EXPLORATIONS IN STM PHENOMENOLOGY :
“INVERSION” TECHNIQUES FOR STM DATA
ANALYSES

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by
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With the advent of Scanning Tunneling Microscopy (STM), the STM has provided us with unprecedented information on the electronic properties of a sample at the atomic level. Because of the STM’s accessibility to the microscopic scale, an experiment on a macroscopic sample provides vast amounts of data. To understand the condensed matter physics underlying the vast STM data on a macroscopic sample, one needs analysis techniques for STM that make use of the aforesaid accessibility to the atomic scale. In this thesis, our aim is to devise analysis techniques that we term as “Inversion” techniques: a technique that extracts information regarding the Hamiltonian/physics of the sample from the STM data with minimal assumptions.

In Chapter 2, we show that the local density of states (LDOS) measured in a STM experiment, at a single tip position contains oscillations as a function of energy, due to quasiparticle interference, which is related to the positions of nearby scatterers. We call them quasiparticle echoes. We propose a method of STM data analysis based on this idea, which can be used to locate the scatterers. In the case of a superconductor, the method can potentially distinguish the nature of the scattering by a particular impurity.

In Chapter 3, we demonstrate an analysis scheme again based on quasiparticle interference around a point impurity, that extracts the lifetime of a quasiparticle by using the LDOS data around the impurity in a STM experiment. This data analysis scheme would augment the Fourier-Transform Scanning Tunneling Spectroscopic methods which provide us with the quasiparticle dispersion. Thus, point impurities can be used as probes to
extract quasiparticle lifetimes from STM experiments and this would complement other experimental methods such as Angle Resolved Photo-emission Spectroscopy (ARPES). We explain in detail how the scheme works in the case of metals and outline the extension to the superconducting case.

In Chapter 4, we deal with a specific part of STM phenomenology of the high temperature superconductor, $\text{Bi}_2\text{Sr}_2\text{Ca}_1\text{Cu}_2\text{O}_8+x$. It concerns the high-energy features outside the gap seen in the STM experiments on BSCCO. Jinho Lee et al (Nature 442, 546 (2006)) showed that these features were a result of a bosonic mode’s coupling to the electrons in the (believed to be) relevant $\text{CuO}_2$ layer. The nature of the bosonic mode is still not resolved. Using a simplified model of $d$-wave BCS quasiparticles coupled to Einstein oscillators with a momentum independent electron-boson coupling, we try to answer: a) how to extract the frequency of the bosonic mode, and b) how to extract an estimate of the electron-boson coupling strength.
BIOGRAPHICAL SKETCH

The author was born on the thirteenth of July in 1983 to Shri Prasanta Kumar Pujari and Shrimati Arundhati Pati in the town of Sambalpur, India, where his ancestors have lived for a long time. His hometown is the steel township of Rourkela located in the interiors of the eastern Indian state of Orissa, a three hour train ride away from Sambalpur.

Growing up in a planned township where education was valued above all else must have left an impact on him, but his primary memories consist of happy days spent in play - be it sports, study, gossip - with dear friends and his sister, Saswati Pujari, and the loving times spent with family. He also recalls an early affinity to science and thought. One of the catalyzing events that made physics a call for him were the fond conversations about the “great theories of physics” with his cousin, Parthasarathi Pani. Even though they did not have any real understanding of those theories, the sense of wonder and mystery for our immense universe was easily felt by them.

Fortunately, the author got a chance to pursue physics at Bombay. He majored in Engineering Physics at IIT Bombay. The four years spent in the serene campus of IIT Bombay and the crazy city of Bombay were formative both for the scientist and the worldly fellow in him. Some of his few strong friendships started there.

Post Bombay, he has spent the last six years in Ithaca. As a part of the Cornell community and Ithaca community, he will remember these six years for the rest of his life. During these years, not only has he the feeling of maturing as a physicist, but also as a man. Also, if fate would have it, he has found the perfect woman for him. He hopes he is made for her.
This document is dedicated to Maa, Bapa and Pujnan.
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A century ago, the human species was starting to grasp at the quantum laws that govern the grand universe that surrounds us - from our immediate neighborhoods to the farthest reaches we have yet seen - at a most fundamental level, i.e. whatever shape the final theory takes, it most likely is going to be a quantum theory. Along with the principle of Relativity, it forms the fundamental building block of today’s physics. Given this, it is remarkable that within just the passage of hundred years - though every bit eventful - we have come to this stage of understanding and, equally impressively, inventiveness that we comprehend of the majority of humans as belonging to one big planetary community. Quantum theory had a great role to play in this historical process, by not only making possible the growth of technologies like the Computer or Electronics/Optics for Communications but also by fundamentally altering our view of the physical world. I feel lucky and thankful to have been a part of this continuing historical and scientific and human process during my graduate studies.

During my personal journey as a physicist, I am indebted infinitely to my gurus. First and foremost, I thank Prof. Christopher L. Henley. As my mentor at Cornell, he has shaped me in ways that have always revealed in hindsight to be the correct mixture of bitterness and sweetness needed to mold the wayward ways of indisciplined youth. I can not hope to match even a fraction of the measure of his contributions to physics, but I am more confident that I have imbibed to a certain degree his unique and independent brand of scientific spirit. I also hope I take with me the discipline and rigor that I have seen him apply to the process of physics.

I am also extremely thankful to Prof. Michael Lawler and Prof. Eun-Ah Kim. Their encouragement during the search for a post-doc position was invaluable. Learning field theory with Michael was great fun too!
I thank Prof. J. C. Davis and Prof. Erich Mueller who were kindly a part of my special committee. The active collaboration with Prof. Davis and his group members, especially Milan Allan, on STM experiments has been a pleasure.

I also happily recall all sorts of conversations, physics or otherwise, and good times spent with the members of the physics department and outside who have passed through Cornell during my stay. They know who they are.

And as for family and friends, one can not even hope to begin.
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C.1 a) The contour is composed of the small circles enclosing the poles of $1/(e^{i/T} - 1)$ situated at the bosonic Matsubara frequencies $\Omega_m = 2\pi m T$. The un-circled pole represents pole/s due to the rest of the integrand in Eq. C.2. b) The contour in a) can be continuously deformed to the contour shown in b) without crossing any poles, since the contribution at infinity is zero. c) The contour in b) can further be trivially deformed now to enclose the previously un-circled pole in a).

C.2 In this schematic, the shaded area represents the number of states from 0 to $E'$.
The fundamental bedrock on which this graduate thesis rests is a phenomenon that arose only with the birth of Quantum Mechanics. The phenomenon is Quantum Mechanical Tunneling. This phenomenon has no classical analogue. Physicists realized early in the twentieth century that Quantum mechanics allows for tunneling through a potential barrier. Yet, it was experimentally accessible only around the middle of the last century, coincident with the development of semiconductors which led to the development of transistors and diodes. Soon tunneling was seen in metal-insulator-metal junctions and also metal-insulator-superconductor junctions. In 1980s, tunneling led to the development of the Scanning tunneling microscope (STM) which allowed for the first time to image the electronic properties of a material at the unprecedented level of the atom.

Since then, STM has become a powerful tool of condensed matter allowing for probing all kinds of materials at sub-nanoscale from metals to semiconductors to strongly correlated matter to superconductors. Given the increasing use of STM in condensed matter experiments, the phenomenology of STM has naturally assumed importance. STM phenomenology - like any phenomenology - comprises of questions that can be grouped under the following two umbrella questions:

1. What kinds of information can the STM afford us with?
2. What kinds of physical hypothesis can explain the results of the various STM experiments?

The theorist is well placed to help the experimenter in this pursuit partly because STM instrumentation is quite involved requiring systems to manipulate metallic tips.
which are atomically sharp at the sub-nanoscale. In many cases, the experiments are at really low temperatures requiring a know-how of low temperature instrumentation like handling Helium, etc. Also, STM makes available atomic-scale information about a macroscopic sample that leads to vast amount of data. Making sense of the physics operating behind the immensity of the data is a challenging task. Thus, it makes sense that theorists dutifully join the STM experimenters in mining the vastness of STM data for understanding.

As a theorist, I will in this thesis tackle the first kind of question: what kinds of information does the STM afford us with? Or in other words, what kinds of information regarding the hamiltonian/physics of the sample can be gleaned out of STM data? Such a question is what we term as an “Inversion” problem. (We term the second kind of question as a “Forwards” problem.) Thus, the aim of this thesis is to come up with “Inversion” techniques for STM data analysis that can be applied - hopefully - to a range of STM experiments. In the remainder of the Introduction, we will elaborate on this thesis. In the subsequent chapters, we will devote our attention to the particular attempts we have made in this direction.

1.1 Pre-requisites

In order to follow the work to be covered in the following chapters, a basic grounding in Condensed matter theory should suffice. For basic theory, graduate courses on Solid State and an understanding of the basics of many-body theory is ideal. For basic condensed matter concepts, one should go to classic texts such as Ashcroft and Mermin’s Solid State Physics, P. W. Anderson’s Basic Concepts of Condensed Matter, etc. I learnt Many-body theory from the excellent text of G. Rickayzen titled “Green’s Functions in
Condensed Matter”. Other sources are Gerald D. Mahan’s “Many-particle physics”, the classic text of Abrikosov, Gorkov and Dzyaloshinskii (though their notation is slightly old-fashioned compared to that used these days), etc.

In relation to the theory of STM, one can find helpful pedagogical introductions in various texts and reviews. The source I found helpful is Ref. [1].

1.2 Philosophy

1.2.1 “Inversion”

The overarching philosophy that underlies this thesis can be stated as the extraction of the most general quadratic Hamiltonian \(^1\) pertaining to the sample, taking into account its known properties and chemistry, that is consistent with the observations of an STM experiment on the sample. We call this philosophy or program as “Inversion” also.

The motivation for setting out with this program comes from the fact that STM (and all other probes) can only measure specific observables. The observable that an STM gives us is the Local Density of States (LDOS) of electrons at a definite spatial location on the sample surface. The LDOS is defined as

\[
n(\vec{r}; \omega) \equiv -\frac{1}{\pi} \text{Im} \left[ \int dt \ e^{i\omega t} \langle c(\vec{r}, t) c^\dagger(\vec{r}, 0) \rangle \right]
\]  

(1.1)

where \(c^\dagger, c\) is the electron annihilation and creation operators respectively. F.T. stands

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\(^1\)The restriction to a quadratic Hamiltonian, i.e. only one-body operators, is a simplifying starting point of the Inversion program analogous to how mean-field theories are good starting points to understand many condensed matter systems. In Chapter 3, we go beyond the quadratic requirement in a restricted sense - by allowing for complex parameters in the Hamiltonian while respecting Hermiticity to take into account the electron/quasiparticle lifetime that ultimately arises out of underlying many-body effects. In Chapter 4, we explicitly deal with many-body physics (interaction of \(d\)-wave BCS quasiparticles with Einstein oscillators).
for Fourier Transform and the expectation is taken in the ground state at zero temperature (at finite temperatures, one has to calculate a thermal average). In an STM experiment, what is actually measured is the tunneling current as a function of applied voltage between an atomically sharp metallic tip and the sample at the location of the tip. The LDOS can be shown to proportional to the derivative of the tunneling current with respect to the applied voltage (See the Appendix of Ref. [1]). This step has some built-in assumptions: 1) The electrons in the STM tip only hop to and from the atom below the tip. The more true this assumption, the more local the measurement. 2) The proportionality constant depends on the type of metal used for the tip, through the density of states of electrons in the tip and matrix elements for the kinetic coupling between the tip and the sample. Practically, by verifying that the extracted LDOS is same for different kinds of STM tips, one makes certain that the extracted LDOS is reliable information (See Footnote 22 of Ref. [2]).

The nontrivial part of the Inversion program lies in the backing out of the parameters of the Hamiltonian that are consistent with the observed LDOS. Indeed, there can be more than one set of parameters which might be consistent with the observed LDOS, in which case the Inversion program can not tell us uniquely the Hamiltonian, and we will have to look to other experimental probes in order to resolve the ambiguity. The flip side of this drawback is that if there is information that we can get through an Inversion analysis of STM data with absolute certainty, then it will be uniquely true of the sample’s Hamiltonian, i.e. other experimental probes will have to confirm the conclusion of that

\[^2\]Imagine two systems: a) a homogeneous d-wave BCS Superconductor, and b) a homogeneous d-density wave [3] material. We assume a particle-hole symmetric dispersion for the underlying electrons such that \(\epsilon(\vec{k} + (\pi, \pi)) = -\epsilon(-\vec{k})\). Then the states connected by either order parameters are equal in energy. In the case of the superconductor, the d-wave order parameter connects an electron at \(|\vec{k}, \uparrow\rangle\) to a hole at \(|-\vec{k}, \downarrow\rangle\). In the case of the d-density wave, the d-density wave order parameter connects an electron at \(|\vec{k}, \uparrow\rangle\) to an electron at \(|\vec{k} + (\pi, \pi), \uparrow\rangle\). Therefore, the dispersion of the quasiparticles due to the presence of the two different order parameters are identical, i.e. \(E(\vec{k}) = \sqrt{\epsilon(\vec{k})^2 + \Delta(\vec{k})^2}\). Similarly, one gets identical coherence factors \(u(\vec{k}) = \frac{1}{2} \left(1 + \frac{\epsilon(\vec{k})}{E(\vec{k})}\right)\) and \(v(\vec{k}) = \frac{1}{2} \left(1 - \frac{\epsilon(\vec{k})}{E(\vec{k})}\right)\). Thus, the LDOS for the quasiparticles obtaining from these two cases are identical and will have same signatures in the STM spectra.
Inversion analysis.

We shall now discuss one such well-established analysis technique which can be said to fall under the Inversion category. This will give us a flavor of the Inversion philosophy and also serve as a paradigmatic example for the techniques proposed in the main body of this thesis. Our example is the so called Fourier Transform Scanning Tunneling Spectroscopy or FT-STS. This method enables us to extract the dispersion of the electrons (more correctly, Fermi Liquid quasiparticles) of the sample under consideration. This spectroscopic method has been applied successfully to both metals and superconductors [4, 5, 6, 7]. The method essentially works by Fourier Transforming a spatial map of STM data at a particular energy. If there are well-defined quasiparticles in the sample, then it turns out that particular wave-vectors in the Fourier Transform are higher in intensity depending on the dispersion relation. From this, one can extract the dispersion of the electrons in the sample. This is quite a powerful method especially considering that STM is real-space probe, yet capable of giving information that are usually thought of as momentum-space information. Also, as emphasized before, dispersion extracted this way is unambiguous and results on dispersion from other probes (e.g Angle-Resolved Photoemission Spectroscopy or ARPES) have to be in agreement with this method, given that the assumption of the existence of well-defined quasiparticles is true. This method is described in more detail in Chapter 3 and Ref. [8].

