}_{k'} + \hat{g}_{k} \cdot \hat{g}_{k'}) K_{kq}^\xi(q, i\omega_n).$$

The QPI functions $A_{\alpha\alpha}^q$ and $A_{\alpha\alpha}^q$ are even and $A_{\alpha\alpha}^q$ is odd in $q$. The latter needs some special consideration. The real space density corresponding to Eq. (22) is given by

$$\frac{\delta N_{\alpha}(q, i\omega_n)}{\delta N_{\alpha}(q, i\omega_n)} = -\frac{1}{\pi} \int V\left(q\right) A_{\alpha0}^q(q, i\omega_n) \exp(iqr)dq,$$

$$\delta N_{\alpha}(q, i\omega_n) = -\frac{1}{\pi} \int V_{cu}(q) A_{\alpha0}^q(q, i\omega_n) \cos(qr)dq.$$

**Fig. 5.** (Color online) Total charge- QPI ($\tilde{A}_{\alpha0}(q, \omega)$) for different scattering processes: first column from non-magnetic impurities, second column from magnetic impurities, and the third row shows mixed non-magnetic/magnetic impurity scattering. a-c) for the normal state. j-l) The same quantity for third row shows mixed non-magnetic/magnetic impurity scattering. a-c) for the normal state. j-l) The same quantity for the superconducting state. d-f) represent the diagonal contributions ($\tilde{A}_{\alpha}^q(\omega)$) and g-i) represent the off-diagonal contributions ($\tilde{A}_{\alpha}^q(\omega)$) of the total charge- QPI for the superconducting state. Here $\omega = -0.2t$. The QPI functions $A_{\alpha\alpha}^q$ and $A_{\alpha\alpha}^q$ are even and $A_{\alpha\alpha}^q$ is odd in $q$. The latter needs some special consideration. The real space density corresponding to Eq. (22) is given by

$$\frac{\delta N_{\alpha}(q, i\omega_n)}{\delta N_{\alpha}(q, i\omega_n)} = -\frac{1}{\pi} \int V\left(q\right) A_{\alpha0}^q(q, i\omega_n) \exp(iqr)dq,$$

$$\delta N_{\alpha}(q, i\omega_n) = -\frac{1}{\pi} \int V_{cu}(q) A_{\alpha0}^q(q, i\omega_n) \cos(qr)dq.$$
Likewise the even part $V_{\text{eq}}(\mathbf{q})$ leads to the finite real space density contribution for the charge- $(A_{0}^{\text{eq}})$ or spin- $(A_{0}^{\text{sp}})$ QPI functions. In particular for constant $V_{\text{eq}}(\mathbf{q}) = V_{\text{eq}}$ no real space spin density modulation can appear from non-magnetic scattering. We mention that the complementary cross- QPI case, an equivalent charge pattern induced by pure magnetic scattering and described by $A_{0}^{\text{eq}} = A_{0}^{\text{sp}}$ is also possible when $V_{\text{m}}(\mathbf{q})$ contains odd contributions. From this analysis we expect that QPI for non-centrosymmetric superconductors derived here exhibits a wealth of new effects due to the inversion symmetry breaking Rashba term.

### 5.2 QPI spectrum with full t-matrix theory

For strong scattering the t-matrix becomes frequency dependent and even resonances may form at impurity sites [42] which cannot be described within Born approximation. It is also important to ask whether the $\mathbf{q}$- space pattern is strongly dependent on the absolute scattering strength and relative strength of $V_{\text{eq}}$ and $V_{\text{m}}$, because this influences the usefulness of QPI for the investigation of the gap function. Such questions cannot be answered within Born approximation and therefore we now resort to the full t-matrix treatment for QPI functions given in Eq. (20). In the special case that the impurity scattering contains only terms due to nonmagnetic and the $z$-component of exchange scattering the expressions for the QPI which are assumed $\mathbf{q}$-independent according to

$$
\tilde{V} = V_{\text{c}}\hat{\rho}_{0} + V_{m}\hat{\rho}_{z}.
$$

We will only calculate the charge QPI function $\tilde{A}_{0}(\mathbf{q}, i\omega_{n})$ given in Eq. (20) using the full t-matrix of Eq. (13). From the evaluation of matrix products and trace in Nambu space we obtain

