Influence of Superconducting Order Parameter on Quasi-Particle Interference

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Abstract

Superconductors are important to study due to their many applications. Superconductivity arises when electron pairs, so-called Cooper pairs, form in the material. To understand the mechanism behind the formation of the Cooper pairs, the pairing symmetry, described by the order parameter, must be found. One method to experimentally determine the order parameter is through quasi-particle interference. Quasi-particle interference (QPI) is a real space perturbation due to a defect and can be experimentally imaged using scanning tunneling microscopy (STM), where an atomic sized tip is scanned over a surface at a bias measuring the tunneling current through the sample surface. QPI can also be theoretically calculated using a tight-binding model describing the electronic structure and then using an interpolation between unit cells using wave functions to carry intra-unit cellular information, so-called Continuum QPI (CQPI). This report studies the influence of different superconducting order parameters in a one-band cuprate-like material on theoretically calculated phase-referenced Fourier transformed CQPI (PRFT-CQPI). The results show that this method gives qualitatively distinct results depending on the order symmetry, suggesting that it can be used to experimentally determine the superconducting gap symmetry. The results are also compared with experiment and with previously published CQPI calculations.
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1 Introduction

Superconductivity is an immensely useful phenomenon where a material can carry electrical current without resistance. There are many known superconducting materials, however, all known superconductors only exhibit this property at very low temperatures, necessitating liquid nitrogen or helium, making it difficult to make use of this property outside of specialist applications.

Superconductivity was first discovered in the early 20th century by Heike Kamerlingh Onnes when investigating the temperature dependence of the resistivity of mercury using liquid helium as a cooling method [1]. This is however at a temperature of 4.2K.

Possible future applications for room temperature superconductors include transmission lines, reducing energy loss. Superconducting magnets also have many possible applications, magnetic levitation trains, for example, have been proposed. This would be a train that has a superconducting system onboard which repels the tracks it travels on to reduce friction, both speeding up a train and reducing the amount of energy necessary to propel it. There are also applications in medicine, for example to create the magnetic fields used in magnetic resonance imaging.

The first theoretical description of superconductivity was published more than 50 years after its discovery. The theory, proposed by Bardeen-Cooper-Schrieffer (BCS), describes the phenomenon as a result of electrons pairing up due to a phonon mediated interaction, so-called Cooper pairs [2]. So far this is the only theory which can predict the critical temperature of superconductors with reasonable accuracy.

In the 80s, the first cuprate high-temperature superconductor was discovered [3]. The term cuprate loosely classes together materials which include Copper anions. This class of materials exhibit superconducting properties at temperatures as high as 133 K. Higher critical temperature materials have been found but only at very high pressures, as opposed to ambient pressure [4]. Since the cuprates had such a high critical temperature, they were researched heavily in order to understand the mechanism behind their superconductivity, which has since been discovered to be electrons condensing into Cooper pairs due to an exchange interaction between the electrons. These materials also have a different order parameter to that of the previously discovered superconductors [5]. The order parameter describes the pairing symmetry of the Cooper pairs, and in the case of an exchange mediated Cooper pair, which largely interacts with the nearest neighbor, a $d$-wave pairing was found. Compared to the previous superconductors, where the pairing symmetry is an isotropic $s$-wave, the $d$-wave undergoes sign-changes in $k$-space, thus making phase information important to distinguish between different order parameters.

There is a whole range of possible superconducting order parameters and it is not exclusive to isotropic $s$-wave. This means that to discover new materials, reliable methods of experimentally determining the order parameter of a material is necessary for the field to progress. Only three methods are able to do this while including phase information: the tri-crystal experiment [5], used to identify the order parameter of the cuprates, neutron scattering [6], and quasi-particle interference [7].

Quasi-particle interference (QPI) is the real-space perturbation in the local density
of states (LDOS) due to a defect in a material. QPI is measured using a real-space imaging method called Scanning Tunneling Microscopy (STM), where an atomic sized tip is scanned across the surface of a material measuring the tunneling current producing an image of the LDOS of the material surface. The LDOS with a defect to simulate QPI, can be theoretically calculated using Green’s function formalism, which provides both an experimental and theoretical method that produce the same product.

The goal with this project is to show how QPI can potentially be used in characterization of superconducting order parameters in materials.

This is done through theoretical calculations of QPI in cuprates using the Continuum QPI method (CQPI), where interpolation with wave functions is used to include information smaller than the unit cell which results in higher accuracy between experimental and theoretical results than in the conventional QPI method. This report studies the CQPI images generated through calculations by taking the Fourier transform of the CQPI (FT-CQPI) and comparing scattering vectors in the FT-CQPI to those in the Fermi surface. Phase information is also studied through so-called Phase-referenced FT-CQPI (PRFT-CQPI), where the method shows sign-changes in the FT-CQPI maps, providing a way to compare sign-changing order parameters.
2 Theory

2.1 Superconductivity

Superconductivity is the phenomenon of a material exhibiting no resistance to an electric current. This property occurs in materials below the material’s critical temperature \( T_c \), for example single element materials such as mercury (4.15K), lead (7.19K), and niobium (9.26K) and compound materials such as magnesium diboride (39K), iron selenide (60-100K) and BSCCO (up to 104K).