1.2.2 “Forwards”

Another well-used and opposite route to any kind of phenomenology can be labeled as “Forward”. In a Forward analysis, one usually makes a supposition or hypothesis about the Hamiltonian of the sample. One then works out the observable of interest given the
hypothesis and compares it to the observed data. The degree of agreement between the two serves as an indicator of the plausibility of the hypothesis. Indeed, much of physics can be thought of as this kind of activity. We will consider some specific examples of such Forward analyses in the context of STM phenomenology that I encountered during my graduate studies, as a study on the contrast of Inversion and Forward approaches to STM studies.

“Anomalous” impurity

Earlier, we briefly mentioned the FT-STS method as an Inversion method. It was applied to the high temperature superconductor \(\text{Bi}_2\text{Sr}_2\text{Ca}_1\text{Cu}_2\text{O}_{8+x}\) (BSCCO) to extract the dispersion relation of the electron. The extracted dispersion was in good agreement with ARPES results. For extracting the dispersion through FT-STS, one just needed particular wave-vectors in the Fourier Transform to “light up” or be higher in intensity with respect to the background. In order to explain the relative magnitude of these peaks in the Fourier Transform, the hypothesis of an “anomalous” impurity was put forward by Nunner \textit{et al}, Ref. [9]. An anomalous impurity, in analogy with an ordinary impurity being thought of as a highly localized modulation of the chemical potential, can be thought of as a highly localized modulation of the pairing potential. This is discussed in more detail in Chapter 2. Their hypothesis that such anomalous impurities are present in BSCCO samples allowed an explanation for why certain peaks in FT-STS of BSCCO were higher in intensity than others. In Chapter 2, we suggest a possible inversion route to tell from STM data whether a particular impurity is ordinary or anomalous.
Phenomenological Modeling of Lifetime

Another work relevant to the phenomenology of BSCCO is the issue of the so-called “coherence” peaks resulting because of the $d$-wave superconductivity observed across high temperature superconductors. It is usual in the STM literature to use the gap between the coherence peaks as representing the $d$-wave gap magnitude as measured in the STM spectra. But, unlike ideal BCS quasiparticles which lead to singular coherence peaks in LDOS spectra, the observed coherence peaks are not sharp but rounded, and the amount of “rounding” also varies from location to location. To explain this, Alldredge et al in Ref. [10] put forth a “forward” hypothesis by positing an intrinsic lifetime broadening of the electrons that go into the making of the $d$-wave Cooper pair in BSCCO. They modeled the lifetime broadening phenomenologically, and were able to fit around a million spectra to a very good degree. Following this work, Graser et al have argued how the assumed phenomenological model for the intrinsic lifetime might be tenable in the context of high temperature superconductivity [11]. This forms another direction in which a forwards analysis has been used, though the broadening issue can not be considered settled since BSCCO (and other Cuprates) are inhomogeneous at nanoscale (with extremely short coherence lengths) and hence, there are possibly other sources of broadening lurking about. In Chapter 3, we discuss a possible inversion route to getting at the intrinsic lifetimes from STM data.

Numerical Modeling of Bosonic Modes in $Bi_2SrCa_2CuO_{8+\delta}$

Our third and final example of a forwards analysis is concerning high-energy features seen in STM data of BSCCO [12] which were shown to be a result of a bosonic mode’s coupling to the electrons in the (believed to be) relevant $CuO_2$ layer. In order to explain the observed high-energy features of BSCCO, Zhu and Balatsky [13] did a forwards
analysis by setting up a model of $d$-wave BCS quasiparticles coupled to various kinds of bosonic modes, both phononic and spin-waves, with several realistic functional forms for the electron-boson coupling. They numerically calculated the effect of such bosonic modes on the LDOS for the electrons and compared it to observed data. On the basis of the comparison of calculated LDOS of the model setup and observed data, they tried to answer which model bosonic mode is the best candidate for the observed one. We discuss this issue and review their work in more detail in Chapter 4. We also tackle an experimentally relevant inversion question - how to extract the bosonic mode’s frequency from the STM experiment? This question was incidentally not addressed in Zhu-Balatsky’s primarily numerical work [13].

In the above three examples, the reader can see that we have touched on various corners of high temperature superconductivity’s phenomenology, and that too mainly of BSCCO. Covering even a basic review of the whole of high temperature superconductivity’s phenomenology is a huge task. We are not going to attempt to do so. In the context of STM phenomenology of Cuprates and this thesis, the reader will find the review Ref. [14] quite pertinent.

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3A historical side-note: It might appear that the work to be covered in the following chapters were conceived as a reaction to each of the three examples of phenomenological modeling of experiments. Historically, this is only true of Chapter 4 on the bosonic modes in BSCCO to an extent. Chapter 2 was preceded by conversations on the vision of the Inversion program between Prof. Henley and Ron Maimon. From these conversations, Prof. Henley already had had a semi-classical notion of Quasiparticle Echoes described in Chapter 2. Thereafter, these were observed in numerical experiments on both normal metals and BCS superconductors. Chapter 3 on Lifetime extraction from STM data owes its origin to the pursuance of the Inversion program. The issue of Lifetimes in BSCCO were floating in the author’s consciousness and this definitely played a part when the Inversion question of Lifetime extraction revealed itself.
BIBLIOGRAPHY


CHAPTER 2
QUASIPARTICLE ECHOES

The text of this chapter is a reproduction of a paper written on the same subject in 2010. The reference to the paper is Phys. Rev. B 82, 035109.

2.1 Introduction

Scanning Tunneling Microscopy (STM), which measures the “local density of states” (LDOS) as a function of position and energy set by the bias voltage, has opened the door to imaging the sub-nanoscale topography and electronic structure of materials, including normal metals [1] and especially cuprate superconductors [2, 3, 4, 5, 6, 7, 8, 9].

The dispersion relations of (Landau or Bogoliubov) quasiparticles may be extracted from STM data on normal metals [10, 11] and superconductors [13], via the inverse method called Fourier transform scanning tunneling spectroscopy (FT-STS) [10, 13], or directly in real space [11]. This technique is based on the fact that impurities produce spatial modulations of the LDOS in their vicinity – standing waves in the electronic structure that generalize the Friedel oscillations found in metals at the Fermi energy. In the cuprates BSCCO and CaCuNaOCl [13], experiments showed these quasiparticle oscillations were dominated by eight wavevectors that connect the tips of “banana” shaped energy contours in reciprocal space, the so-called Octet model as explained theoretically [12]. For optimally doped samples, the dispersion inferred from these wavevectors agrees well with $d$-wave BCS theory indicating the existence of well-defined BCS quasiparticles in this regime.

The central observation of this chapter is that the same Friedel-like oscillations of the LDOS, analyzed in the space/momentum domain by FT-STS, are also manifested in the
energy/time domain. Our analysis shows that the small impurity-dependent modulations of the LDOS have a period, in energy, inversely proportional to the time required by a quasiparticle wavepacket to travel to the nearby impurities and back – hence we call it “quasiparticle echo”. From this, in principle, one can determine the location and (in a superconductor) the nature of the point scatterers in a particular sample.

The basic idea of the LDOS modulations may be understood semiclassically. The LDOS \( N(\vec{r}; \omega) \) is defined as \((-1/\pi)\text{Im}G(\vec{r}, \vec{r}; \omega)\), the time Fourier transform of the local (retarded) Green’s function \( G(\vec{r}, \vec{r}; t) \). Imagine a bare electron wavepacket (centered on energy \( \omega \)) is injected at time \( t = 0 \) at point \( \vec{r} \) in a two-dimensional material: the Green’s function expresses its subsequent evolution. Assuming there are well-defined quasiparticles at this energy with dispersion \( E(\vec{k}) \); then for every wavevector \( \vec{k} \) on the energy contour \( E(\vec{k}) = \omega \), the wavepacket has a component spreading outwards at the group velocity \( \vec{v}_g(\vec{k}) \equiv \nabla_{\vec{k}}E(\vec{k})/\hbar \). When this ring reaches an impurity at \( \vec{r}_{\text{imp}} \), it serves as a secondary source and the reflected wavepacket arrives at the “echo time”

\[
T_e \equiv 2\frac{|\vec{R}|}{|\vec{v}_g(\vec{k})|} \tag{2.1}
\]

for the \( \vec{k} \) such that \( \vec{v}_g(\vec{k}) \parallel \vec{R} \equiv \vec{r}_{\text{imp}} - \vec{r} \). This creates a sharp peak at \( t = T_e \) in \( G(\vec{r}, \vec{r}; t) \) [see Fig. 2.1 (d)], and hence modulations as a function of \( \omega \) in its Fourier transform \( N(\vec{r}; \omega) \) with period \( \Delta \omega = 2\pi\hbar/T_e \) [14]. Generically, for a particular impurity direction, \( |\vec{v}_g| \) varies with energy, so the the modulation in \( \delta N(\omega) \) due to the impurity is “chirped” correspondingly.
2.2 Normal Metal

We illustrate the quasiparticle echo first by a numerical calculation for a normal metal, defined by the lattice Schrödinger equation for the wavefunction $u_i$ on site $i$:

$$\sum_j (t_{ij} + \mu_i \delta_{ij}) u_i = Eu_i. \quad (2.2)$$

Here the $t_{ij}$'s are intersite hoppings and the $\mu_i$'s are on-site potentials (including the chemical potential); in this paper, we assume they are translationally invariant except at discrete (and dilute) impurity sites. We take the specific case of nearest-neighbor hopping $t$ at half-filling, so the the dispersion is $\epsilon(k_x, k_y) = -2t(cos k_x + cos k_y)$, and we place one (repulsive site potential) impurity at the origin. To numerically calculate the LDOS, we used the Recursion method [16] which is summarized in Appendix A.1. The Recursion method is well-suited for the calculation of LDOS for cases without translational symmetry.

Fig. 2.1(a) shows the impurity case LDOS which has echo oscillations on top of what otherwise would have been clean case LDOS, visible along the sides of the peak. Note that, for us to see more than one oscillation within the bandwidth, the impurity must be at least several sites away; hence the oscillations always have small amplitude and are best viewed by subtracting the clean LDOS. Throughout the paper, energy is in units of $t$ and time in units of $t^{-1}$ with $t = 1$ and $\hbar = 1$.

For a given energy $\omega$, we define $\Delta \omega(\omega)/2$ as the separation of the zeroes that bracket $\omega$ in the (subtracted) $\delta N(\omega)$ trace, and let $T_e(\omega) \equiv 2\pi \hbar/\Delta \omega(\omega)$. We chose $E = 0.7t$ and $\vec{R}$ in the [1,1] direction, for which the group velocity is $v_g = 2.785t/\hbar$. Then, using $\delta N(20, 20; \omega)$, $\delta N(30, 30; \omega)$, and $\delta N(40, 40; \omega)$ [the first and last trace of these are shown in Fig. 2.1(c,d)], we read off $\Delta \omega/2 = 0.1545$, 0.103, and 0.077, from which $v_g T_e/2 = 20.04 \sqrt{2}$, 30.05 $\sqrt{2}$, and 40.22 $\sqrt{2}$, respectively. The proportionality between
the oscillation rate and the actual distance confirms the semiclassical explanation of these modulations.

### 2.2.1 “Echolocation” of Impurity

Using these quasiparticle echoes, we can locate the position of impurities by measuring the LDOS wiggles at a few points in the vicinity. At each point, we extract the wiggle period $\Delta \omega$ and hence the echo time $T_e = 2\pi/\Delta \omega$. Then (2.1) defines a locus of possible impurity locations, $\{ \vec{v}_{\text{group}}(\vec{k}) T_e/2 : \epsilon(\vec{k}) = \omega \}$. The intersection of the loci from STM
spectra taken at multiple points \( \vec{r} \) will locate \( \vec{r}_{\text{imp}} \) uniquely. Furthermore, via a more exact derivation of the LDOS modulations (see below), the amplitude of the LDOS modulations tells the scattering strength of the impurities (in Born approximation they are proportional to each other). Once an impurity has been pin-pointed, the higher-energy STM spectrum at that point may independently identify the chemical nature of the impurity, e.g. in cuprates [15] and thus may reveal which kinds of impurities are important for the scattering of quasiparticles.

As a test, we evaluated the subtracted LDOS at three points \( \vec{r}_A = (-30, 0) \), \( \vec{r}_B = (-20, 20) \), and \( \vec{r}_C = (15, 30) \), with the impurity at \( \vec{r} = 0 \). From the half-periods of the wiggles at energy \( \epsilon = 0.7t \), (extracted as before) we found the respective echo times \( T_A = 39.9 \), \( T_B = 20.4 \) and \( T_C = 36.7 \). The three scaled loci(scaled by half the respective echotimes), shown in Fig. 2.2 e), intersect at \( (0,0) \) as can be seen graphically, thereby demonstrating the idea of echolocation. We call it “Echolocation” since we are inferring echo times and then translating them to distances in space, akin to Echolocation by radar or by bats/dolphins, which similarly depends on the echo times. A more careful numerical analysis can be done to extract errors in echolocation as well.

We emphasize again that this method locates impurities as seen by quasiparticle interference and, hence, is new information extracted from STM. Moreover, even though we may or may not have a detailed understanding of the STM spectra near the impurity, this method is not limited to it as it uses far-from-impurity measurements to locate the impurity. Hence, potentially, this method can overcome the limitations of and/or confirm the predictions for impurities’ recognition from their spectral signatures or comparisons with near-impurity data(e.g. see [21]’s Sec IX in context of Cuprates)
Figure 2.2: (a) Schematic of few measurements around an impurity. The arrowheads represent the STM Tip positions. After measurement, we get (b) \( \delta N(\vec{r}_A; \omega) \), (c) \( \delta N(\vec{r}_B; \omega) \) and (d) \( \delta N(\vec{r}_C; \omega) \). Extracting the echotimes for each measurement at \( \omega = 0.7t \), we locate the impurity, shown as a black dot, in the first panel. Note, that the locus of impurity locations changes with \( \omega \), and is of the shape shown only at \( \omega = 0.7t \).