$$
\tilde{A}_{0}(\mathbf{q}, i\omega_{n}) = \frac{1}{N} \sum_{\mathbf{k}} \text{Tr}_{\sigma} \left[ (t_{d}^{*}(i\omega_{n})G_{kG_{k-\mathbf{q}}} - t_{d}(i\omega_{n})F_{kF_{k-\mathbf{q}}}) + (\tilde{t}_{d}^{*}(i\omega_{n})G_{k}\sigma_{z}G_{k-\mathbf{q}} - \tilde{t}_{d}(i\omega_{n})F_{k}\sigma_{z}F_{k-\mathbf{q}}) \right. \\

\left. - \tilde{\sigma}_{a}(i\omega_{n}) \left( G_{k}\sigma_{x}F_{k-\mathbf{q}} + F_{k}\sigma_{x}G_{k-\mathbf{q}} \right) - \sigma_{a}(i\omega_{n}) \left( G_{k}(i\sigma_{y})F_{k-\mathbf{q}} + F_{k}(i\sigma_{y})G_{k-\mathbf{q}} \right) \right].
$$

In the case of purely nonmagnetic scattering ($V_{m} = 0$) $\tilde{t}_{d}(i\omega_{n}) = \tilde{\sigma}_{a}(i\omega_{n}) = 0$ and the expression reduces to

$$
\tilde{A}_{0}(\mathbf{q}, i\omega_{n}) = \frac{1}{N} \sum_{\mathbf{k}} \text{Tr}_{\sigma} \left[ (t_{d}^{*}(i\omega_{n})G_{kG_{k-\mathbf{q}}} - t_{d}(i\omega_{n})F_{kF_{k-\mathbf{q}}}) \right. \\

\left. - \frac{2}{N} \sum_{\mathbf{k}} \tilde{\sigma}_{a}(i\omega_{n}) \left( G_{k}\sigma_{x}F_{k-\mathbf{q}} + F_{k}\sigma_{x}G_{k-\mathbf{q}} \right) \right].
$$

In the following discussion we restrict to the tetragonal Rashba systems where $\mathbf{g}_{k} \cdot \hat{z} = 0$, i.e. the Rashba vector is perpendicular to the impurity moment ($S_{z}$) associated with magnetic scattering $V_{m}$. In this case terms involving $t_{d}(i\omega_{n})$ do not appear in $\tilde{A}_{0}(\mathbf{q}, i\omega_{n})$. The general case with all three components of the Rashba vector $\mathbf{g}_{k}$ present is treated in [7]. Using the Green's function matrices in Eq. (4) and performing the traces in spin space this leads to $(\mathbf{k}' = \mathbf{k} - \mathbf{q})$

$$
\tilde{A}_{0}(\mathbf{q}, i\omega_{n}) = t_{d}^{*}(i\omega_{n}) \frac{1}{N} \sum_{\mathbf{k}} \left[ G^{\mathbf{k}'}_{-}G^{\mathbf{k}'}_{+} + (\mathbf{g}_{k} \cdot \mathbf{g}_{k'})G^{\mathbf{k}'}_{-}G^{\mathbf{k}'}_{+} \right] + t_{d}(i\omega_{n}) \frac{1}{N} \sum_{\mathbf{k}} \left[ F^{\mathbf{k}'}_{+}F^{\mathbf{k}'}_{-} + (\mathbf{g}_{k} \cdot \mathbf{g}_{k'})F^{\mathbf{k}'}_{+}F^{\mathbf{k}'}_{-} \right] \\

- \frac{2}{N} \sum_{\mathbf{k}} \mathbf{g}_{k} \cdot \hat{z}_{a}(i\omega_{n}) \left( G^{\mathbf{k}'}_{k}\sigma_{x}F_{k-\mathbf{q}} + F^{\mathbf{k}'}_{k}\sigma_{x}G_{k-\mathbf{q}} \right) G^{\mathbf{k}'}_{k}F^{\mathbf{k}'}_{k}.
$$