The standard theory of superconductivity is BCS (Bardeen-Cooper-Schreiffer) theory which describes electron pairs as condensing into so-called Cooper pairs [2]. The theory shows that at any attraction between two electron pairs, Cooper pairs form. In the conventional case, the pairing symmetry of the Cooper pairs is isotropic, so-called \( s \)-wave symmetry. The symmetry is described by the order parameter of the superconductor.

In many superconductors, the mechanism behind Cooper pairs is a phonon interaction. However, with the discovery of the high temperature superconductivity in cuprates, this description was no longer universal, and a different mechanism had to be found to describe this novel material. In cuprates, the mechanism behind Cooper pairs is an exchange interaction, resulting in an order parameter that is no longer isotropic and undergoes sign changes.

Unconventional superconductors are those whose order parameter has a lower symmetry than the crystal symmetry. Many different kinds of order parameters have been speculated, since both the spin part and the orbital part may have some sort of \( k \)-dependence.

The order parameters used in this report are

\[
\Delta_k = \Delta_0 \\
\Delta_k = \frac{1}{2} \Delta_0 (\cos(k_x a) - \cos(k_y a)) \\
\Delta_k = \frac{1}{2} \Delta_0 \sin(k_x a) \sin(k_y a) \\
\Delta_k = \Delta_0 \sin(2\pi k_x) \\
\Delta_k = \frac{1}{\sqrt{2}} \Delta_0 (\sin(2\pi k_x) + i \sin(2\pi k_y))
\]

where \( \Delta_0 \) is the magnitude of the superconducting gap.

\( s \)-wave symmetry is the isotropic pairing state described in BCS theory and is the most conventional superconducting state, describing many superconductors such as aluminium, lead, and niobium. \( d \)-wave symmetry has been confirmed in some materials, such as the cuprates, and \( p \)-wave is yet to be confirmed in a material. Chiral \( p \)-wave symmetry \((p_x + ip_y)\) is of interest in quantum computing [8].
Figure 1: Pairing symmetries in momentum space: (left) s-wave, (center) $d_{x^2-y^2}$ -wave, and (right) $d_{xy}$ -wave.

### 2.1.1 Cuprates

Cuprates are materials with copper anions, commonly in the form of CuO$_2$ layers, and are high-temperature superconductors. A single electronic band is sufficient to describe their electronic structure. It has been found that the superconducting order parameter of cuprates has d-wave symmetry of the type $d_{x^2-y^2}$ [5].

The first cuprate to be discovered was Ba-La-Cu-O [9]. Quickly thereafter BSCCO, or Bi-Sr-Ca-Cu-O was discovered and is now a commonly studied material with ARPES and STM due to cleaving well and giving good surfaces. It is a family of cuprates, with chemical formula Bi$_2$Sr$_2$Ca$_{n-1}$Cu$_n$O$_{2n+4+x}$. Generally, the $T_c$ increases as $n$ increases, up to a point called optimal doping, where $T_c$ reaches a maximum.

It was in cuprates that quasi-particle interference was first shown to be a method of studying superconductivity [10]. This is thus an ideal material to study the influence of different superconducting gap symmetries on QPI, even though it is known what the superconducting order parameter is for cuprates.

Scattering vectors in cuprates are usually set out according to the octet model [11], where seven scattering vectors connect eight points in the Fermi surface as represented in Figure 2. Points of high symmetry in $k$-space are defined as in Figure 2.

### 2.1.2 Superconducting Hamiltonian

The Hamiltonian for electronic structure of a superconducting system can be written in Nambu formalism as a matrix consisting of the real and mirrored non-superconducting Hamiltonian on the diagonal and the superconducting order parameter on the off-diagonals, as

$$H^{SC} = \begin{pmatrix} H(k) & \Delta_k \\ \Delta_k^* & -H(-k) \end{pmatrix}$$

(6)

where $\Delta_k$ is the order parameter. Calculations of this are projected onto the particle sector.
2.2 Scanning Tunneling Microscopy

Scanning Tunneling Microscopy (STM) is an experimental technique for studying the electronic structure of the surface of materials. An STM uses an atomically sharp tip, held a few Ångströms above the surface of the sample. A voltage between the tip and the surface is applied to induce a tunneling current, which is measured. The tip is then scanned over the real space to make an image of the surface, called a topographic map, see Figure 3. Measurements are usually taken at very low temperatures to be able to take sharp images.