### 2.2.2 Analytic derivation

Adopting the T-matrix formalism, we can obtain an analytic form for the LDOS modulations. Formally, the difference in dirty LDOS and clean LDOS for a single point impurity is given by

\[
\delta N(\vec{r}; \omega) = -\frac{1}{\pi} \text{Im} \left[ G_0(\vec{r} - \vec{r}_{\text{imp}}; \omega) T(\omega) G_0(\vec{r}_{\text{imp}} - \vec{r}; \omega) \right]
\]  

(2.3)

where \( G_0(\vec{r}, \vec{r}_{\text{imp}}; \omega) \equiv G_0(\vec{r} - \vec{r}_{\text{imp}}; \omega) \equiv G_0(\vec{R}; \omega) \) is the free propagator; LDOS modulations are due to interference between the two \( G_0 \) factors.

\[
G_0(\vec{R}; \omega) = \lim_{\delta \rightarrow 0^+} \int_{B.Z.} dk_x dk_y \frac{e^{i\vec{k} \cdot \vec{R}}}{(2\pi)^2} \frac{1}{\omega + i\delta - \epsilon(\vec{k})}
\]  

(2.4)
The integrand is singular all along the energy contour $\epsilon(\vec{k}) = \omega$, which we also parametrize as $\vec{k}_e(s)$, where $s$ is the arc-length in reciprocal space. By the change of variables $z \equiv e^{ik_y}$ we convert the inner $(k_y)$ integral to a complex contour integral in the $z$ plane (rewriting $\epsilon(k_x, k_y)$ as an analytic function of $z$); for $k_x$ values found on the energy contour, the $z$ path encounters two poles, one inside and one outside, depending on the sign of $\delta$. Extracting the residue and absorbing factors, we get

$$G_0(\vec{R}; \omega) = \frac{1}{2\pi i} \oint \eta(s) ds \frac{e^{i\vec{k}_e(s) \cdot \vec{R}}}{\hbar v_g(\vec{k}_e(s))} + G_{\text{non-singular}} \quad (2.5)$$

where $\eta(s) = 1$ on the half of the energy contour where $\text{sgn}(\delta) = \text{sgn}(|v_g(\omega, s)|)$ and zero on the other half (See Appendix A.2 for a detailed explanation). The non-singular term $G_{\text{non-singular}}$ comes from the integrals over $k_y$ which do not cross the energy contour.

At large $\vec{R}$, the two-dimensional BZ integration will be dominated by those $\vec{k}$ [18] on the energy contour where the phase in the numerator is stationary, i.e. $\vec{v}_g(\vec{k}) \parallel \vec{R}$: let us call such a point $\vec{k}_R$ (so it is a function of the direction $\vec{R}$ and of $\omega$). Using standard formulas of the stationary phase approximation [19] we get asymptotically

$$G_0(\vec{R}; \omega) = \frac{-i e^{i\pi/4}}{v_g} \sqrt{\frac{1}{2\pi k_0 |\vec{R}|}} e^{i\vec{k}_R(\vec{R}, \omega) \cdot \vec{R}}. \quad (2.6)$$

Here $\kappa^{-1}$ is the curvature $d^2\vec{k}_e/ds^2$ of the energy contour at $\vec{k}_R$.

Using (2.1) and (2.3), we finally get

$$\delta N(\omega) = \frac{T}{2\pi^2 v_g^2 k_0 R} \cos \left( 2\vec{k}_R(\vec{R}, \omega) \cdot \vec{R} \right). \quad (2.7)$$

valid in the limit of a distant impurity. (All factors are actually functions of $\vec{R}$ and $\omega$: these arguments are shown only in the rapidly varying factors.) As we change $\omega$ to $\omega + \delta \omega$ keeping $\vec{R}$ fixed, the chain rule gives $\vec{k}_R(\omega + \delta \omega) = \vec{k}_R(\omega, \omega) = v_g^{-1} \delta \omega \vec{R}$ so, with $\phi = \vec{k}_R \cdot \vec{R}$, we get

$$\cos \left( 2\vec{k}_R(\vec{R}, \omega + \delta \omega) \cdot \vec{R} \right) \rightarrow \cos(\phi + T \delta \omega). \quad (2.8)$$
This confirms the simple semiclassical prediction $\Delta \omega = 2\pi/T_e$ (see Eq. (2.1)) for the modulation period due to echoes. The same quasiparticle interference is responsible for the spatial oscillations evident in (2.7) and the energy oscillations in (2.8).

2.3 Echoes in Superconductors

Additional relevant issues arise in case of superconductors. To discuss these, we use a mean-field Bogoliubov-DeGennes (BDG) Hamiltonian with/without a single point impurity as shown below.

$$\sum_j \begin{bmatrix} t_{ij} + \mu_i \delta_{ij} & \Delta_{ij} \\ \Delta_{ij}^* & -t_{ij} - \mu_i \delta_{ij} \end{bmatrix} \begin{bmatrix} u_i \\ v_i \end{bmatrix} = E \begin{bmatrix} u_i \\ v_i \end{bmatrix}$$

(2.9)

where we are using a lattice formulation of BDG equations. The $u_i$s and $v_i$s represent particle and hole amplitudes on site $i$, $t_{ij}$s and $\mu_i$s represent the intersite hoppings and site chemical potentials respectively, and $\Delta_{ij}$ represent the off-diagonal order parameter amplitude. We discuss $d$-wave superconductors ($d$SC’s) to highlight this method’s application to cuprates. For dSCs, $\Delta_{ij}$ is nonzero only on nearest-neighbor bonds and $\Delta_{i,\hat{x}\hat{x}} = -\Delta_{i,\hat{y}\hat{y}}$ because of the $d$-wave nature. Our normal state is the same nearest neighbor tight binding model on the square lattice with $t = 1$ and off-diagonal hopping amplitudes set to $|\Delta| = 0.1$. The Recursion method was extended to superconductors in [17] and is used for our numerics. In Fig. 2.3 c) and d), we show the LDOS(after subtracting the clean LDOS shown in Fig. 2.3 a)) at $20 \sqrt{2}$ distance from an impurity along the $(1, 1)$ direction for the case of a potential scatterer and an anomalous pair potential scatterer (which scatters an electron into a hole and vice versa) respectively.

In contrast to the normal case, there are two different wiggles: a fast one and a slow one. The reason for this is that the dSC quasiparticle dispersion gives rise to two
Figure 2.3: Quasiparticle echoes in a $d$-wave SC. (a) no impurity $N_0(\omega)$ showing the $d$-wave gap, (b) A caricature of the two different group velocities along (1,1) direction for $d$-wave Bogoliubov dispersion, (c) $\delta N_{ORD}(20,20;\omega)$ for an ordinary impurity and (d) $\delta N_{ANO}(20,20;\omega)$ for an anomalous impurity.

different group velocities in the (1, 1) direction [20]. We also note that the fast wiggles exist only within the gap while the slow wiggles are both inside and outside the gap. In Fig. 2.3 b), we show the constant energy contours for the quasiparticle dispersion given by $E(\vec{k}) = \sqrt{\epsilon(\vec{k})^2 + \Delta(\vec{k})^2}$, the gradient of which is the quasiparticle group velocity. From Fig. 2.3 b), we see that along (1, 1), the banana-shaped energy contours in the first and third quadrants give one velocity (which corresponds to the slow wiggles), while the contours in the second and fourth quadrants give a slower velocity (which corresponds to the fast wiggles). For $E > |\Delta|$, there are no longer “banana” contours, so we get only one group velocity (similar to the normal case) and hence only one kind of wiggle is seen in Fig. 2.3(c,d) outside the cusps.
Once the impurity is located using the loci intersection method described before, one can study the LDOS data around the impurity to infer the impurity’s strength and whether it is ordinary (magnetic/nonmagnetic) (cf. Ref. [21] and references therein) or anomalous [22]. This distinction is already visible in individual spectra: provided the normal state is particle-hole symmetric, one gets particle-hole symmetric echo oscillations $\delta N_{\text{ANO}}$ from an anomalous impurity, since it scatters electrons into holes and vice versa [Fig. 2.3(d)]; this is not the case for $\delta N_{\text{ORD}}$ from an ordinary impurity [Fig. 2.3(c)].

A second diagnostic distinguishing (nonmagnetic) ordinary scatterers from anomalous ones is the real-space pattern of the surrounding standing waves in the LDOS, which is best seen in Born Approximation. In this limit, the impurity T-matrix is of the form (in the 2×2 Nambu notation) $U_{\text{imp}}\tau_3$ or $\Delta_{\text{imp}}\tau_1$ for the ordinary or anomalous cases, respectively. Then the echo oscillations take the respective forms

$$\delta N_{\text{ORD}} \propto U_{\text{imp}}(G_{11}^2 - G_{12}^2); \quad \delta N_{\text{ANO}} \propto \Delta_{\text{imp}}(2G_{11}G_{12}).$$

(2.10)

Here, the $G_{i,j}$s are the matrix elements of the usual free propagator $G_0(\vec{k}; \omega) = (\omega^2 - E(\vec{k})^2)^{-1}[\omega + \epsilon(\vec{k})\tau_3 + \Delta(\vec{k})\tau_1]$ thus in real space

$$G_0(\vec{R}; \omega) = \frac{\pi i}{(2\pi)^2} \oint \eta(s) \frac{ds}{2} g(\vec{k}(s, \omega)) + G_{\text{non-singular}}$$

(2.11)

where $g(\vec{p}; \vec{R}, \omega) \equiv 1 + \frac{1}{\omega}(\epsilon(\vec{p})\tau_3 + \Delta(\vec{p})\tau_1)$.

We can carry out the stationary phase approximation as before, but instead we numerically calculated the propagator using Eq. (2.11), since we are interested in LDOS information around(close) to the impurity. In Fig. 2.4, we show $\delta N$ around an impurity over a grid of 20x20 lattice points(shown one quadrant with others related by symmetry).

We see that certain of the real-space oscillations, present in case of the ordinary impurity, are suppressed in the case of a d-wave anomalous impurity. This is the same
effect as the suppression of certain “octet” vectors [13, 12] for the case of d-wave anomalous impurity as argued in [22]’s Eq. 10 and the following paragraph. Our real-space analysis qualitatively duplicates that of Ref.[22] illustrating how the real-space QPI and our energy-domain echoes are complementary manifestations of the same phenomenon.

2.4 Conclusion and Discussion

In conclusion, we have introduced a method of STM data analysis in the energy domain as a phenomenological tool for the study of real materials, complementary to FT-STS. Since it is based on the same quasiparticle interference effects already used successfully in FT-STS, we have confidence that the signals will be observable. They should be particularly strong in materials with an energy-dependent group velocity in some range of energies, such as d-wave superconductors and also graphene [23].

Since the echo analysis can be done in local patches of the sample (unlike FT-STS which fourier transforms over a larger region), we can locally verify the existence of quasiparticles at various energies through QPI. In particular, in cuprates, echoes might
be used to check the hypothesis of quasiparticle extinction [24] above a certain energy. Furthermore, we have argued that echo analysis might reveal the nature of specific impurities [25] in a sample, information which hitherto was (at best) known statistically.


[18] If the contour included a point with $v_g(\vec{k}_e(s)) = 0$, that point might also make a singular contribution.


[20] The (1,1) direction was chosen to bring out the difference in the two quasiparticle velocities most clearly. Along other directions, there are two velocities but they are very similar in magnitude and, hence, it is difficult to distinguish the two different wiggles. For this reason, possibly in a real experiment, one might have to look for echoes in certain directions.


[25] In this paper, we illustrated echolocation only for the case of isolated point-like impurities. Real STM data will typically contain a superposition of LDOS wiggles from several nearby impurities; it is necessary (and not too difficult) for the analysis method to separate these contributions.
CHAPTER 3
LIFETIME EXTRACTION

This chapter is adapted from a preprint version of the same work that has been uploaded at the online archive, www.arxiv.org. The URL for the preprint is “http://arxiv.org/abs/1104.1749”.

3.1 Introduction

Scanning Tunneling Microscopy (STM), apart from providing direct local real space information on electronic properties, has also been successfully used to extract momentum space properties of the sample through the application of Fourier Transform Scanning Tunneling Spectroscopy (FT-STS) [1] as we also mentioned in the introduction to the thesis. Through FT-STS, one is able to extract the dispersion of the underlying well-defined quasiparticles or carriers. FT-STS assumes the existence of well-defined quasiparticles in the system and it is the interference of these quasiparticles that is utilized in FT-STS.

In this chapter, we try to extend the domain of momentum space properties that can be extracted using STM. The central result is the demonstration of a data analysis scheme that would give us the lifetime information of the charge carriers in a sample as a function of momentum (and energy) from data collected in an STM experiment. Previously, ARPES is the tool that has been used successfully to get lifetime information on the carriers in a sample by measuring the one-particle electron spectral function directly in momentum space. Extracting lifetime from STM - a real space probe - thus would add value by providing an independent method that complements and checks the ARPES method.
Previous attempts at reconciling lifetime broadening effects on STM data mainly consist of writing down viable fitting forms for the lifetime function that explain STM data, rather than extracting it out of the data like one does in an ARPES experiment by quantifying the width of the peaks in ARPES spectra (See e.g. [2]. In the context of metals/Fermi liquids, Ref. [3] have fitted STM data on Silver and Copper with a model for thermal broadening of the electrons [4]. Refs. [5] and [6] are prominent examples in the phenomenology of high temperature superconductors.