Inserting the explicit expressions for the normal and anomalous Green’s functions in Eq. (5) we finally obtain a QPI function that consists of two contributions,

$$
\tilde{A}_{0}(\mathbf{q}, i\omega_{n}) = \tilde{A}_{0}^{\text{(d)}}(\mathbf{q}, i\omega_{n}) + \tilde{A}_{0}^{\text{(a)}}(\mathbf{q}, i\omega_{n}),
$$

originating in the diagonal $(d)$ and anti-diagonal $(a)$ terms of the t-matrix in Eqs. (13).

$$
\tilde{A}_{0}^{\text{(d)}}(\mathbf{q}, i\omega_{n}) = \frac{1}{4N} \sum_{\mathbf{k} \xi \xi'} \left[ 1 + \xi \xi' (\mathbf{g}_{k} \cdot \mathbf{g}_{k'}) \right] t_{d}^{*}(i\omega_{n})(i\omega_{n} + \xi_{k})t_{d}(i\omega_{n} + \xi'_{k}) \frac{\Delta_{k_{\xi}} \Delta_{k'_{\xi'}}}{[(i\omega_{n})^{2} - E^{2}_{k_{\xi}}][(i\omega_{n})^{2} - E^{2}_{k'_{\xi'}}]},
$$

$$
\tilde{A}_{0}^{\text{(a)}}(\mathbf{q}, i\omega_{n}) = -\frac{1}{2N} \sum_{\mathbf{k} \xi \xi'} \xi \xi' \mathbf{g}_{k} \cdot \hat{z}_{a}(i\omega_{n}) \frac{t_{d}(i\omega_{n} + \xi_{k})t_{d}(i\omega_{n} + \xi'_{k})}{[(i\omega_{n})^{2} - E^{2}_{k_{\xi}}][(i\omega_{n})^{2} - E^{2}_{k'_{\xi'}}]}.
$$

---

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We can check this result for the Born approximation where \(t_0(\omega_n) = t_0(\omega_n) = V_c\) and \(\tau_d(\omega_n) = \tau_d(\omega_n) = 0\) (see also 7). Then the fraction in the first equation is given by \(V_c A_{00}(\omega_n)\), furthermore \(A_0^0(\omega_n) = 0\) and therefore \(\delta N_0(\omega_n) = V_c A_{00}(\omega_n)\) reduces to the previous result in Eq. (22). For nonmagnetic scattering only \((V_m = 0)\) the anti-diagonal (a) contribution in Eq. (32) simplifies because \(\tau_d(\omega_n) = 0\). Then we may write

\[
\delta N_0(\omega_n) = \sum_{\mathbf{k}\xi^\prime} \frac{-\xi^\prime g_{k\xi}^0 g_{k\xi}}{2N} \frac{t_0(\omega_n)(\omega_n + \epsilon_{\mathbf{k}\xi}) A_{\mathbf{k}\xi^\prime}}{[(\omega_n)^2 - E_{\mathbf{k}\xi}^2][(\omega_n)^2 - E_{\mathbf{k}\xi^\prime}^2]}.
\]

Note that the even in the general case the anti-diagonal QPI contribution \(A_0^0(\omega_n)\) is only nonzero in the superconducting phase because it is due to Andreev-type scattering processes that require the presence of a condensate. Since the superconducting gap has nontrivial \(A_{2u}\) symmetry one has to expect that \(\delta N_0(\omega_n)\) is not fully symmetric.

In the strong scattering case bound states or resonances in the superconducting gap can appear which may be investigated by the calculation of the charge of the local density of states (LDOS), \(\delta N_0(\omega)\), at the impurity site. It is given by the integral over the real space density oscillations or the momentum space integral over the corresponding charge- QPI function according to

\[
\delta N_0(\omega) = -\frac{1}{\pi} \text{Im} \left[ \frac{1}{N} \sum_{\mathbf{q}} \tilde{A}_0(\mathbf{q}, \omega_n) \right].
\]

The total LDOS is then given by \(N_0(\omega) = N_0(\omega) + \delta N_0(\omega)\) where \(N_0(\omega) = -(1/\pi) \text{Im} [g(\omega_n)] \omega_n \rightarrow \omega + i\delta\) is the background DOS (per site) of quasiparticle states.