Scanning tunneling spectroscopy takes a spectrum by measuring the current in one position and varying the voltage applied between the tip and the surface. This gives a spectrum of the local density of states as a function of electron energy, commonly called and I-V curve, whose derivative is $dI/dV$ which is proportional to the LDOS [12].

$$\frac{dI(V, r)}{dV} \propto \rho(eV,r)$$

2.3 The Spectral Function

The spectral function is a measure of the probability of a particle with momentum $\mathbf{k}$ to have energy $\omega$. This is given by

$$A(k_x, k_y, \omega) = \frac{-1}{\pi} \text{Tr} \text{Im} G(k_x, k_y, \omega)$$

where $G(k_x, k_y, \omega)$ is the Green’s function. This shows that a particle can have an energy distributed around a mean, according to the Heisenberg uncertainty principle. This can be plotted at fixed $\omega$ with varying $k_x$ and $k_y$ or along a fixed path in $k$-space, like with band structure, and $\omega$ along the other axis.
2.4 Local Density of States

The local density of states (LDOS) is the spatially-resolved density of states. The differential conductance measured by STM is proportional to the LDOS and the LDOS can also be calculated theoretically with Green’s function formalism.

The LDOS can be calculated from a Hamiltonian $H^0(\mathbf{k})$, often chosen as a tight binding model. This is done through Green’s function formalism, defined as

$$
G^0(\mathbf{k}, \omega) = \frac{1}{\omega - H^0(\mathbf{k}) + i\Gamma} \tag{9}
$$

where $\omega$ is the energy, $H^0(\mathbf{k})$ the Hamiltonian describing the system, and $\Gamma$ the energy broadening. By definition, the local density of states is the imaginary part of the Green’s function

$$
\text{Im} G^0(\mathbf{k}, \omega) = \delta(\omega - E(\mathbf{k})) = N^0(\omega) \tag{10}
$$

and with a summation over $\mathbf{k}$ we get the LDOS as

$$
\rho(\omega) = \sum_{\mathbf{k}} \text{Im} G^0(\mathbf{k}, \omega) = \sum_{\mathbf{k}} \delta(\omega - E(\mathbf{k})) \tag{11}
$$

2.5 Quasi-particle interference

Quasi-particle interference (QPI) is the spatial perturbation to the LDOS due to defects or boundaries. This is because electrons, in the presence of an impurity, produce real-space oscillations in the local density of states which can be detected using STM. The Fourier transform of the impurity LDOS gives well defined scattering vectors $\mathbf{q} = \mathbf{k} - \mathbf{k}'$ where $\mathbf{k}$ and $\mathbf{k}'$ are constrained to the single particle band structure. QPI is then a quantity that can be obtained from experimental STM measurements and theoretical calculations, thus provides a way to compare experiment and theory.
A Hamiltonian including a point-like defect at unit cell $\mathbf{R}_\alpha$

$$H(\mathbf{R}) = H^0(\mathbf{R}) + V^{\text{imp}} \delta(\mathbf{R}_\alpha)$$

where $H^0(\mathbf{R})$ is the Hamiltonian in unit cell $\mathbf{R}$ describing the unperturbed system and $V^{\text{imp}} \delta(\mathbf{R}_\alpha)$ describes the perturbation due to the defect using a Kronecker delta function.

Similar to the non-interacting case shown in Equation 9, we can write the retarded Green’s function as

$$G^R(\mathbf{R},\mathbf{R}',\omega) = \frac{1}{\omega - H^0(\mathbf{R} - \mathbf{R}') - V\delta(\mathbf{R}_\alpha) + i\Gamma}$$

which is the probability of a particle with energy $\omega$ at $\mathbf{R}$ to propagate to position $\mathbf{R}'$ at energy $\omega$. Here $i\Gamma$ is an energy broadening term. This equation is not analytically solvable as is, however with some approximations it is.

Rewrite the equation, taking out the impurity term:
\[ G^R(R, R', \omega) = \left( \frac{1}{\omega - H^0(R - R') + i\Gamma} \right) \left( \frac{1}{1 - \frac{V\delta(R_\alpha)}{\omega - H^0(R - R') + i\Gamma}} \right) \]  \hspace{1cm} (14)

A Taylor expansion on the second parenthesis yields

\[ \frac{1}{1 - \frac{V\delta(R_\alpha)}{\omega - H^0(R - R') + i\Gamma}} = 1 + \frac{V\delta(R_\alpha)}{\omega - H^0(R - R') + i\Gamma} + \frac{V^2\delta(R_\alpha)}{(\omega - H^0(R - R') + i\Gamma)^2} + \frac{V^3\delta(R_\alpha)}{(\omega - H^0(R - R') + i\Gamma)^3} + \ldots \]  \hspace{1cm} (15)

Where each term is a product of the unperturbed Green’s function, \( G^0(R - R', \omega) \).