3.2 Setup (Normal Metal)

We start by describing the basic setup of the scheme starting using the simpler case of normal metals. We imagine the system to be composed of Landau quasiparticles described by a propagator of the form

\[ \tilde{G}_0(k; \omega) = \frac{1}{\omega - i\eta(k; \omega) - \epsilon(k)} \] (3.1)

Self-energy processes - e.g. due to electron-electron interaction as in a Fermi Liquid or through scattering off a bosonic mode like a phonon - lead to a finite lifetime for the quasiparticle. Self-energy is generally referred to as \( \Sigma(k; \omega) \). The imaginary part of \( \Sigma(k; \omega) \) leads to a finite lifetime. We call it as \( \eta(k, \omega) \) in the denominator of Eq. (3.1), i.e.

\[ \eta(k, \omega) = Im[\Sigma(k; \omega)] \]. Also, the real part of the self-energy shifts the chemical potential and we assume that the dispersion term \( \epsilon(k) \) is this shifted dispersion [7]. Our aim is to extract \( \eta(k, \omega) \) from STM data. We might have the knowledge of the dispersion \( \epsilon(k) \) either via FT-STS on the same data or through an ARPES experiment.

Apart from the quasiparticles, there is one point impurity in the system which scatters the quasiparticles. Without loss of generality, we set the origin of the impurity to zero, \( r_{imp} = 0 \). In a real situation, we are imagining there to be a dilute amount of impu-
rities in the sample so that multiple impurity scattering is not important. In other words, we are using a point impurity as a probe to extract quasiparticle properties. For a single point impurity, we can solve the impurity problem via the T-matrix approach [8], and the propagator is

\[ G(r, r'; \omega) = G_0(r, r'; \omega) + G_0(r, r_{\text{imp}} = 0; \omega) \cdot T(\omega) \cdot G_0(r_{\text{imp}} = 0, r'; \omega) \]  (3.2)

where \( G_0(r, r'; \omega) = (2\pi/L)^2 \sum_k \tilde{G}_0(k; \omega) e^{ik(r-r')} \) \( \equiv G_0(r-r'; \omega) \) \(^1\) is the free propagator, and the impurity effect is captured by the “T-matrix” \( T(\omega) \), which is given by \( T(\omega) = U/(1 - UG_0(r_{\text{imp}}, r_{\text{imp}}; \omega)) \) where \( U \) is the impurity strength. It is in the second term of the above equation Eq. (3.4) that we have Quasiparticle Interference (QPI) which is utilized in FT-STS. Furthermore, since the STM measures the LDOS \( n(r; \omega) \) or the imaginary part of the real space propagator, i.e.

\[ n(r; \omega) = -\frac{1}{\pi} \text{Im}[G(r, r; \omega)], \]  (3.3)

therefore, the operating equation for the rest of the chapter is

\[ G(r, r; \omega) = G_0(r, r; \omega) + G_0(r, 0; \omega) \cdot T(\omega) \cdot G_0(0, r; \omega) \]

\[ = G_0(0; \omega) + G_0(R; \omega) \cdot T(\omega) \cdot G_0(R; \omega). \]  (3.4)

We will quickly review the key notions underlying FT-STS, since our method also utilizes QPI. STM measures LDOS as a spatial map over the surface for a range of energies. FT-STS’s main operating principle is that the peaks in the Fourier transform of local density of states (LDOS) map (say at energy \( \omega \)) are situated at particular wave-vectors. These wave-vectors connect points on the \( \epsilon(k) = \omega \)'s contour for which the product of the density of states (also called Joint density of states) is high. This can be understood by looking at the Fourier transform of the interference term in Eq. (3.4) (see

\(^1\)Lower case \( r \) refers to actual position co-ordinates, while in the future, upper case \( R \) will refer to difference of two lower case \( r \)'s and \( R \) will only appear in the argument of the free (assumed to be translationally invariant) Green’s function \( G_0 \).
Eq. (1) of [9] and the following paragraph). If the quasiparticles have finite lifetimes, the resultant effect in FT-STS will be a broadening of the FT-STS peaks. The broadening of the FT-STS peaks has been seen in experiments, e.g. Ref. [10]. Moreover, the “shapes” of these FT-STS peaks contain information about the momentum dependence of the lifetime \( \eta(k; \omega) \). It seems that extracting the \( k \)-dependence of \( \eta(k; \omega) \) from the FT-STS method is a hard task because, apart from other possible broadening factors like inhomogeneity (e.g. STM data in cuprates), one has the difficulty of deconvolving the output of FT-STS - the QPI term is a product in real space - without the prior knowledge of \( \eta(k; \omega) \). Instead we work in real space, our main tactic being to extract \( G_0(R; \omega) \) from QPI, and STM data is most suited for this.

We now list down the main steps of the analysis scheme and in what follows we give their essential technicalities along with pictorial demonstrations. In the appendices to this chapter, we include further technical details and proofs required in those steps.

1. From LDOS/\( n(r; \omega) \) map, we have to construct a \( G(r, r; \omega) \) map.

2. Once we have the \( G(r, r; \omega) \) data, we will have to “invert” Eq. (3.4) in order to extract \( G_0(R; \omega) \). To invert Eq. (3.4), we need

   (a) a way to find \( G_0(0; \omega) \)

   (b) a way to find the correct phases of \( G_0(R; \omega) \) as will be explained soon.

3. Once this is done, we Fourier transform to get \( \tilde{G}_0(k; \omega) \) and, thence, \( \eta(k; \omega) \).

In the following Sections 3.3-3.6, we show results of this method for various cases of (normal metallic) dispersion and lifetimes. We also recapitulate the steps achieved in each section as boxed text at the end of the sections, to serve both as a summary and a step-by-step guide to the scheme. Then, we discuss what kind of data sets are desirable and how the method extends to the superconducting case.
3.3 Step 1: “Kramers-Kronig”-ing the LDOS

Our starting point is the experimental data set which consist of LDOS maps $n(r, \omega)$ over a range of energies.

The first step of the analysis method is to convert the LDOS data to $G(r, r; \omega)$. This will be achieved through a Kramers-Kronig relation that the propagator satisfies,

$$\text{Re}[G(r, r; \omega)] = P \int n(r; x)/(\omega - x)$$

(3.5)

where the principal value integral is over the real line. Since the LDOS is nonzero only within a finite bandwidth [11], this integral is over a finite range of energies. In general, in a real experiment one might have information only over part of the bandwidth in which case, we can definitively apply this method only to an energy range that is well within the measured energy range, where even the incomplete spectrum can be fruitfully used as demonstrated in Fig. 3.1. This is very often the/one of the interesting energy ranges(e.g. around the Fermi energy for metals or the nodal energy for cuprates). We can also apply some form of extrapolation to construct LDOS data over the full bandwidth [12]. Kramers-Kronig has been applied successfully to other spectroscopies, e.g. Electron Microscopy (see [13]), thus giving us reason that they be applied to STM data as well.
Figure 3.1: In this figure, we demonstrate the effect of Kramers-Kroning to an example LDOS where we limit the integral by a finite cut-off, $\text{Re} \{ G(\omega) \} = P \int_{-\Lambda}^{\Lambda} \frac{n(r; x)}{(\omega - x)}$, Eq. 3.5. The example LDOS (see inset) is for a nearest-neighbour hopping model at half-filling, $\tilde{G}_0(k; \omega) = (\omega - i0.1t + 2t(Cos[k_x] + Cos[k_y]))^{-1}$ and $t = 1$. Around the Fermi energy ($\omega = 0$ in this case), we see that even for $|\Lambda| = 3$, $\text{Re} \{ G \}$ agrees well up to around $|\omega| = 1$. One can quantitatively show that this error is at most $\log \left| \frac{\Lambda + \omega}{\Lambda - \omega} \right| \approx 2|\omega/\Lambda|$ in units of $n$ and we do much better than that (see Appendix B.1).

**Step 1:**

*Input* - The LDOS map $n(r; \omega)$.

*Output* - Map of $G(r, r; \omega)$.

*Method* - At each spatial point $r$, Real part of $G(r, r; \omega)$ is calculated using

$\text{Re} \{ G(r, r; \omega) \} = P \int n(r; x)/(\omega - x)$, Eq. 3.5.

*Problem* - In the experiment, the range of energies over which the measurements are made might not be the full bandwidth.

*Solution* - The error in $\text{Re} \{ G(r, r; \omega) \}$ systematically goes down as the the fraction of spectral weight under the measured energy range increases, and as $\omega$ becomes well within the measured energy range. See Appendix B.1 for details. This allows us to get reasonable $\text{Re} \{ G(r, r; \omega) \}$ for an energy range well within the measured energy range (See Fig. 3.1).
We now discuss the second step: how to invert Eq. (3.4) at a fixed energy. From now on, the energy index $\omega$ is of passing concern and we will denote it as $\omega_{\text{fixed}}$.

### 3.4 Step 2: Finding $G_0(0; \omega_{\text{fixed}})$

At that fixed energy $\omega_{\text{fixed}}$, the first step is to find out the first term on the right hand side of Eq. (3.4), $G_0(0; \omega_{\text{fixed}})$. Since, we are assuming that the free propagator is that of a translationally invariant system, therefore $G_0(0; \omega_{\text{fixed}})$ is just a complex number, which is independent of $R$. This will be done a minimization procedure where a cost function would penalize incorrect guesses for $G_0(0; \omega_{\text{fixed}})$. Given a $G_0(0; \omega_{\text{fixed}})$ guess, we can solve for $T(\omega_{\text{fixed}})$ by solving Eq. (3.4). Furthermore, we can calculate the impurity strength $U$ from $T(\omega_{\text{fixed}})$. Once $T(\omega_{\text{fixed}})$ is known, we can solve for $G_0(R; \omega_{\text{fixed}})$.

\begin{equation}
G_0(R; \omega_{\text{fixed}}) = G_0(0; \omega_{\text{fixed}}) \sqrt{\frac{G(r, r, \omega_{\text{fixed}}) - G(0, 0, \omega_{\text{fixed}})}{G(0, 0, \omega_{\text{fixed}}) - G_0(0; \omega_{\text{fixed}})}}. \tag{3.6}
\end{equation}

Using Green’s function theory, one can show that the magnitude $|G_0(R; \omega_{\text{fixed}})|$ monotonically decays to zero for large $R$ (exponentially in $R$ in one dimensions and as square root of $R$ in two dimensions, see Appendix B.2) for dispersion that have convex energy contours. We demonstrate this effect in 1D and also show the effect of incorrect $G_0(0; \omega_{\text{fixed}})$ on extracted $|G_0(R; \omega_{\text{fixed}})|$ in Fig. 3.2. We see how an incorrect guess for $G_0(0; \omega_{\text{fixed}})$ spoils the monotonic decay of $|G_0(R; \omega_{\text{fixed}})|$.

\footnote{The argument $R$ is the surface distance of STM tip from the impurity site. In the following, $R = r$ because we have set $r_{\text{imp}} = 0$.}

\footnote{The reason for the deviation from the monotonic decay of $|G_0(R; \omega_{\text{fixed}})|$ due to an incorrect value of $G_0(0; \omega_{\text{fixed}})$ is as follows: Given our (incorrect) guess of $G_0(0; \omega_{\text{fixed}})$, we can decompose the extracted (incorrect) $G_0(R; \omega_{\text{fixed}})$ as $G_0(R; \omega_{\text{fixed}}) = G_0(0; \omega_{\text{fixed}})^{\text{correct}} + G_0^{\text{error}}$ where $G_0^{\text{error}}$ is a constant. Therefore,

\[ |G_0(R)| = |G_0(0; \omega_{\text{fixed}})^{\text{correct}}| + |G_0^{\text{error}}| + 2|G_0(0; \omega_{\text{fixed}})^{\text{correct}}||G_0^{\text{error}}| \times \cos(\text{Arg}[G_0(0; \omega_{\text{fixed}})^{\text{correct}}] - \text{Arg}[G_0^{\text{error}}]), \]
This motivates a minimization using a cost function that penalizes deviation from the smooth decay of extracted $|G_0(R;\omega_{\text{fixed}})|$ for finding the correct $|G_0(0;\omega_{\text{fixed}})|$. A good start guess for $G_0(0;\omega_{\text{fixed}})$ is to take a spatial average of $G(r,r;\omega_{\text{fixed}})$ over the whole data set around the impurity at $\omega_{\text{fixed}}$. One can show that the error in the guessed $G_0(0;\omega_{\text{fixed}})$ is $O[1/L^2]$ ($O[1/L^d]$ in $d$ dimensions, see Appendix B.4) suppressed compared to the correct $G_0(0;\omega_{\text{fixed}})$, and if the window were infinite, the spatial average of $G(r,r;\omega_{\text{fixed}})$ would exactly equal the correct $G_0(0;\omega_{\text{fixed}})$.

Now we discuss one particular implementation of the Cost function to measure the monotonic decay of extracted $|G_0(R;\omega_{\text{fixed}})|$. In one-dimension, the cost function for a one-dimensional list of values for $|G_0(R;\omega_{\text{fixed}})|$ (that is extracted given a guess $G_0(R =$ (we have suppressed the $\omega_{\text{fixed}}$ argument) and it is the final cosine term which spoils the monotonicity even for large $R$. Moreover, the $|G_0^{\text{error}}|$ term would also not let the Green’s function decay to zero as $R \to \infty$.

Figure 3.2: Above is shown $|G_0(R;\omega_{\text{fixed}})|$ on a 200-site window around an impurity extracted with various start guesses for $G_0(0;\omega_{\text{fixed}})$. For the figure above, we chose a one-dimensional nearest-neighbour hopping model at half-filling,  $	ilde{G}_0(k;\omega) = (\omega-i0.1r+2i(Cos[k,i]))^{-1}$ (with $t=1$) and $\omega_{\text{fixed}} = 0.5$. 
\( 0; \omega_{\text{fixed}} \)) is constructed as

\[
\text{Cost}(\{z_r\}) = \sum_r \frac{|z_{r+1} + z_{r-1} - 2z_r|^2}{||(z_{r+1} + z_{r-1})/2||^2}
\]  

(3.7)

where the list is \( \{z_r\} \) and sum runs over all 3-tuples. Looking at Fig. 3.2, we heuristically see how the above cost function is constructed. For every 3-tuple of points, the function is minimized when the numerator \(|z_{r+1} + z_{r-1} - 2z_r|\) is zero. This corresponds to the 3-tuple lying in a straight line. Thus, if there is non-monotonicity, there will be 3-tuples in the list which deviate from being “straight” as in the Fig. 3.2. This non-monotonic behaviour will then be penalized by the cost function. The denominator \(|(z_{r+1} + z_{r-1})/2|\) is used to suitably normalize the cost function so as to make it independent of the scale of \( \{z_r\} \).