6 Numerical results and discussion

In the presentation of numerical results we focus on the charge-QPI \(\tilde{A}_0(\mathbf{q}, \omega_n)\) which is in any case experimentally the most easily accessible quantity. We discuss primarily the results obtained by using the full t-matrix theory for which we have derived a closed and explicit representation previously. We emphasize that we do not give an exhaustive discussion here of all possible situations that may occur on changing the electronic \((t_1, t_2, g)\), superconducting \((\psi_0, \psi_1, \psi_0)\) and impurity scattering parameters \((V_c, V_m)\) and also the polarization channels \(\alpha, \beta\). We rather fix the first two sets of parameters to obtain a realistic model of CePt_3Si and then study a few typical QPI spectra as function of frequency (bias voltage) \(\omega\) and scattering parameters \((V_c, V_m)\). We will mostly investigate the nonmagnetic scattering \(V_c\) only and restrict to the scalar charge QPI function, i.e., we focus on the \((\alpha, \beta) = (0, 0)\) channel of Eq. (17). The salient features of the additional spin-QPI and cross-QPI have been discussed previously within Born approximation [28]. They are experimentally more difficult to access because they require the spin polarization of both the impurity spin, e.g. by a small external field as well as a spin analyzer for the tunneling current.

The underlying model is summarized by the panels of Fig. 1 which show the Rashba split bands (a) and Fermi surface (b) in the normal state. The model parameters are chosen [34,35] such that the M-point Fermi surface of CePt_3Si is reproduced qualitatively. The dashed lines show the nodes of the gap functions \(\Delta_{\mathbf{k}\xi}\). The gap parameters are tuned such that nodes for \(\Delta_{\mathbf{k}\xi}\) appear on the \(\epsilon_{\mathbf{k}\xi}\)-FS sheet. The existence of nodes is suggested e.g. by thermal conductivity measurements [37]. The surfaces of constant quasiparticle energies in the superconducting phase (c) consist of thin sheets with points of large curvature in \(\mathbf{k}\)-space. The connecting \(\mathbf{q}\) vectors of these extremal points are the ones which will show up prominently in the QPI spectra.

A basic ingredient of the QPI theory are the momentum integrated Green’s functions given in Eq. (12). The energy dependence of \(f\) and \(g\) is shown in Fig. 2. In Fig. 2a the real and imaginary part of \(-g(\omega_n)\) in the normal state are plotted where the unperturbed density of states (DOS) of Rashba bands is given by

\[
N_0(\omega) = -\frac{1}{\pi} \text{Im} [g(\omega_n)]_{\omega_n \rightarrow \omega + i\delta} = \frac{1}{N} \sum_{\mathbf{k}\xi} \delta(\omega - \epsilon_{\mathbf{k}\xi}).
\]

This indicates that all calculations, also for QPI spectrum, are done for zero temperature by analytic continuation to the real axis. Numerically we use a finite imaginary part \(\delta = 0.005 t_1\). The DOS has two peaks at \(\omega \approx \pm t_1\) which are due to the van Hove singularities at X and M points in Fig. 1a. In the superconducting state the DOS (Fig. 2b) changes considerably due to the gap opening of the order
|Δκ| ≃ t₁. Due to the large gap and the strong particle-hole asymmetry of the dispersion around the Fermi level the nodal V-shape of the DOS is asymmetric around ω = 0 and exists only for small frequency ω ≪ |Δκ|. The corresponding anomalous Green’s function −f(ω) is shown in Fig. 2c.

From the momentum integrated Green’s functions the t-matrix components of Eq. (14) that determine the QPI functions can directly be obtained once the scattering model is fixed by (V₀, Vₘ) parameters. The element tₙ(ω) which enters in the diagonal part of the QPI function is shown in Fig. 2 for the normal (a) and superconducting state (b). Its imaginary part still resembles the DOS with a cutoff at the lower M-point band edge and the peak due to the X-point singularity.