Here, a change of notation is made, since the non-interacting Green’s function is invariant under translation. This can be rewritten, taking care of the order of multiplication, to

\[ G^R(R, R', \omega) = G^0(R - R', \omega) + G^0(R - R', \omega) V\delta(R_\alpha) G^0(R - R', \omega) + G^0(R - R', \omega) V\delta(R_\alpha) G^0(R - R', \omega) V\delta(R_\alpha) G^0(R - R', \omega) + \ldots \]  \hspace{1cm} (16)

Now, since the Kronecker delta function is non-zero only for \( R' = R_\alpha \), rewrite the above as

\[ G^R(R, R', \omega) = G^0(r - R', \omega) + G^0(r - R_\alpha, \omega) V G^0(R_\alpha - R', \omega) + G^0(r - R_\alpha, \omega) V G^0(R_\alpha - R_\alpha, \omega) V G^0(R_\alpha - R', \omega) + \ldots \]  \hspace{1cm} (17)

Let \( R_\alpha = 0 \) and write the infinite series as

\[ G^R(R, R', \omega) = G^0(R - R', \omega) + G^0(R, \omega) T(\omega) G^0(R', \omega) \]  \hspace{1cm} (18)

with the \( T(\omega) \) matrix defined as

\[ T(\omega) = V[1 + G^0(0, \omega)V + (G^0(0, \omega)V)^2 + (G^0(0, \omega)V)^3 + \ldots] \]  \hspace{1cm} (19)

which is equivalent to
\[ T(\omega) = \frac{V}{1 - VG^0(R = 0, \omega)}. \] (20)

The \( T(\omega) \) matrix describes all possible scattering of the point-like impurity, described by \( V \).

Now, by taking the imaginary part of the Green’s function, the LDOS can be found as

\[ N^0(\omega) + \delta N(R, \omega) = \text{Im}[G^R(R, R', \omega)] = \text{Im}[G^0(0, \omega)] + \text{Im}[G^0(R, \omega) T(\omega) G^0(-R, \omega)] \] (21)

where one term is the unperturbed part of the Green’s function and the other the perturbation which is spatially dependent and due to the impurity. This second term is the QPI since it is oscillations due to the impurity, and can be calculated, after a Fourier transform to the \( q \)-space as

\[ \delta N(q, \omega) = \text{Im} \sum_k [G^0(k, \omega) T(\omega) G^0(k + q, \omega)] \] (22)

This would give the FT-QPI map. Here one can see that the oscillations have a direction and wavelength described by the scattering vector \( q \) connecting two constant energy states of the electronic structure.

This equation above, Equation 22, calculates what is called the discrete or lattice QPI, since it utilizes a discrete lattice composed only of the coordinates of the center of the unit cells. However, since an STM measures the LDOS with a continuous \( r \), the discrete QPI will not agree very well with the experimental measurement. In addition, Equation 22 does not take into account the vacuum tail of the wave functions above the surface towards the tip position, ignoring any tunneling matrix effects due to the overlap between the surface and tip wave functions. A continuum QPI (CQPI) calculation is necessary to compare experiment with theory.

### 2.5.1 Continuum QPI

The continuum LDOS describes the QPI as a function of a continuous variable through a continuum transformation from the lattice Green’s function. This accounts for different positions and orbital character of the states. With the continuum calculation, the interaction of wave functions are considered over several unit cells, and such, they must be specified. They can be taken from density functional theory calculations or as Gaussian or Slater-like functions.

The interpolation is given as [13]

\[ G(r, r', \omega) = \sum_{R, R'} G^R(R, R'; \omega) w_R(r) w_{R'}(r') \] (23)
where \( w_R(r) \) and \( \tilde{w}_R'(r') \) are the wave functions carrying intra unit cell spatial information. This gives that

\[
\rho(r,\omega) = \frac{-1}{\pi} \text{Im} G(0,0,\omega). \quad (24)
\]

In practice, a CQPI calculation discretizes each unit cell into a certain number of pixels, and for each pixel inside the unit cell, calculates the local density of states due to the wave function at the center of the unit cell, but also from neighboring unit cells within a cut off. This is shown qualitatively in Figure 6 (right) alongside the wave function (left) used in calculations in this report.

The difference between DQPI and CQPI is that the latter carries information within the unit cell, while the former is limited to unit cell discretization. This can be clearly seen in Figure 7, where the DQPI and CQPI are presented for a 7x7 unit cell lattice. In the case of DQPI, this results in only 7x7 pixels, while the CQPI is shown with 15x15 pixels in each unit cell, totaling 105x105 pixels.

### 2.5.2 Phase-referenced QPI

The Fourier transform \( \tilde{g}(q,\omega) \) of the conductance map, i.e. the FT-QPI, measured by the STM is complex valued, and most commonly the modulus is taken since the intensity is used to identify scattering vectors. However, the phase of the Fourier transform (FT) carries information about the order parameter and the defect. Since the order parameter information is of interest and not the defect, using phase-referenced Fourier transform is useful. Phase-referenced FT (PRFT) makes it pos-
Figure 7: (left) Discrete QPI and (right) continuum QPI for 7x7 unit cells. The limitation with DQPI is that it cannot carry information smaller than a unit cell, which makes it poor to compare to STM QPI images, which measure continuously and is better compared with CQPI.