We generalize this to two dimension by evaluating the one-dimensional cost using the same formula for all one-dimensional slices of a two-dimensional data set either along \( x \) or \( y \) direction. We do it in this way because the two-dimensional data set is symmetric with respect to interchanging \( x \) and \( y \) when there is no error. In the error-full case, we can pre-process the data set to impose the symmetries of the square lattice. Thus the Cost function is

\[
\text{Cost}(\{z_{x,y}\}) = \sum_{y} \sum_{x} \frac{|z_{x+1,y} + z_{x-1,y} - 2z_{x,y}|^2}{||(z_{x+1,y} + z_{x-1,y})/2||^2}
\]  

(3.8)

We show an example implementation of this cost function for test case data in Appendix B.3.
Step 2:

Input - A two-dimensional Map of $G(r, r; \omega_{fixed})$

Output - A complex number $G_0(0; \omega_{fixed})$

Method - This is done through a minimization procedure using a cost function whose input is a guess "$G_0(0; \omega_{fixed})$". The minimization procedure is based on the monotonic decay of $|G_0(R; \omega_{fixed})|$ to zero for large $R$ (See Appendix B.2). For each value of $\omega_{fixed}$, the magnitude of $G_0(R; \omega_{fixed})$ is calculated by finding the absolute value of $\sqrt{(G(r, r; \omega_{fixed} - G_0(0; \omega_{fixed}))/G(0, 0; \omega_{fixed} - G_0(0; \omega_{fixed}))}$ (See Eq. 3.6).

Implementation - One way to construct the Cost function is using

$\text{Cost}([z_{x,y}]) = \sum_x \sum_y \frac{|z_{x+1,y} + z_{x-1,y} - 2z_{x,y}|^2}{|z_{x+1,y} + z_{x-1,y}|/2|^2}$ (See Eq. (3.7)) where $\{z_{x,y}\}$ is the two-dimensional data set corresponding to $|G_0(R = (x, y); \omega_{fixed})|$ calculated using the guess "$G_0(0; \omega_{fixed})$" (See also Appendix B.3).

A good start guess for $G_0(0; \omega_{fixed})$ is the spatial average of $G(r, r; \omega_{fixed})$ over the whole data set around the impurity (See Appendix B.4).

3.5 Step 3 : Finding phases of $G_0(R; \omega_{fixed})$

With the correct $G_0(0; \omega_{fixed})$, we use Eq. (3.6) to get $G_0(R; \omega_{fixed})$. Because of the square root, we have an ambiguity of a $\pi$ phase for the phase of $G_0(R; \omega_{fixed})$. Capturing this phase is crucial to get the correct $\tilde{G}_0(k; \omega_{fixed})$ upon Fourier transforming. To get the correct phase, we start with the observation that the phases have to be smooth and well-behaved as a function of $R$ because $G_0(R; \omega_{fixed})$ is differentiable with respect to $R$ [14]. We use this property to fix the phase of the square of $G_0(R; \omega_{fixed})$, i.e. we select
that branch of the argument function when evaluating the phase of \( G_0(R; \omega_{\text{fixed}})^2 \) which maintain the aforesaid smoothness. We start by making a spatial list of the phases as given by the \( \text{Arg}(z) \) function which restricts the phase obtained to one branch of the Argument function. Then, we start at \( R = 0 \). As we move away from the origin, we multiply phase factors of \( e^{i 2m\pi} \) to \( G_0(R; \omega_{\text{fixed}})^2 |e^{i \phi_{\text{principal}}} \) for all \( R \), the \( m \)'s being so chosen that if \( |R'| > |R| \) then \( \phi_{\text{principal}}' + 2\pi m' > \phi_{\text{principal}} + 2\pi m \). We implemented the choosing of \( m \)'s as shown in the following flowchart:

1. Define a monotoniser function that takes two arguments that lie between \((-\pi, \pi]\) and keeps adding \( 2\pi \) to the second argument till it becomes greater than the first argument. \( \text{mono}(x, y) : \text{Do } y = y + 2\pi \text{ Till } y > x \).

The following steps are done in each of the symmetry-related octants in space and we write down the steps for the octant \( y > 0 \) and \( x > y \).

2. Start at origin \((0, 0)\). Move a step along x-axis to \((x, y) = (1, 0)\). Then, \( \text{mono}(\phi_{\text{principal}}(\vec{R} = (x - 1, y)), \phi_{\text{principal}}(\vec{R} = (x, y))) \).

3. Then do \( \text{mono}(\phi_{\text{principal}}(\vec{R} = (x, y)), \phi_{\text{principal}}(\vec{R} = (x, y + 1))) \) along y-direction till \( y = x \).

4. Move a step along x-axis. Do \( \text{mono}(\phi_{\text{principal}}(\vec{R} = (x - 1, y)), \phi_{\text{principal}}(\vec{R} = (x, 0))) \) where the y of the first argument is highest integer such that \( x > \sqrt{(x - 1)^2 + y^2} \).

5. Repeat step 3) and 4) till the whole octant is covered.

Similar phase fixing is done for all the octants. Once this is done, the phase of \( G_0(R; \omega_{\text{fixed}}) \) is just half that of the phase-fixed \( G_0(R; \omega_{\text{fixed}})^2 \). Since, the phase of \( G_0(R; \omega_{\text{fixed}})^2 \) has been made well-behaved, the phase of \( G_0(R; \omega_{\text{fixed}}) \) will also be well-behaved which is what was desired. In Fig. 3.3, we show the result of doing the phase-fixing to numerically calculated \( G_0(R; \omega_{\text{fixed}})^2 \) and also directly to \( G_0(R; \omega_{\text{fixed}}) \) and find
that they are in the correct ratio of two.

Step 3:

Input - A two-dimensional map of $G_0(R; \omega_{\text{fixed}})$ with incorrect phases

Output - A two-dimensional map of $G_0(R; \omega_{\text{fixed}})$ with phases fixed

From Step 2, we have the “raw” (phases incorrect) $G_0(R; \omega_{\text{fixed}})$ using

$$G_0(0; \omega_{\text{fixed}}) \sqrt{G(r, r; \omega_{\text{fixed}} - G_0(0; \omega_{\text{fixed}})/G(0,0; \omega_{\text{fixed}} - G_0(0; \omega_{\text{fixed}}))}$$

(See Eq. 3.6) calculated using the correct $G_0(0; \omega_{\text{fixed}})$.

Problem - Upon taking the square root, there is an ambiguity of a $\pi$ phase.

Solution - We take advantage of the smoothness of $G_0(R; \omega_{\text{fixed}})$ as a function of $R$ (See also Appendix B.5).

Method - The phases are fixed as follows: As we move away from the origin/impurity, we multiply phase factors of $e^{i2m\pi}$ to the square of $G_0(R; \omega_{\text{fixed}})$, i.e.

$$G_0(R; \omega_{\text{fixed}})^2 = |G_0(R; \omega_{\text{fixed}})^2|e^{i\phi_{\text{principal}}'}$$

for all $R$, where $\phi_{\text{principal}}'$ is the phase as calculated using the Arg($z$) function which restricts the phase obtained to one branch of the Argument function. The $m$’s are so chosen as to ensure that if $|R'| > |R|$, then $\phi_{\text{principal}}' + 2\pi m' > \phi_{\text{principal}} + 2\pi m$.

The phase of $G_0(R; \omega_{\text{fixed}})$ is then half that of the phase-fixed $G_0(R; \omega_{\text{fixed}})^2$

(See the Flowchart in the text of this section above).
Figure 3.3: In the panels above we show the phases of $G_0(R; \omega_{\text{fixed}})$ (a) and b)) and $G_0(R; \omega_{\text{fixed}})^2$ (c) and d)) in the first quadrant of size 30x30 lattice sites around an impurity at a $\omega_{\text{fixed}}(= -t)$. a) and c) show the phases as evaluated by the Arg(z) function restricted to one branch. b) and d) show the smooth phases as reconstructed using the reconstruction algorithm. The ratio of phases in b) and d) is identically two over the whole quadrant, even though the ratio of phases in a) and c) does not behave in such a regular manner. $\epsilon(k) = -2t(Cos[k_x] + Cos[k_y])$ and $\eta(k, \omega_{\text{fixed}} = -t) = 0.1t$ in this example.
3.6 Step 4 : $G_0(R; \omega_{\text{fixed}})$ to $\eta(k; \omega_{\text{fixed}})$

With the correct phases, we are now ready to Fourier transform the extracted $G_0(R; \omega_{\text{fixed}})$ to get $\tilde{G}_0(k; \omega_{\text{fixed}})$ and $\eta(k; \omega_{\text{fixed}})$ with our knowledge of $\epsilon(k)$. By doing the above scheme for a range of energies, we can extract $\eta(k; \omega)$ over the aforesaid range of energy. Moreover, the extracted $\tilde{G}_0(k; \omega)$ also has to satisfy the condition that $\omega - \text{Re}[\tilde{G}_0(k; \omega)^{-1}]$ depends exclusively on momentum if $\text{Re}[\Sigma(k; \omega)]$ has a weak dependence on $\omega$. In Fig. 3.4, we show how this method performs with and without error and we see that it performs well for error magnitudes less than 0.25\%. Perhaps one can still improve on the robustness of the scheme to error. For the panels Fig. 3.4 a-d, the form of $\eta$ had no momentum dependence, and this kind of fitting form has been proposed in [6] for Cuprates and has been theoretically discussed in [15]. In general, we expect the lifetime function to have few (low) harmonics of $k$ similar to the dispersion. Thus, our analysis scheme would serve the purpose of finding the most general $\eta(k; \omega)$ that is consistent with STM data. We can extract an approximate analytic form for $\eta$ by doing a least-squares fit of the extracted $\eta$ to a function of $k$ containing a few harmonics in the Brillouin zone. The approximate analytic form can then be compared to theoretical proposals.
Step 4:

Input - Phase-fixed two-dimensional map of $G_0(R; \omega_{\text{fixed}})$

Output - $\eta(k, \omega_{\text{fixed}})$

Method - We Fourier transform $G_0(R; \omega_{\text{fixed}})$ to get $\tilde{G}_0(k; \omega_{\text{fixed}})$. From $\tilde{G}_0(k; \omega_{\text{fixed}}) = (\omega_{\text{fixed}} - i \eta(k, \omega_{\text{fixed}}) - \epsilon(k))^{-1}$ (See Eq. (3.1)), the lifetime is then extracted as $\eta(k, \omega_{\text{fixed}}) = -\text{Im}[\tilde{G}_0(k; \omega_{\text{fixed}})^{-1}]$.

Doing the Steps 1-4 for various values of $\omega_{\text{fixed}}$ in a range of energies gives the dependence of $\eta(k, \omega)$ on $\omega$ in that energy range.

Additionally, $\omega_{\text{fixed}} - \epsilon(k) = \text{Re}[\tilde{G}_0(k; \omega_{\text{fixed}})^{-1}]$. If we have the knowledge of $\epsilon(k)$ from a different experiment, the previous relation can serve as another check on the efficacy of the recipe.

3.7 Some Remarks on Desired Data Sets

At this point, it seems valuable to comment on what kind of data sets would be ideal for such an analysis. In Fig. 3.5, we show an example of data set seen in a real experiment. We show how it is similar to a theoretical data set(calculated numerically) which has a lifetime broadening. Thus, we would expect that if we observe a few of the “Friedel oscillation”-like rings around the point impurity, this analysis scheme should work. Moreover, if FT-STS applied to a single point impurity data shows reliable QPI peaks, then we believe that the data set would have good enough spatial resolution to resolve the momentum dependence of lifetime $\eta$ to the same momentum resolution as that of the FT-STS results. We can improve on this by taking an average over data sets around multiple point impurities to improve signal to noise.
Figure 3.4: In these figures we are plotting $|\omega_{\text{fixed}} + i\eta(k, \omega_{\text{fixed}}) - \epsilon(k)|^{-1}$ as a function of $\vec{k}$ over a Brillouin Zone $(0, 2\pi) \times (0, 2\pi)$ at $\omega_{\text{fixed}} = -t$ for the above plots). In a) we show the input form resulting out of our choice of input for $\eta$, where $\epsilon(k) = -2t(Cos[k_x] + Cos[k_y])$ (nearest-neighbour hopping) and $\eta(k, \omega_{\text{fixed}} = -t) = 0.1t$; in b) we show the form extracted using the proposed analysis scheme when no noise was added to the STM data calculated numerically. One sees the limitation in momentum resolution in the form of “blockiness” introduced by having a finite window. This “blocky” momentum resolution gets better or worse with greater or smaller window sizes. In c) and d) we show the results of the analysis scheme to data with 1% and 0.05% Gaussian errors added respectively. We have done similar analyses for different energy values and different forms of $\eta$ and in e), f) and g), we show the corresponding results for $\epsilon(k) = -2t(Cos[k_x] + Cos[k_y]) - 4(0.2t)(Cos[k_x] * Cos[k_y])$ (nearest and second-nearest neighbour hopping) and $\eta(k, \omega_{\text{fixed}} = -t) = 0.25t + 0.1t$ (nearest-neighbour hopping).
3.8 Extension to the Superconducting Case

Now, we will sketch how this method of analysis can be extended to superconducting case using d-wave superconductors (pertinent to cuprates’ STM phenomenology) as our example. In Nambu’s two component notation, the free superconducting propagator looks like

\[
\tilde{G}_0(k;\omega)^{-1} = \begin{pmatrix}
\omega - i\eta_e(k, \omega) - \epsilon(k) & \Delta(k) \\
\Delta(k)^* & \omega - i\eta_h(k, \omega) + \epsilon(k)
\end{pmatrix}
\] (3.9)

where \(\epsilon(k)\) is the bare dispersion and \(\Delta(k)\) is the (d-wave) gap of the cuprate in question. These are assumed to be known (through other experiments). As before, we want to determine the electron/hole lifetime. The first simplification is the relation

\[
\eta_h(k, \omega) = -\eta_e(k, -\omega).
\] (3.10)