In Fig. 4 we show the QPI spectrum for nonmagnetic (V₀) scattering and increasingly negative frequencies or voltages (from left to right). The top and bottom rows show the total charge-QPI function ˜Λ₀(q, iωₙ) in the normal and superconducting state, respectively. The latter has two contributions, the diagonal ˜Λₓₓ₀(q, iωₙ) shown in the second row and the anti-diagonal part ˜Λₓₓ₋₁(q, iωₙ) presented in the third row (it vanishes identically in the normal state according to Eq. (32)). The first row basically shows the “2kf” contour resulting from scattering across the M-point constant energy surfaces in Fig. 1b. The dimensions of these contours decrease with increasingly negative frequency when the bottom of the band at the M-point is approached. In addition one can clearly see a diagonal cross feature that results from small wave vector intra band (ξ = ξ’) scattering parallel to the M-point sheet.

In the superconducting state (second row) the QPI looks very different due to the breakup of constant quasi-particle surfaces caused by the gap opening (see Fig. 1c). The maximum amplitude of the spectrum is dominated by the wave vectors q that correspond to connections between points of maximum curvature on the broken sheets as indicated in Fig. 4e. Therefore the QPI spectrum is a kind of map of the reconstructed surfaces of constant quasiparticle energies and highly specific for the node structure of the gap function. In particular the wave vector q₁ corresponds to scattering connecting opposite sites of the accidental gap node. The observation of such QPI feature would be a clear evidence for the existence and position of the node points (lines in 3D which are so far only conjectures from low temperature transport measurements).

In the third row we show the anti-diagonal contribution in the superconducting state which has similar overall features as the second row. One additional aspect is that it exhibits directly the spatial (reflection) symmetry breaking of the triplet ˜Δ₂u state. However the anti-diagonal part has considerably lower amplitude than the diagonal one so that the total QPI function ˜Λ₀(q, iωₙ) corresponding to the experimental conductance is dominated by the diagonal part. It is shown in the last row of Fig. 4 for the superconducting state.

The frequency dependence of QPI pattern in Fig. 4 is only shown for the nonmagnetic (V₀) scattering. In general the scattering potentials enter in the combinations V₀ ± Vₘ into the t-matrix elements of Eq. (14). Therefore we now fix the frequency to ω = −0.2t₁ and investigate the QPI spectrum as function of various scattering strengths (V₀, Vₘ). We compare purely nonmagnetic (V₀) scattering as before, equal scattering strength V₀ = Vₘ and purely magnetic (Vₘ) scattering in Fig. 5 (V₀, Vₘ are given by t₁ units). We show again the total charge-QPI function ˜Λ₀(q, iωₙ) of the normal and superconducting state in the top and bottom row, respectively. The latter has diagonal and anti-diagonal contributions which are shown in the second and third row, respectively. We observe that the amplitude of the QPI functions vary considerably with (V₀, Vₘ) combination, however the momentum pattern stays surprisingly similar in the three cases, determined by the shape of split Fermi surface sheets and the nodal gap structure. This supports the view that also in the non-centrosymmetric superconductors the QPI spectrum may be used to investigate the SC gap structure and is not veiled by the influence of the details of scattering mechanism.

In addition to the composition of the scattering potential it is important to understand the effect of its overall strength. Most QPI investigations use only the Born approximation corresponding to weak scattering potentials. On the other hand for strong scattering the integrated QPI spectra or LDOS may exhibit resonance peaks as function of frequency under suitable conditions. It is therefore important to know to which extent the momentum and
frequency pattern of $\tilde{A}_0(q, i\omega_n)$ depends on the strength of the scattering potential and the type of approximation. In Fig. 6 we show the comparison of weak scattering in Born approximation (top row) and strong scattering in full t-matrix theory (bottom row) for the SC state. From the comparison we conclude that for all frequencies the $q$-space pattern of QPI function are remarkably similar although the amplitudes are reversed (Fig. 6d-f is the ‘negative’ of Fig. 6a-c). This may be understood from the limit of $t_d(i\omega_n)^*$ in Eq. (32) which is $V_c > 0$ in Born approximation and $-1/g(i\omega_n)$ in the strong scattering t-matrix approximation. In the frequency range shown in Fig. 6 this quantity is $< 0$ according to Fig. 3b. Our results of Figs. 5,6 suggests that the observed QPI pattern is rather insensitive to the details of the scattering mechanism and is mainly determined by Fermi surface structure and superconducting gap nodes. Fig.6 thereby represents the extreme case of very strong scattering. However this conclusion is also valid for cases of intermediate scattering strength. Therefore we believe that also in the case of noncentrosymmetric superconductors the STM-QPI technique may be used to investigate the symmetry of the superconducting gap.