Possible to compare the FT-QPI map at positive and negative energies to study the sign-change of the order parameter. The PRFT references the phase of the FT at energy $\omega$ at an energy $\omega_0$. In a superconductor, it is useful to consider the QPI for $\omega < 0$ and reference to $\omega_0 = |\omega|$.

$$\tilde{g}_{PR}(\mathbf{q}, -\omega) = |\tilde{g}(\mathbf{q}, -\omega)| \text{ Re} [e^{i(\theta_{\mathbf{q}, -\omega} - \theta_{\mathbf{q}, \omega})}]$$

(25)

The Fourier transform of the conductance map is thus modulated by a phase factor, +1 for in-phase oscillations and -1 for out-of-phase oscillations. This method removes any global phase arising, for example, from the position of the defect in the frame of the image.
3 Method

The quasi-particle interference maps are generated using the continuum calculation presented in sections 2.5 and 2.5.1. From the continuum QPI calculation, the local density of states real space map is found. This is then Fourier transformed into a FT-QPI map. The PRFT-QPI is calculated by using Equation 25. The density of states and spectral function are also calculated.

The one-band tight-binding Hamiltonian used to describe cuprates in this report is given by

$$H(k) = t_1(\cos(k_x) + \cos(k_y)) + t_2 \cos(k_x) \cos(k_y) + t_3(\cos(2k_x) + \cos(2k_y)) + t_4 \cos(2k_x) \cos(2k_y) + \ldots$$

(26)

where the hopping parameters $t_1, t_2, \ldots$ must be specified. Nine hopping parameters are used, with the parameters taken from [14]. Only in-plane hopping is used, since out-of-plane hopping is a magnitude smaller than in-plane.

From [14], the optimal doping is at $n = 0.85$ (15% hole doped) which gives a Fermi level at -0.36963 eV. For all Cuprate figures in this report with the exception of the ones directly compared to the results of [14], the Fermi level is set at 0 eV, corresponding to a doping of $n = 1.12$ (12% electron doped).

Parameters that could be fixed by parameters from Kreisel et al.[14] have been chosen as such. These are the superconducting gap at $\Delta = 0.033$ eV and $V_{imp} = 0.3$ eV unless otherwise stated.

The orbitals are described by Slater-like type wave functions. Cuprates have mainly $d_{x^2-y^2}$ type orbitals, given as a Slater-type wave function as

$$w(r) = \sqrt{\frac{15}{12\pi}} \frac{x^2 - y^2}{2r^2} e^{-|r|/w}$$

(27)

where $r = \sqrt{x^2 + y^2 + h^2}$. $w$ is specified by the parameter radius and $h$ by the parameter zheight. The parameters chosen for definition of the wave function are a radius of 0.6 and a zheight of 1, see Figure 6, chosen to be similar to the wave function used in [14]. There is one wave function centered on the Cu atom centered in the unit cell.

The number of $k$-points is 4096, lattice size is 64x64 with each unit cell discretized at 3x3 for the continuum calculation. The energy broadening $\Gamma = 0.001$ eV, which is approximately 4K in temperature. For computational efficiency the sums over the nearest neighbour unit cells only run up to a cut off, which is here set to 4.
4 Results

Calculations using the cuprate model with different superconducting order parameters are presented to investigate whether PRFT-CQPI patterns are unique and if they allow to distinguish between different order parameters.

4.1 Normal state electronic structure

The normal state of the cuprate, which occurs above $T_c$, is presented here. The band structure and density of states are shown in Figure 8 where a van Hove singularity, which occurs due to a saddle point in the band structure, is shown at -0.55 eV. In Figure 9, the spectral function and the FT-CQPI map are shown at the Fermi level. Here, the distinct cuprate banana shapes are shown in the spectral function. In the FT-CQPI map the scattering vectors expected from the octet model are present, as shown by the red arrows.

![Figure 8: Spectral function (left) and DOS (right) of cuprate in the normal state with a van Hove singularity at -0.55 eV. Inset shows no gaps at the Fermi level.](image)

4.2 S-wave superconductivity

S-wave superconductivity is the conventional type of superconductivity well described by BCS theory. Including a superconducting gap with s-wave symmetry, Equation 1, in the tight-binding model described above, opens up energy gaps at both places in the Brillouin zone where the band crosses the Fermi level, Figure 10. The superconducting gap has a U-shape as seen in the DOS in Figure 10. Due to
energy broadening, the corners at the bottom of the U-shape are curved as opposed to sharp, which they would be in the case of no broadening. Due to the gap in the DOS, the behavior of the Spectral function and the FT-QPI map, shown in Figure 11, is such that they have large intensity near the coherence peaks and very low intensity at energies inside the gap. Apart from the intensity decreasing due to the gap, here is no other change from superconductivity in the features of the Spectral function or the FT-CQPI maps. This is because the s-wave symmetry is isotropic.

4.3 D-wave superconductivity

Cuprates have been shown to have \(d_{x^2-y^2}\) pairing symmetry. Here both \(d_{x^2-y^2}\) and \(d_{xy}\) symmetries are presented.