The proof of this relation is outlined in Appendix B.6 and, it follows by showing 
\(\Sigma_{22}(-\omega - i\delta) = -\Sigma_{11}(\omega + i\delta)\).
This relation implies \( G_0(R, \omega)_{22} = -G_0(R, -\omega)_{11} \) and \( G_0(R, \omega)_{12} = G_0(R, -\omega)_{12} \). Now, as before, we imagine there is a point impurity which result in a two-component T-matrix. One can show that this T-matrix has no off-diagonal entries (for an ordinary potential impurity) since \( G_0(R = 0, \omega)_{12} = 0 \) owing to the d-wave symmetry of the gap function. One can further show that \( T_{22}(-\omega) = -T_{11}(\omega) \) and, resultantly, \( G(r, r; \omega)_{22} = -G(r, r; -\omega)_{11} \). For \( r = r_{\text{imp}} \), we have \( G_{11} = G_{0,11} + T_{11}G_{0,11}^2 \) and \( G_{22} = G_{0,22} + T_{22}G_{0,22}^2 \). Using \( G(r, r; \omega)_{22} = -G(r, r; -\omega)_{11} \), we can thus determine \( T_{11} \) and \( T_{22} \) given a guess for \( G_0(R = 0, \omega)_{11} \) (which will again be determined by demanding the monotonicity of \( G_0(R, \omega)_{11} \)). For \( r \neq r_{\text{imp}} \), we have

\[
G_{11}(r, r; \omega) = G_0(0, \omega)_{11} + T_{11}(\omega)G_0(r - r_{\text{imp}}, \omega)_{11}^2 + T_{22}(\omega)G_0(r - r_{\text{imp}}, \omega)_{12}G_0(r - r_{\text{imp}}, \omega)_{21} \tag{3.11}
\]

\[
G_{22}(r, r; \omega) = G_0(0, \omega)_{22} + T_{22}(\omega)G_0(r - r_{\text{imp}}, \omega)_{22}^2 + T_{11}(\omega)G_0(r - r_{\text{imp}}, \omega)_{12}G_0(r - r_{\text{imp}}, \omega)_{21}. \tag{3.12}
\]

Again using \( G(r, \omega)_{22} = -G(r, -\omega)_{11} \), now with the knowledge of \( T_{11} \) and \( T_{22} \), we can solve the above equations for \( G_0(R, \omega) \) upto a phase of \( \pi \) (which we reconstruct as before) at each \( \omega \) for all \( r \) in the dataset, following which we Fourier transform to extract \( \tilde{G}_0(k, \omega) \) and \( \eta_e(k, \omega) \).

### 3.9 Conclusion

In conclusion, we demonstrated an analysis scheme which holds promise to extract lifetimes from STM data in various systems ranging from metals and semiconductors to strongly correlated compounds to superconductors. Some final remarks are in order. We demonstrated the proposed analysis scheme in case of a point impurity, but it can be extended to the case of an extended impurity too. The resulting complica-
tion will be that now we would have to guess more than just $G_0(R = 0; \omega)$ (e.g. if the impurity extends over two adjoining sites $r_1$ and $r_2$, then $G(r, r; \omega)$ will be a function of $G_0(0; \omega) = G_0(r_1, r_1; \omega) = G_0(r_2, r_2; \omega)$ and $G_0(1; \omega) = G_0(r_1, r_2; \omega)$). This scheme is inherently local, where we would be analyzing data around a single impurity. Thus, it would really utilize the local information that STM affords us with. There have been other examples of data analysis done on STM data previously to extract local information([17],[18]). In this sense, we would do better than ARPES where the signal is averaged over an area of the sample equal to the beam size, if and only if the STM experiment has good signal to noise. Similarly, we can overcome inhomogeneity issues for dirty systems, in which case we would concentrate this analysis on a homogeneous patch similar in spirit to Hudson’s analysis [18] and to a previous work, Echolocation [19] also described in Chapter 2.
BIBLIOGRAPHY


[7] It is this “renormalized” dispersion that is measured in FT-STS and ARPES.


[11] Practically, even though the LDOS might not be exactly zero outside the bandwidth, we saw that if the spectral weight of the spectrum within the bandwidth is approximately greater than 0.95, which can be expected to be true for well-defined quasiparticles, the Kramers-Kroning essentially works. Moreover, as we show in Fig. 3.1, this issue matters even less for an energy range much smaller than the bandwidth. We are assuming in the above that we have a one-band dispersion.
The knowledge of the dispersion can serve as a guide in this regard. Furthermore, we can have an iterative set-up where the result of the analysis scheme using the extrapolated full-bandwidth LDOS data can be used to make a new and better extrapolation to ensure convergence.

Optical excitations in electron microscopy, F. J. Garca de Abajo, Rev. Mod. Phys., 82, 209 (2010).

This can most simply be seen by looking at the equation of motion for a non-interacting Green’s function on the continuum (Fourier transformed with respect to time): \((\zeta + \nabla^2/2m)G_0(R; \zeta) = \delta(R)\). Thus, \(G_0(R; \zeta)\) is differentiable for \(R \neq 0\). At \(R = 0\), \(G_0(R; \omega)\) can be non-differentiable, and this manifests as a kink in the phase of Green’s function at \(R = 0\) for both continuum and lattice. (See Appendix B.5 for a discussion on how this argument applies to the interacting case).


In this chapter, we turn our attention towards a different corner of STM phenomenology. The research work to be covered in this chapter owes its origin to the experimental work concerning the issue of “high-energy” features found in the LDOS data of $\text{Bi}_2\text{Sr}_2\text{Ca}_1\text{Cu}_2\text{O}_{8+x}$ (BSCCO), a high-temperature Superconductor [1]. As Jinho Lee et al found in their pioneering experiment, these features are located at an energy scale greater than the so called coherence peak’s energy scale (see Fig 1 of Ref. [1]). They showed that the high-energy feature was due to a coupling of the d-wave quasiparticles to a bosonic mode. The bosonic mode was also shown to be a phononic mode of the Oxygen atoms (it is still unclear whether the apical or in-plane oxygen are involved in the bosonic mode) using the isotope effect which showed the expected shift in the bosonic mode frequency when the oxygen in the samples were substituted isotopically. The bosonic mode frequency was itself extracted by showing the constancy of the energy difference between the high-energy feature due to the bosonic mode and the coherence peak, even though both the high-energy feature and coherence peak spatially vary significantly over the sample. From an inversion perspective, the question that we ask in this chapter is a) how should one extract the bosonic mode’s frequency, and b) how can one try to extract the electron-boson coupling strength.
4.1.1 History of Bosonic Modes in Conventional Superconductors

Historically, the issue of high-energy features in tunneling data of superconductors due to a bosonic mode played an important role in the quantitative confirmation of the phononic mechanism of Cooper pairing in conventional (s-wave) superconductors like Lead, Mercury, etc. including the correct prediction of Transition temperatures ($T_c$). Tunneling data from Superconductor-Insulator-Metal junctions apart from showing a clear BCS gap to excitations in the superconductor also showed features at energies higher than the gap. These features were located precisely at an energy separated from the gap energy scale by the pairing phonon’s frequency.

Understanding these high-energy features though required a formulation that went beyond the basic BCS theory. Basic BCS theory is a weak-coupling theory in the sense that even an infinitesimal electron-electron attraction (caused by a weak electron-phonon coupling) can produce Cooper pairing. The electron-phonon coupling in materials (Lead, Mercury) with most prominent (non-BCS) deviations at high energy was estimated to be large compared to materials (like Aluminum) where BCS theory was in good agreement. It required the formulation of strong-coupling Superconductivity, achieved by Eliashberg [2], to understand the gap and the high-energy features coming from the strong electron-phonon coupling. The formalism is powerful enough to handle situations like: 1) the pairing phonon is dispersing, 2) the density of states of electrons is not a simple function of energy, 3) the electron-phonon coupling has a complicated momentum dependence, etc. McMillan-Rowell [3] used the Eliashberg formalism to invert the tunneling data to extract the the pairing phonon’s $\alpha^2 F(\Omega)$, which is the product of $F(\Omega)$ that is the density of states of lattice vibrations and $\alpha^2(\Omega)$ that describes the (momentum-averaged) interactions between the electrons and the lattice.

Quantitative confirmation of the phononic mechanism came from an excellent agree-
ment of the phonon’s $\alpha^2 F(\Omega)$, as extracted using McMillan-Rowell procedure from tunneling data coming from different junctions, e.g. for Lead, extraction was done using Lead-Insulator-Lead, Aluminum(superconducting)-Insulator-Lead and Metal-Insulator-Lead junctions. Also, the energies of the transverse and longitudinal modes as seen in the peaks in $\alpha^2 F(\Omega)$ were found to be in agreement with the energies that were expected from the dispersion curves for phonons as measured by inelastic neutron scattering. See the Refs. [3, 4, 5] to learn the details of this important piece of work in the history of superconductivity.

### 4.1.2 Further details of the BSCCO experiment

In the case of BSCCO, the method used to extract the bosonic mode’s frequency in the Lee et al experiment was to find the difference between the energy value of the inflection point before the hump of the boson dip-hump feature and the energy of the coherence peak. This scheme’s choice was attributed to a similar scheme to detect molecular vibrational mode frequencies using electron tunneling [6, 7]. This scheme or method is known as Inelastic Electron Tunneling Spectroscopy (IETS). We quote below a paragraph from Ref. [7] which explains the physics behind this method:

“In 1966 it was discovered that vibrational spectra can be obtained from molecules adsorbed at the buried metal-oxide interface of a metal-oxide-metal tunneling junction. In that experiment, the tunneling current $I$ was measured as a function of voltage $V$ across the junction. Small, sharp increases in the ac tunneling conductance, $dI/dV$, were observed when the energy of the tunneling electrons reached the energy of a vibrational mode for molecules in the junction. This increase is the result of electrons losing their energies to the vibrational mode, giving rise to an inelastic tunneling chan-
nel, which is forbidden when tunneling electrons have energies below the quantized vibrational energy. In the experiment, a peak at each vibrational energy was observed in $d^2I/dV^2$. This method, known as inelastic electron tunneling spectroscopy (IETS), has been applied to a wide range of systems and has led to a better understanding of molecules in the adsorbed state.”

The application of this method to the extraction of the boson frequency seems *ad hoc* and slightly confusing in the first glance, since the high-energy features were also said to be “possible strong-coupling superconductivity signatures of Electron- Boson Interaction” in Lee it et al’s paper, Ref. [1]. Applying IETS methodology to a possible Eliashberg-like feature seems to need reconciliation. This issue is one of the motivations behind the work in this chapter.

### 4.2 A Weak-Coupling Model: Set-Up and Assumptions

We will now describe our attempt to investigate the issue of how to extract the bosonic mode’s frequency in such an STM experiment.

1. Our central assumption is that the bosonic mode has no role in the establishment of the d-wave superconductivity, it being established through some mechanism that is unknown. The mechanism of superconductivity in high temperature SCs is still famously an open question. Lee *et al* [1] are conservative about the role of the observed phononic mode’s contribution to the establishment of superconductivity. We quote from the concluding paragraph of their paper:

   “Taken together, these data present some intriguing new possibilities. The first is that superconducting energy gap disorder $\Delta(r)$ is a consequence of heterogene-
ity in the pairing potential caused by disorder in the frequencies and coupling constants of pairing-related vibrational modes. But the strong dependence of superconducting electronic structure on hole density while the [Boson’s frequency] $\Omega(r)$ distributions remain unchanged (Fig. 4) appears to argue against this point of view.”

As we said before, we assume that the boson has no role in superconductivity and that the sample has d-wave quasiparticles independently of the boson. This assumption motivates a weak-coupling viewpoint.

2. The next step is to posit the presence of a bosonic mode. Our philosophy is to consider the simplest case for the bosonic mode. This has the advantage - as we attempt to show in the rest of the chapter - of making the underlying mathematics and the predictions thereof quite transparent. Thus, we choose

(a) An Einstein oscillator for the bosonic mode,

(b) A momentum independent electron-boson coupling.

This simplification of momentum independence of the bosonic mode is legitimate since the central issue we are addressing is the extraction of bosonic mode’s frequency which is an energy related question $^1$.

**Digression : Relation to Strong Coupling Eliashberg Theory**

The strong-coupling formalism [2, 3] had been necessary to explain the high-energy features in s-wave SCs because the same pairing phonon led to the gap and the high-energy feature, hence necessitating a self-consistent scheme that gave the non-zero gap as well

$^1$To investigate momentum dependent properties of the bosonic mode, one would need to do something like FT-STS with the boson feature. This has been attempted by Lee et al. We do not address the issue of momentum dependence in this work.
as the high energy feature. In our setup, we ask how the boson - through the electron-boson coupling - affects the d-wave quasiparticle propagator. If the electron-boson coupling is small, then we can do perturbation theory. We require no self-consistency unlike Eliashberg theory, since we have assumed an already established gap (through some mechanism that does not involve the boson). This is the main reason why we can do a weak-coupling calculation.

As will be shown in the next section, we proceed by calculating the self-energy due to the boson at lowest order and by working out its properties, we tackle the inversion questions of 1) extracting the boson’s frequency as reflected in the LDOS spectrum, and 2) extracting an estimate for the electron-boson coupling strength.

**Digression : Elastic vs. Inelastic Processes**

In this work, we only consider the elastic (virtual) process whereby a phonon is emitted and re-absorbed by the BCS quasiparticle. It is diagrammatically represented by the following Feynman diagram Fig. 4.2 a). We are not taking into account the following inelastic (real) process Fig. 4.2 b). This process corresponds to inelastic emission or absorption of phonons (that might be extraneous to the CuO$_2$ layer). These two processes can, in principle, have different signatures in the STM spectra. This issue is not being resolved in this work.

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2We also mention that few of the reasons that made Eliashberg formalism tractable (e.g. 1) s-wave nature of gap, 2) Migdal’s theorem which allowed a small parameter $m/M$ due to a separation of energy scales of the underlying normal metal’s (free) electron mass ($m$) and the lattice ions mass ($M$)) can’t be ported directly to the case of Cuprates which are high temperature superconductors. One would have to devise analogous simplifications for the d-wave case of cuprates, where the nature of the underlying normal state is not yet clear.
4.3 Self-Energy due to the Boson

In this section, we discuss the self energy corrections to the $d$-wave BCS quasiparticle by an Einstein oscillator at lowest order in the electron-boson coupling. Firstly, we set up the formalism and work out the full analytical expression for the self energy $\Sigma$. Secondly, we work out the analytic form of the boson feature presaged by it.