Finally we also show the total LDOS as function of energy (Fig. 7) which is obtained from the integrated QPI spectrum according to Eq. (34). The change $\delta N(\omega)$ due to normal impurity scattering is shown in Fig. 7a and the total LDOS $N(\omega)$ in comparison to the unperturbed quasiparticle DOS $N_0(\omega)$ is presented in Fig. 7b for the superconducting phase. The changes are relatively small and in particular do not show the development of a separate resonance peak for the parameter range investigated. This may be due to the nodal structure of the gap which leads to considerable imaginary part in $t_d(\omega)$ even at small frequencies (Fig. 3b).

7 Conclusion and outlook

In this work we have derived the full t-matrix theory of quasiparticle interference in non-centrosymmetric superconductors. Unlike in common, purely numerical treatments we have succeeded to give a closed analytical representation for the full t-matrix that shows explicitly how the combination of normal and magnetic scattering determines the QPI spectrum, and in particular how the non-diagonal Andreev scattering terms in QPI appear beyond Born approximation as an effect of the condensate. For our closed expression for the charge-QPI function only one remaining momentum space integration to obtain the integrated normal and anomalous Green’s functions needs to be performed numerically. Our theory is valid for an arbitrary combination and strength of non-magnetic and magnetic scattering potentials where the impurity spin is polarized perpendicular to the Rashba-vector $g_k$. So far the non-centrosymmetric QPI problem has only been treated within Born approximation [28] where the frequency dependence of the scattering is neglected. It therefore remained an open problem whether this influences the interpretation of the momentum dependence of QPI pattern. Our results show the the latter is remarkably stable and qualitatively unchanged by frequency variation and modification of the combination of scattering potentials ($V_c, V_m$).

Furthermore the QPI structure pattern and characteristic wave vectors connected with gap features are almost identical in the Born approximation and full t-matrix theory. Consequently for practical purposes one may assume that the frequency dependence and momentum dependence of QPI pattern shows no strong interdependence and this holds true for arbitrary scattering strengths. Therefore our theory demonstrates that QPI may be used as a stable method in non-centrosymmetric superconductors to investigate the symmetry of the superconducting gap function and its accidental node positions which cannot be determined by the other applicable methods.

We have discussed the results of our analytical t-matrix and QPI spectrum theory for typical situations without giving a full systematic survey of the predictions as function of model (scattering potential, gap function) parameters. For that program to be carried out in a sensible way first experimental results for NCS superconductors are needed for orientation. As a starting point one should consider the normal (and nonmagnetic) state and see whether the predictions in Fig.4a-c can be verified, i.e. whether the simple 2D FS model used here is a reasonable simplification. In a next step it is necessary to verify that the influence of small-moment magnetic order (which has been neglected here) is unimportant. And only as final step one may hope to gain insight into the question of accidental node existence and their postions by employing a more extensive search in the parameter space of the the model analyzed here.

We finally mention that our theory is not restricted to the tetragonal Ce-based 131 compounds but may straightforwardly be extended to cubic non-centrosymmetric compounds [43] like Li$_2$Pd$_{13}$B and Li$_2$Pt$_{13}$B with general Rashba vector as discussed in 7.