The average LDOS for s-wave and d-wave symmetries is presented in Figure 12. Here the U-shape of the s-wave is distinct from the V-shapes of the two d-wave symmetries. The \(d_{x^2-y^2}\) order parameter has a broader gap at low LDOS while the \(d_{xy}\) has a clear V-shape. The peaks are at \(\pm 0.034\) eV, \(\pm 0.027\) eV and \(\pm 0.03\) eV for \(s\), \(d_{x^2-y^2}\), and \(d_{xy}\) respectively. The slight asymmetry, with slightly higher peaks at \(\omega < 0\), is due to the underlying non-superconducting DOS, as seen in Figure 8, since there is a van Hove singularity at \(-0.55\) eV and the DOS slants towards this peak. The height of the peaks can be understood from how much area of the non-superconducting DOS the gap displaces, since \(d_{x^2-y^2}\) is wider at the bottom than \(d_{xy}\), the \(d_{x^2-y^2}\) peaks will be larger.
Figure 10: (right) Spectral function with insets showing the gaps due to superconductivity and (left) density of states of cuprate with s-wave order parameter.

Figure 11: FT-CQPI maps with corresponding spectral function as inset for cuprate with s-wave symmetry. Due to isotropic symmetry, the gap is in all directions and the intensities fade in the gap.
Figure 12: Average LDOS for \textit{s}-wave, \textit{d}_{x^2-y^2}-wave, and \textit{d}_{xy}-wave superconducting symmetries. Peaks are at ±0.034 eV, ±0.027 eV and ±0.03 eV respectively. \textit{s}-wave shows the distinct U-shape, while \textit{d}-wave symmetries shows the V-shape. The slight asymmetry in the peak heights is due to the underlying DOS, as seen in the DOS of the non-superconducting case.

4.3.1 \textit{d}_{x^2-y^2}-wave symmetry

This is the order parameter curates have been shown to have through the tri-crystal experiment which utilized the phase changes occurring in the order parameter [5]. The spectral function and DOS are presented in Figure 13. Compared to the \textit{s}-wave case, here only one band crossing the Fermi level is gapped, occurring between symmetry points M and X. In Figure 15, where the spectral functions are shown as insets, the gap is also seen occurring between M and X. In the DOS, the gap is present and has the V-shape of the \textit{d}-wave gap.

In Figure 14, the Continuum Local Density of States is presented as a function of energy at three locations in real space: on top of the impurity, on top of a nearest neighbor of the impurity, and far away from the impurity at an impurity free site as well as the average CLDOS over all real space. The gap is present in all CLDOS, however there is an asymmetry at the coherence peaks of all sites that cannot be due to the non-superconducting DOS. The impurity free site and the Average CLDOS show a negligible asymmetry, with peak energy at similar \(\omega\) values and no height difference between the coherence peaks. The impurity free site will have larger overall values due to being taken on top of an atom, while the average CLDOS averages over the whole real space. The energies of the coherence peaks at the impurity site and the nearest neighbour site have shifted by 0.002 eV, the impurity site coherence peaks by -0.002 eV and the nearest neighbor by +0.002 eV. The coherence peak in the spectrum at the impurity site is approximately 50% larger at positive energy than negative energy, and the spectrum at the nearest neighbour site is approximately 30% smaller.

The FT-CQPI maps of the \textit{d}_{x^2-y^2} pairing symmetry are shown in Figure 15 with red
arrows showing the scattering vectors. At -30 meV and 30 meV, the FT-CQPI maps do not have distinct features of superconductivity, and look similar to maps outside of the gap and also the non-superconducting case. In the spectral functions at these energies, there is not yet a gap present either. At -20 meV and 20 meV, there are distinct patterns different from the maps close to the coherence peaks. At -20 meV the intensity is stronger than at 20 meV, which is expected from the DOS. Intensity peaks are very clear at these energies. The scattering vectors shrink as the energy approaches the Fermi level, which is expected from the spectral functions as seen in the inset figures. Crosses, located on the Bragg peaks, can be identified, which do not appear in the non-superconducting case.

Line cuts of the FT-CQPI maps are taken at three locations, through the central Bragg peaks, through the Bragg peaks of the 1st and 2nd order, and half way between these points, and are presented in Figure 16. They all show how the FT-CQPI maps change in the gap and remain unchanged outside the gap.

The Phase-referenced FT-CQPI maps are presented in Figure 17 alongside the corresponding spectral functions with the pairing symmetry overlaid in red and blue. Scattering vectors are also shown as solid lines for vectors that are not sign changing and dashed lines for those that are sign changing. In the PRFT-CQPI maps the red represents an area that is not sign changing and blue an area that is. For energies -20 meV and -10 meV, the scattering vectors match very well between the spectral function and the PRFT-CQPI, however at -30 meV the PRFT-CQPI is qualitatively completely red, exhibiting no sign change.

Figure 13: Spectral function (left) and density of states (right) for $d_{x^2-y^2}$ pairing symmetry in cuprate.
Figure 14: Local density of states at impurity site (red circle), nearest neighbor site (blue triangle) and impurity free site (green star) with $d_{x^2-y^2}$ wave symmetry.