4.3.1 Formalism

In the following, we might use “momentum” interchangeably with “wavevector” and “energy” interchangeably with “frequency”, i.e. $\hbar = 1$.

We start with $d$-wave BCS quasiparticles. They can be modeled by a Hamiltonian of the form

$$H = \sum_{k,\sigma} \epsilon(k)c_{k,\sigma}^{\dagger}c_{k,\sigma} + \Delta(k)c_{k,\sigma}c_{-k,-\sigma} + h.c.$$  \hspace{1cm} (4.1)
In the $2 \times 2$ Nambu formalism, the corresponding $d$-wave BCS propagator is

$$G_0(k; i\omega_n)^{-1} = \begin{pmatrix} i\omega_n - \epsilon(k) & \Delta(k) \\ \Delta(k)^* & i\omega_n + \epsilon(k) \end{pmatrix}. \quad (4.2)$$

where $\omega_n$ is a fermionic Matsubara frequency. $\epsilon(k)$ is the dispersion and $\Delta(k)$ is $d$-wave gap and is assumed to be of the form

$$\Delta(k) = \frac{\Delta_0}{2} (\cos(k_x) - \cos(k_x)). \quad (4.3)$$

**Note :-** The coherence peaks in the LDOS corresponding to the bare propagator occur at energy values $E_{coh}$ close to $\pm \Delta_0$.

Our Einstein oscillator is described by a propagator of the form

$$D(\vec{q}; i\Omega_m) = \frac{1}{2} \left( \frac{1}{i\Omega_m - \Omega_0} - \frac{1}{i\Omega_m + \Omega_0} \right) \equiv D(i\Omega_m). \quad (4.4)$$

where $\Omega_m$ is a bosonic Matsubara frequency and $\Omega_0$ is the mode frequency of the oscillator.

Now, if there is a momentum independent electron-boson coupling with matrix element $g$, then the electronic self energy due to the boson at the lowest order in the electron-boson coupling is given by

$$\Sigma(\vec{k}; i\omega_n) = -\frac{T}{N_L} \sum_{\vec{q}, \Omega_m} g^2 D(i\Omega_m) \tau_3 G_0(\vec{k} - \vec{q}; i\omega_n - i\Omega_m) \tau_3$$

Because $D(\vec{q}; i\Omega_m) \equiv D(i\Omega_m)$ is independent of momentum, the momentum index $\vec{q}$ in Eq. (4.5) above is summed over. Therefore, the self energy is independent of momentum and depends only on energy,

$$\Sigma(\vec{k}; i\omega_n) \equiv \Sigma(i\omega_n) \quad (4.5)$$
This simplification is expedient for us as we are concerned with the effect of a boson on the LDOS with respect to energy so as to figure out how to extract the boson’s mode frequency. The above self energy equation can be algebraically shown to be (See details of the algebra in Appendix C.1)

\[
\Sigma(E) = -\frac{ig^2}{2N_L} \sum_{\vec{q}} \frac{1}{(E + \Omega)^2 - E(\vec{q})^2} \begin{pmatrix}
E + \Omega + \epsilon(\vec{q}) & -\Delta(\vec{q}) \\
-\Delta(\vec{q}) & E + \Omega - \epsilon(\vec{q})
\end{pmatrix}
\]

\[
+ \frac{\Omega}{(E - E(\vec{q}))^2 - \Omega^2} \begin{pmatrix}
1 + \frac{\epsilon(\vec{q})}{E(\vec{q})} & \frac{\Delta(\vec{q})}{E(\vec{q})} \\
-\frac{\Delta(\vec{q})}{E(\vec{q})} & 1 - \frac{\epsilon(\vec{q})}{E(\vec{q})}
\end{pmatrix}
\]

(4.6)

where \(E(\vec{q})^2 = \epsilon(\vec{q})^2 + \Delta(\vec{q})^2\).

### 4.3.2 Asymptotic Form near \(E_{coh} + \Omega_0\)

Since we are anticipating, in view of Ref. [1], the high-energy feature due to the boson around energy \((E_{coh} + \Omega_0)\), we will try to understand the properties of the self energy around that energy value \(^3\).

\(^3\)To calculate the value of the Self-energy for real-valued energies, we in the usual way take a limiting procedure by including an infinitesimal positive imaginary part to real \(E\).
We recall that the expression for the self energy (See Eq. 4.6) is

$$\Sigma(z) = -\frac{ig^2}{2N_L} \sum_{\vec{q}} \frac{1}{(z + \Omega_0)^2 - E_{\vec{q}}^2} \begin{pmatrix} z + \Omega + \epsilon_{\vec{q}} & -\Delta_{\vec{q}} \\ -\Delta_{\vec{q}} & z + \Omega_0 - \epsilon_{\vec{q}} \end{pmatrix}$$

$$+ \frac{\Omega_0}{(z - E_{\vec{q}})^2 - \Omega_0^2} \begin{pmatrix} 1 + \frac{\epsilon_{\vec{q}}}{E_{\vec{q}}} & -\frac{\Delta_{\vec{q}}}{E_{\vec{q}}} \\ -\frac{\Delta_{\vec{q}}}{E_{\vec{q}}} & 1 - \frac{\epsilon_{\vec{q}}}{E_{\vec{q}}} \end{pmatrix}$$

$$= -\frac{ig^2}{2} \int_{-\pi/a}^{\pi/a} \int_{-\pi/a}^{\pi/a} a^2 d\vec{q} \frac{1}{(2\pi)^2 (z + \Omega_0)^2 - E_{\vec{q}}^2} \begin{pmatrix} z + \Omega + \epsilon_{\vec{q}} & -\Delta_{\vec{q}} \\ -\Delta_{\vec{q}} & z + \Omega_0 - \epsilon_{\vec{q}} \end{pmatrix}$$

$$+ \frac{\Omega_0}{(z - E_{\vec{q}})^2 - \Omega_0^2} \begin{pmatrix} 1 + \frac{\epsilon_{\vec{q}}}{E_{\vec{q}}} & -\frac{\Delta_{\vec{q}}}{E_{\vec{q}}} \\ -\frac{\Delta_{\vec{q}}}{E_{\vec{q}}} & 1 - \frac{\epsilon_{\vec{q}}}{E_{\vec{q}}} \end{pmatrix}$$

(4.7)

where we remind that $q_x$ and $q_y$ in the integral above have dimensions of momenta or inverse length running from $(-\pi/a, \pi/a)$ and $a$ is the lattice constant.

By examining the above expression Eq. (4.7), we can see that the second term makes a singular contribution to self energy around the energy value $E_{coh} + \Omega_0$. Understanding the form of this singular contribution is the goal of this section.

We start with the off-diagonal terms. $\Delta_{\vec{q}}$ has $d$-wave symmetry while rest of the terms have $s$-wave symmetry with respect to ninety degree rotations in the zone. Therefore, upon integrating over the whole zone, the off-diagonal integrals are exactly zero. The consequence of this is that an Einstein oscillator with a momentum-independent electron-boson coupling can not lead to $d$-wave superconductivity. Let us imagine decreasing the the gap magnitude continuously to zero (i.e. taking the limit $\Delta_0 \to 0$ where $\Delta_{\vec{q}} = (\Delta_0/2)(\cos(q_x) - \cos(q_y))$). Even in this limit, the off-diagonal terms would equal zero. Thus, this mode can not give rise to $d$-wave superconductivity. Notice this argument does not apply for $s$-wave superconductivity, but would apply for $p$-wave superconductivity.

For the diagonal terms, we need not pay attention to the terms in the numerators.
as they are regular and do not contribute to the singularity. The denominator of the integrand can be expanded as

\[
\frac{\Omega_0}{(z - E_{\bar{q}})^2 - \Omega_0^2} = \frac{1}{2} \left[ \frac{1}{z - \Omega_0 - E_{\bar{q}}} - \frac{1}{z + \Omega_0 - E_{\bar{q}}} \right].
\]  

(4.8)

Upon this expansion, we realize that it is the \(1/(z - \Omega_0 - E_{\bar{q}})\) term which is singular at \(E_{coh} + \Omega_0\). Thus, we are looking at an integral of the form

\[
-\frac{ig^2}{4} \int_{-\pi/a}^{\pi/a} \int_{-\pi/a}^{\pi/a} \frac{1}{a^2} \frac{d\bar{q}}{(2\pi)^2} \frac{1}{z - \Omega_0 - E_{\bar{q}}} 
\]  

(4.9)

In Fig. 4.2, we plot a contour plot of \(E_{\bar{q}}\) over the zone and show a zoomed in portion around one of the saddle points.

It is such saddle points which are responsible the singularity at \(E_{coh} + \Omega_0\) and they are the same saddle points which are responsible for the coherence peaks in the bare LDOS (i.e., without the boson mode coupled to the BCS quasiparticles). We will expand \(E_{\bar{q}}\) around this saddle point and write it as

\[
E_{\bar{q}} = E_{coh} + (v'_x(q_x - q_x^{saddle})^2 - v'_y(q_y - q_y^{saddle})^2)
\]  

(4.10)

where \(v'_x > 0, v'_y > 0\) are numerical constants (with dimensions of energy per momenta squared) depending on the details of the dispersion of the BCS quasiparticles. The notation \(v'\) is used because they represent the second derivative of the dispersion and the first derivative being the group velocity is generally notated as \(v\). For a general saddle point, the \(q_x\) and \(q_y\) variables need not be aligned with the \(x\) and \(y\) directions of the reciprocal lattice. In our case, it turns out to be so as can be seen from the Fig. 4.2. This expansion is valid only out to a momenta cut-off around the saddle point, say \(K_x\) and \(K_y\). After shifting origin and rescaling of axes and introducing the cut-offs, the singular part of the self energy takes the form

\[
-\frac{ig^2}{4 \sqrt{v'_x v'_y}} \int_{-\sqrt{v'_x}K_x}^{\sqrt{v'_x}K_x} \int_{-\sqrt{v'_y}K_y}^{\sqrt{v'_y}K_y} \frac{a^2 d\bar{q}}{(2\pi)^2} \frac{1}{z - (q_x^2 - q_y^2)}
\]  

(4.11)
Figure 4.2: In these figures, we illustrate the saddle points in the dispersion of $d$-wave quasiparticles that are responsible for the singularity in the bosonic self energy. The bare dispersion of the $d$-wave BCS quasiparticles was chosen to be $t_1 = 1, t_2 = -0.2749, t_3 = 0.0872, t_4 = 0.0938, t_5 = -0.0857$ and $\mu = -0.8772$ and $\Delta_0 = 0.2$. In a), the whole Brillouin Zone is shown and is chosen as $(0, 2\pi) \times (-\pi, \pi)$. The box highlights one of the saddle points of which there are four in number. In b), we zoom in to the box to show the structure of the saddle point more clearly. We are assuming that the lattice constant $a = 1$. 
where $z = (E - \Omega_0 - E_{coh}) + i\eta$ where $\eta$ has to be taken to $0^+$ to evaluate the integral on the real line. Another simplification we will now make is in our choice of the cut-offs We will stipulate that the cut-offs are so chosen so that $\sqrt{v'_x}K_x = \sqrt{v'_y}K_y$. One particular choice could be $\sqrt{v'_x}K_x = \sqrt{v'_y}K_y = \sqrt{v'_x} + v'_yK^4$.

The first step is to convert the integral into a form that looks like an energy (as opposed to momenta) integral as follows

$$
-\frac{ig^2a^2}{4(2\pi)^2\sqrt{v'_xv'_y}} \int dE' g(E') \frac{1}{z - E'}
$$

where $g(E')$ is the density of states or the number of states between $E'$ and $E' + dE'$ divided by $dE'$. The evaluation of $g(E')$ is done in Appendix C.2 and we cite the result,

$$
g(E') = -\log \left[ \frac{E'}{4(\sqrt{v'_xv'_y})K_xK_y} \right] + \text{terms regular at } E' = 0.
$$

Now, we do the energy integral in Eq. 4.12 using contour integration. We do the integral over a semi-circular contour on the top half of the Argand plane as shown in Fig. 4.3. Thus, the integral is proportional to the residue of the pole at $z$ implying

$$
\Sigma(z) = \frac{g^2a^2}{(2\pi)\sqrt{v'_xv'_y}} \log \left[ \frac{(z - \Omega_0 - E_{coh}) + i\eta}{4(\sqrt{v'_xv'_y})K_xK_y} \right] + \text{regular terms}
$$

where we have multiplied a factor of 4 since there are four such saddle points contributing to the singular part of the self energy. This is the central result of this section: the asymptotic form of the singular part of the self energy around $E_{coh} + \Omega_0$ is logarithmic.

Above, we glossed over the technical point of what is the contribution to the contour integral (ref. Eq. 4.12) through the semicircular piece at infinity. We notice that the contribution due to that piece is independent of $z$, since in the limit $E' \to \infty$, $z - E' \approx$
Figure 4.3: In this figure, we show the semi-circular contour over which we perform the contour integration to evaluate the energy integral in Eq. 4.12. Since in Eq. 4.12, \( z = (E - \Omega_0 - E_{coh}) + i\eta \) where \( \eta \to 0^+ \), therefore the pole (shown as a cross above) is captured by the contour.

\(-E'\). Hence, this piece gives a constant independent of \( E \) as a contribution to the above expression.