Appendix A

Here we give the complete expression for the charge-QPI function in the full t-matrix case. Contrary to Sec. 5.2 where we treated the tetragonal symmetry case with $g_k = 0$ we now do not pose any condition on the Rashba vector. In the general case we have to add the contributions coming from nonzero $g_k$ to Eq. (32). They are present, e.g., in the cubic non-centrosymmetric superconductors and they are given by $(k' = k - q)$.
The first (diagonal d) and second (anti-diagonal a) terms may be evaluated explicitly as

\[ A^d_0(q, \omega_n) = \frac{1}{2N} \sum_{k \xi \xi'} \xi \xi' \delta \delta' \left( \tilde{t}_d(\omega_n) + i \epsilon_c \tilde{t}_d(\omega_n) + \Delta_{k \xi} \Delta_{k \xi'} \right), \]

\[ A^a_0(q, \omega_n) = -\frac{1}{2N} \sum_{k \xi \xi'} \xi \xi' \delta \delta' \left( \tilde{t}_a(\omega_n) + i \epsilon_c \tilde{t}_a(\omega_n) + \Delta_{k \xi} \Delta_{k \xi'} \right). \]

The total QPI function contributions in the general case of arbitrary \( g_k \) are then given by the sum of Eqs. (32,36), namely \( A^q_0(q, \omega_n) = A^d_0(q, \omega_n) + A^d_0(q, \omega_n) \) and \( A^q_0(q, \omega_n) = A^d_0(q, \omega_n) + A^a_0(q, \omega_n) \). The meaning of the first term becomes clear when we consider the Born approximation. In this case \( t_d(\omega_n) = V_n \), and we get \( A^q_0(q, \omega_n) = V_n A^q_0(q, \omega_n) \) which corresponds to the cross-QPI function of Eq. (22) describing the charge modulation due to exchange scattering \( V_n \) from impurity spins \( S_z \). Note that this is equal to the inverse process (spin modulation from non-magnetic scattering \( V_c \)), i.e. \( A^q_0(q, \omega_n) = A^q_0(q, \omega_n) \). In Born approximation the anti-diagonal contribution \( A^a_0(q, \omega_n) \) vanishes.

In the full t-matrix theory, but assuming only nonmagnetic scattering (\( V_n = 0 \)) this term simplifies and adding it to the tetragonal terms of Eq. (32) we get an expression similar to Eq. (33)

\[ A^q_{00}(q, \omega_n) = -\frac{1}{2N} \sum_{k \xi \xi'} \xi \xi' \delta \delta' \left( g_k t_{ka}(\omega_n) + i g_k t_{ka}(\omega_n) \right) \frac{1}{\left( \omega_n - E_{k \xi} \right) \left( \omega_n - E_{k \xi'} \right)}. \]  

**Appendix B**

Here we give a different form of the full t-matrix QPI functions in Eq. (32) that makes its connection to the result from Born approximation more transparent. Using \( t_d(\omega_n) = t_d(\omega_n)^+ + it_d(\omega_n)^- \) we can write the imaginary part of the diagonal term as

\[ \text{Im} \left[ A^d_0(q, \omega_n) \right] = \frac{1}{4N} \sum_{k \xi \xi'} \left( 1 + \xi \xi' \delta \delta' \cdot g_k \cdot g_k \right) \left[ t_d(\omega_n)^+ \text{Im} \left[ K^{qk}_{\xi\xi}(\omega_n)^- \right] + t_d(\omega_n)^- \text{Im} \left[ K^{qk}_{\xi\xi}(\omega_n)^+ \right] \right]. \]  

where we have now two integration kernels defined by

\[ K^{qk}_{\xi\xi}(\omega_n)^\pm = \frac{(\omega_n + \epsilon_c)(\omega_n + \epsilon_c') \pm \Delta_{k \xi} \Delta_{k \xi'}}{\left[ (\omega_n)^2 - E_{k \xi}^2 \right] \left[ (\omega_n)^2 - E_{k \xi'}^2 \right]}. \]

In Born approximation the scattering reduces to \( t_d(\omega_n)^+ = V_c \) and \( t_d(\omega_n)^- = 0 \). Furthermore \( t_d(\omega_n) \equiv 0 \). Then we have only the diagonal part and \( A^q_0(q, \omega_n) = V_c A^q_0(q, \omega_n) \) where \( A^q_{00}(q, \omega_n) \) is now given again by Eqs.(22,23) with the identification \( K^{qk}_{\xi\xi}(\omega_n) = K^{qk}_{\xi\xi}(\omega_n)^- \). Therefore the \( K^+ \) kernel in the QPI function can only appear beyond Born approximation.

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