Figure 15: FT-CQPI maps of cuprate at energies -30, -20, -10, 10, 20, 30 meV with $d_{x^2-y^2}$ symmetry with scattering vectors in red. Inset is the spectral function at corresponding energy. The scattering vectors shrink as the energy approaches the Fermi energy.
Figure 16: Line cuts of CQPI of cuprate with $d_{x^2-y^2}$ symmetry.

Figure 17: Phase referenced FT-CQPI maps of cuprate with $d_{x^2-y^2}$ symmetry. Solid line scattering vectors are non-phase changing, dashed scattering vectors are sign changing. In the PRFT-QPI map, if the vector points to a blue area, it is sign changing, if red, it is not sign changing. For energies -20 meV and -10 meV, the PRFT-QPI map agrees with the predicted signs, however, at $\omega = -30$ meV it does not agree.
4.3.2 Comparison to published CQPI

A comparison to previous CQPI calculations is made presented in Figure 18, published by Kreisel et al. (2015) [14]. The wave function is chosen to be similar to the one presented in the Supplementary Material of the paper, however, in this report Slater-like wave functions are used while the original paper uses wave functions from ab initio density functional theory calculations. The order parameter is chosen to be the same, of \( d_{x^2-y^2} \) symmetry and with a gap \( \Delta = 0.033 \) eV. The impurity potential is also chosen to be the same, \( V_{imp} = 0.3 \) eV. Energy broadening is set at 1 meV, which corresponds approximately to the thermal broadening in tunneling spectra expected at 4K. The model is also calculated at optimal doping, \( n = 0.85 \).

In Figure 18, the FT-CQPI maps of BSCCO cuprate calculated by [14] are shown alongside the FT-CQPI maps calculated in this report. Most peaks are present in both, and show especially clear correspondence at \( \pm 18 \) meV. There is less similarity between the maps at \( \pm 30 \) meV, this is very close to the coherence peaks, and most likely is due to using different wave functions in the calculation. The intensities are different, however broadly, the high intensity spots occur in both maps, and the general shapes are similar.

Figure 18: Comparison with figures from Kreisel et. al (2015) Supplementary Materials [14], used with permission from the author, of cuprate FT-CQPI maps with some peaks of interest circled with blue added in this report. The figures from Kreisel are to the left in each pair, marked with energy in red text, with the corresponding figure calculated in this report placed to the right in each pair.
4.3.3 $d_{xy}$-wave symmetry

For $d_{xy}$ pairing symmetry, the superconducting gap now occurs between symmetry points X and $\Gamma$, as shown in the spectral function in Figure 19 and in the spectral functions presented as insets in Figure 20.

In the FT-CQPI maps, Figure 20, the scattering vectors in the spectral function show clear peaks in the FT-CQPI maps. The maps at $\pm 30$ meV show structure different from outside the gap. The scattering vectors grow in the gap, and so do the patterns in the FT-CQPI maps, contrasting to $d_{x^2-y^2}$ symmetry where they shrink. Line cuts are presented in Figure 21.

The PRFT-CQPI maps in Figure 22 show correspondence between the sign-changing scattering vectors in the spectral function and the PRFT-CQPI map at -20 and -10 meV, while it does not match up at energy -30 meV.

![Spectral function and DOS for $d_{xy}$-pairing symmetry in cuprate](image)

Figure 19: Spectral function (left) and DOS (right) for $d_{xy}$-pairing symmetry in cuprate.

4.3.4 Comparison to experiment

The PRFT-CQPI calculated in this report is compared to the experimental PRFT-CQPI data published by Gu et al. (2019) [15] in Figure 23. The experiment was done by STM on a BSCCO cuprate. The gap was measured to be $\Delta = 44$ meV, so the maps for comparison are chosen at an energy scaled by 3/4 since they were calculated for a gap $\Delta = 33$ meV. The cuprate with $d_{x^2-y^2}$ order parameter, Figure 17 share many similar features with the experiment, for example, no sign changes along the diagonals. The calculation with $d_{xy}$ order parameter, Figure 22, however,
Figure 20: FT-CQPI maps of cuprate at energies -30, -20, -10, 10, 20, 30 meV with $d_{xy}$ symmetry with scattering vectors in red. Inset is the spectral function at corresponding energy. The scattering vectors shrink as the energy approaches the Fermi energy.

Figure 21: Line cuts of FT-CQPI of cuprate with $d_{xy}$ order parameter.
Figure 22: Phase-referenced FT-QPI map of cuprate with $d_{xy}$ symmetry at -30 meV, -20 meV, and -10 meV. Scattering vectors are shown in red and black, with solid vectors showing non-sign changing scattering vectors and dotted vectors sign changing vectors. In the PRFT-QPI map, if the vector points to a blue area, it is sign changing, if red, it is not sign changing. For energies -20 meV and -10 meV, the PRFT-QPI map agrees with the predicted signs, however, at $\omega = -30$ meV it does not agree.

does not, which is expected, since cuprates have been shown to have $d_{x^2-y^2}$ pairing symmetry.

The experimental PRFT-CQPI shows some additional peaks due to supermodulation, a structural reconstruction of the bulk material, which is not accounted for in the calculation.

Figure 23: Comparison of $d_{x^2-y^2}$ and $d_{xy}$ PRFT-CQPI maps (middle and right) to STM experiment (left) by Gu et al. (2019) [15] under CC4.0 license. Large circles in black added in this report. The paper reports a gap $\Delta = 44$ meV, energies are thus scaled by 3/4 to be comparable, since this reports QPI is calculated with $\Delta = 33$ meV. The experiment, a BSCCO cuprate, matches very well with $d_{x^2-y^2}$ symmetry while $d_{xy}$ symmetry does not share the same features.
4.4 P-wave superconductivity

A chiral p-wave order parameter does not have clear sign-changes as the d-wave symmetries do, which makes it difficult to study in the same way as the d-wave. The $p_x + ip_y$ order parameter would need some sort of color wheel to show the expected sign changes, and this is not illustrated here. The $p_x$ order parameter is simple, however, with a nodal line running vertical through the center, and a sign change over this line.

The gap shapes of all paring symmetries studied in this report are presented in Figure 24. The normal state spectrum shows no gap and with a slope due to details of the band structure. As presented earlier, gap for an $s$-wave order parameter has a U-shaped gap and the two d-wave order parameters have a V-shaped gap. The two d-wave order parameters follow each other up until their coherence peaks, which is what the two $p$-wave cuprates do as well. The gap for the $p_x$-wave order parameter has a V-shape at the bottom of the gap, but curves from the coherence peaks as opposed to the chiral $p$-wave which is similar to the $s$-wave gap but again with a slight curve from the coherence peak.

![Figure 24: Average CLDOS of cuprate with different pairing symmetries.](image)

PRFT-CQPI maps at -20 meV for order parameter $d_{x^2-y^2}$, $d_{xy}$, $p_x$ and chiral p-wave are presented in Figure 25. All maps have differences between them. Only $p_x$ shows C2 symmetry in the map, making it stand out from the remaining. The $\pi/4$ rotation of the sign changes between $d_{x^2-y^2}$ and $d_{xy}$ wave show relatively clearly, with, for example, sign changes in blue along the diagonal for $d_{x^2-y^2}$ and along the vertical and horizontal for $d_{xy}$.

In all of the superconducting FT-CQPI maps, crosses centered on the Bragg peaks are visible. These do not occur on the non-superconducting maps.

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Figure 25: PRFT-CQPI maps for order parameters $d_{x^2-y^2}$, $d_{xy}$, chiral p-wave, and $p_x$ at -20 meV.

4.5 Influence of impurity potential

To understand the influence of the impurity potential on the PRFT-CQPI maps, calculations were done for different impurity potentials. These are presented in Figure 26. As seen in the maps, there is no distinguishable difference between $V_{imp} = 1$, 10, and 100 meV, apart from a magnitude increase in intensity, however at 1000 meV the map clearly changes. The intensity increase corresponds with the theory, where for small $V G^0(0, \omega)$, the T-matrix is approximately equal to $V$. So a magnitude increase in $V$ would mean a magnitude increase in the intensity. The change at $V_{imp} = 1000$ meV could be due to reaching a limit.
5 Discussion

The coherence peaks of the $d_{x^2-y^2}$-wave symmetric cuprate are at a smaller value than the coherence peaks of the $d_{xy}$-wave symmetric cuprate, see Figure 12, and so the FT-CQPI maps look similar to the normal state maps even in the gap when close to the coherence peak. This is due to the nodal planes of the pairing symmetry being aligned and misaligned, respectively, to the wave function.

The PRFT-QPI maps show that this method works for order parameter identification, since the sign-changing scattering vectors are determined by this property. The $\pi/4$ rotation between the $d_{x^2-y^2}$ symmetry and the $d_{xy}$ symmetry can be seen directly in the scattering vectors of the PRFT-QPI maps in the superconducting gap. Both the $d_{x^2-y^2}$ and $d_{xy}$ symmetric cuprates do not agree with the expected sign changes close to the coherence peak, which suggests the PRFT-QPI should be studied firmly in the gap if there is an expectation of correspondence to the sign changes in the spectral function scattering vectors.

Overall, there is a distinction between the PRFT-CQPI patterns of this cuprate model with different order parameters. However, further analysis is necessary to see how these patterns behave due to superconducting order parameter symmetry. These results imply that studying phase-referenced Fourier transformed quasiparticle interference might be a way forward in the characterization of superconducting order parameters prompting further studies on the topic.

Figure 26: PRFT-CQPI at $\omega = -20meV$ with impurity potentials $V_{imp} = 1, 10, 100, 1000$ meV. The lower three potentials are indistinguishable apart from intensity increasing by one magnitude for each magnitude increased in potential.
6  Bibliography