### 4.4 Numerical Results

In this section, we show numerical results to check 1) the predicted logarithmic form of the self energy in the previous section, and 2) the resultant LDOS due to the (self energy corrected) \( d \)-wave BCS quasiparticle.
In the Fig. 4.4 below, we show numerical calculations of the self energy as a confirmation of the logarithmic singularity present in the self energy near $E_{coh} + \Omega_0$ as shown in the previous section. In numerics, we have to settle for finite imaginary parts $\eta$ which lead to the “rounding” of the singularity. As expected of a rounded logarithmic singularity due to a finite imaginary part, the real parts of the self energy components show a rounded logarithmic-kink singularity and the corresponding imaginary parts show rounded up-step edges.
Figure 4.4: In the figures above, we show plots obtained from numerical calculations of Self Energy as a function of Energy for three different values of the imaginary part $\eta$. The three values are $0.005$ (brown), $0.01$ (purple) and $0.02$ (blue) in units of $t_1 = 1$. The $x$-axis are in units of $t_1 = 1$ and the units of $y$-axes in these plots are arbitrary. The bare dispersion of the $d$-wave BCS quasiparticles was chosen to be $t_1 = 1$, $t_2 = -0.2749$, $t_3 = 0.0872$, $t_4 = 0.0938$, $t_5 = -0.0857$ and $\mu = -0.8772$. These values are a six-parameter fit to the band structure as measured in ARPES used previously for optimally doped BSCCO [8]. We chose $\Delta_0 = 0.2$ and the boson frequency $\Omega_0 = 0.25$. In a), we show the bare LDOS without the bosonic mode coupling to show the location of the coherence peaks. In b) and c), we show the real parts of $11$ and $22$ components of the Self Energy. In d) and e), we show the imaginary parts of $11$ and $22$ components of the Self Energy. As we can note, the location of the logarithmic singularity as landmarked by the maximum in the real parts, and the upturn of the “step” in the imaginary parts is $\Omega_0 = 0.25$ separated from the location of coherence peaks in a). Another confirmation of the logarithmic nature of the singularity is that the height of the peaks in the real parts of the Self Energy increases linearly as the imaginary part $\eta$ is decreased geometrically.
In order to understand the effect of such a self energy on the LDOS, we look at the expression for the LDOS due to the self energy corrections of the BCS quasiparticle.

\[
n(E) \equiv -\frac{1}{\pi} \text{Im} \left[ \int_{B.Z} \frac{a^2 d\vec{k}}{(2\pi)^2} G_{11}(\vec{k}; E) \right] \\
= -\frac{1}{\pi} \text{Im} \left[ \int_{B.Z} \frac{a^2 d\vec{k}}{(2\pi)^2} (G_0^{-1}(\vec{k}; E) - \Sigma(E))^{-1} \right] \\
= -\frac{1}{\pi} \text{Im} \left[ \int_{B.Z} \frac{a^2 d\vec{k}}{(2\pi)^2} \left( \frac{E + \epsilon(\vec{k}) - \Sigma_{22}(E)}{E^2 - E(\vec{k})^2} \right) \right] \text{... to lowest order in } g \\
\Rightarrow \delta n(E) = \frac{1}{\pi} \text{Im} [\Sigma_{22}(E) \cdot I(E)] \\
\tag{4.15}
\]

where we call the change in LDOS due the bosonic self energy as \( \delta n(E) \) and

\[
I(E) = \int_{B.Z} \frac{a^2 d\vec{k}}{(2\pi)^2} \left( \frac{1}{E^2 - E(\vec{k})^2} \right). \\
\tag{4.16}
\]

We need just note that since the self energy is independent of momentum (cf. Eq. (4.5)), the self energy term in the numerator of momentum integral of the self energy corrected propagator does not get affected by the momentum integration and the integral \( I(E) \) provides an overall multiplicative factor to the singularity of the self energy (cf. Eq. (4.15)), i.e.

\[
\delta n(E) \propto \text{Im} [\Sigma_{22}(E)] \cdot \text{Re}[I(E)] + \text{Re}[\Sigma_{22}(E)] \cdot \text{Im}[I(E)] \\
\tag{4.17}
\]

In the Fig. 4.5 below, we show representative numerical calculations of the self energy corrected LDOS. We discuss the shape of the feature in more detail in the next section. Here, we note that the feature is a combination of a rounded logarithmic-kink and a rounded up-step edge (cf. Eq. (4.17)).

Now we come to the original inversion question that we asked at the beginning of this chapter : How to extract the bosonic mode’s frequency. It is clear from the Fig. 4.5, that the feature has the dip-hump shape as reported in the literature. But, we see that
Figure 4.5: In this figure, we show the Self Energy corrected LDOS as a function of energy for three different values of $\eta = 0.005$ (brown), 0.01 (purple) and 0.02 (blue) in units of $t_1 = 1$ respectively. The $x$-axis are in units of $t_1 = 1$ and the units of $y$-axes are arbitrary. We see that the inflection after the Boson hump is located at an energy from the coherence peaks separated by the Boson mode frequency. The bare dispersion of the $d$-wave BCS quasiparticles was chosen to be $t_1 = 1$, $t_2 = -0.2749$, $t_3 = 0.0872$, $t_4 = 0.0938$, $t_5 = -0.0857$ and $\mu = -0.8772$. These values are a six-parameter fit to the band structure as measured in ARPES used previously for optimally doped BSCCO [8]. We chose $\Delta_0 = 0.2$ and the boson frequency $\Omega_0 = 0.25$. The straight line segments in the energy range $(0.25, 0.39)$ are numerical artifacts since those data points were not numerically calculated. The LDOS is smooth and featureless in that energy range.

$\Delta_0 + \Omega_0$ occurs after the maximum (hump) of the feature and not before (as in Ref. [1]). Thus, given that the assumptions that we have made are reasonably true, in the experiment of Lee et al [1], the prediction of our model can make a difference of around $>5meV$ in the estimate of the phonon’s frequency (estimated by Lee et al to be 52meV)

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$^5$One can convince that this be so by imagining a combination of a rounded logarithmic-kink and a rounded up-step edge (See Eq. (4.17) and Fig. 4.4).

$^6$In the following section, we describe a fitting scheme based on this observation to extract the boson frequency. We note that a fitting scheme is not an inversion technique, but instead a forwards technique. If we had a better understanding the integral $I(E)$ (cf. Eq. (4.26)), then we could hope to find a definitive analytic criterion for the location of the boson frequency.
and hence is a significant difference.

We believe that if the bosonic mode seen in the experiments does not play any role in the establishment of the $d$-wave superconductivity or, in other words, is not the glue or mechanism for the $d$-wave Cooper pairing, then our weak-coupling calculation - including the simplifying assumptions of an Einstein oscillator for a bosonic mode and a momentum independent electron-boson coupling - is a robust starting point to ask the inversion question regarding the extraction of the boson frequency $^7$. Deviations from these simplifying assumptions might make quantitative differences to the extraction of the boson frequency $^8$, if the primary assumption that the mechanism of the superconductivity is independent of the bosonic mode be true.

### 4.5 Fitting Scheme for the Experimental Boson Feature

In this section, we attempt to fit actual data from the Lee et al experiment using the weak-coupling model that we set up in the previous two sections.

In Fig. 4.6, we show a digitized version of the data corresponding to a typical spectrum shown in the inset of Fig. 1 a) of Ref. [1]. We consider only the positive part of the spectrum for the fitting scheme and the very same fitting scheme (to be described below) can be applied to the negative side and other spectra.

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$^7$Indeed, our calculation is only valid to the lowest order in $g$ and we think that higher order corrections would not affect our conclusions. We have not shown this.

$^8$Even if the electron-boson coupling depends on momentum, it is reasonable to expect that it is a regular function of momentum. Then, the singularity in the self energy will still come from the saddle point in the dispersion of the $d$-wave BCS quasiparticles (See Appendix C.2), thus leading to the same qualitative shape for the boson feature.

If the bosonic propagator has a momentum dependence via the dispersion of the mode $\Omega(k)$, then it is not improbable that the resulting boson feature comprises a superposition of features like in our calculation where each feature comes due to each particular value of bosonic mode energy of the dispersion $\Omega(k)$. Thus, the feature might have an extended dip-hump shape. This conjecture needs to be checked though.
Figure 4.6: In the figure above, we show a typical spectrum for LDOS \( n(E) \) as a function of energy \( E \) (in meV) from the Lee et al experiment [1].

### 4.5.1 Set-Up

We start with our choice of parameters for the \( d \)-wave BCS quasiparticles. The bare dispersion of the electrons in the (nearly sharp) \( d \)-wave BCS quasiparticles \(^9\) was chosen to be

\[
\begin{align*}
  c_1 &= 130.5 \text{meV} \\
  c_2 &= -595.1 \text{meV} \\
  c_3 &= 163.6 \text{meV} \\
  c_4 &= -51.9 \text{meV} \\
  c_5 &= -111.7 \text{meV} \\
  c_6 &= 51.0 \text{meV}
\end{align*}
\]  

\(^9\)Soon for the purposes of controlling the singularities, we will include finite imaginary parts to the \( d \)-wave BCS propagator (cf. Eq. (4.2)). These imaginary parts are interpreted as the inverse lifetime of the quasiparticles. For a quasiparticles to be well defined, the imaginary part included must be much smaller than than the energy of the quasiparticle.
and

\[ \epsilon(\vec{k}) = c_1 + \frac{c_2}{2}(\cos k_x + \cos k_y) + c_3(\cos k_x \cos k_y) \]
\[ + \frac{c_4}{2}(\cos 2k_x + \cos 2k_y) + \frac{c_5}{2}(\cos 2k_x \cos k_y + \cos k_x \cos 2k_y) \]
\[ + c_6(\cos 2k_x \cos 2k_y). \quad (4.19) \]

based on the six-parameter tight-binding fit done on ARPES data in Ref. [8]. The lattice constant \( a \) (dimensions of length) does not play any role in the calculations below and we set it to one. Because of this convention, we will mention momenta as having units of \( \text{length}^{-1} \) and position as having units of \( \text{length} \). These values are a six-parameter fit to the band structure as measured in ARPES used previously for optimally doped BSCCO [8]. Our choice of the \( d \)-wave gap function is

\[ \Delta(\vec{k}) = \Delta_0^2 (\cos(k_x) - \cos(k_y)). \quad (4.20) \]

From Fig. 4.6, we find that the coherence peak on the positive side is located at \( E_{coh} = 39.8\text{meV} \). The coherence peaks come about because of the saddle points in the dispersion of the \( d \)-wave BCS quasiparticles \( E(\vec{k}) = \sqrt{\epsilon(\vec{k})^2 + \Delta(\vec{k})^2} \) (See Fig. 4.2 for an illustration). At such saddle points, \( E(\vec{k}_{saddle}) = E_{coh} \) and we can use this to find the value of \( \Delta_0 \). From using \( E(\vec{k}_{saddle}) = E_{coh} \) we found,

\[ \Delta_0 = 43.2\text{meV}. \quad (4.21) \]

### 4.5.2 Coherence Peak Calibration

Since, the STM measures an \( I - V \) curve and the \( dI/dV \) is proportional to the LDOS, therefore, there is an arbitrariness in the scale of the LDOS, i.e. the y-axis scale in Fig. 4.6. Thus, we need a way to calibrate the scale. This calibration will also be used to do a check on our weak-coupling assumption in a future subsection.
The way we calibrate the y-axis is by making use of the coherence peak. The coherence peak in the LDOS is also a result of a singularity due to the saddle points in the dispersion of the $d$-wave BCS quasiparticles $E(\vec{k})$. The argument runs very similar to that of Section 4.3.2. We have

$$n(E) = -\frac{1}{\pi} \text{Im} \left[ \int_{BZ} \frac{a^2 d\vec{k}}{(2\pi)^2} \frac{E + \epsilon(\vec{k})}{E^2 - E(\vec{k})^2} \right] = -\frac{a^2}{(2\pi)^3} \text{Im} \left[ \int_{BZ} d\vec{k} \left( \frac{1}{E - E(\vec{k})} + \frac{1}{E + E(\vec{k})} \right) \left( 1 + \frac{\epsilon(\vec{k})}{E} \right) \right], \quad (4.22)$$

The $1/(E - E(\vec{k}))$ term in the integrand of Eq. (4.22)’s second line above gives a divergent contribution at the (positive) coherence peak. The $\int d\vec{k}(1 + \epsilon(\vec{k})/E) \times (1/(E + E(\vec{k})))$ contribution in Eq. (4.22) above is regular at that coherence peak and will be taken into account as a regular background term.

Regarding the $\int d\vec{k}(1 + \epsilon(\vec{k})/E) \times (1/(E - E(\vec{k})))$ contribution, we note that

1. due to the $\epsilon(\vec{k})$, the $\int d\vec{k}/(E - E(\vec{k})) \times (\epsilon(\vec{k})/E)$ piece has cancellations since the integrand is positive over part of the zone and negative over the rest. If $\epsilon(\vec{k})$ were to be particle-hole symmetric, then the cancellations would make this piece exactly zero.

2. Moreover, for the saddle point where $E(\vec{k}) = E_{coh}$, we also have $\epsilon(\vec{k}) = 0$. See Fig. 4.2. Thus, the divergence due to the $1/(E - E(\vec{k}))$ is countered by the presence of $\epsilon(\vec{k})$ in the numerator leading to the $\int d\vec{k}/(E - E(\vec{k})) \times (\epsilon(\vec{k})/E)$ piece being regular.

Therefore, this piece can also be absorbed into the background

3. Thus, the only divergent piece is $\int d\vec{k}/(E - E(\vec{k}))$ and the singularity is logarithmic analogous to the algebra in Section 4.3.2. We control the singularity by including an imaginary part $\eta_{coh}$ to $E$. 

66
Putting all this together, the fitting form for the calibration of the coherence peak is

\[ n(E) = \frac{(\alpha_{cal}a^2)}{(2\pi)^2 \sqrt{v_x'v_y'}} \log \left[ \frac{\sqrt{(E - E_{coh})^2 + \eta_{coh}^2}}{4(\sqrt{v_x'v_y'})K_xK_y} \right] \]

\[ + (a_{coh}E + b_{coh}). \]  

(4.23)

where - as defined in Section 4.3.2 - \( v_x'v_y' = 8849.5 \text{meV}^2 \text{length}^4 \) and \( K_xK_y = 0.03 \). \( \alpha_{cal} \) is the calibration coefficient that sets the scale for the y-axis. \( (a_{coh}E + b_{coh}) \) takes account of all regular contributions.  

Using the fitting form in Eq. (4.23), we show in Fig. 4.7 the fit to the coherence peak on the positive energy side of the experimental data (cf. Fig. 4.6). We restrict our attention to the window \( 30 - 50 \text{meV} \) and we recall that \( E_{coh} = 39.8 \text{meV} \).

\[ \text{Figure 4.7: In the figure above, we show the fit of the fitting form in Eq. 4.23 to the positive coherence peak in the experimental data in the energy window 30 - 50meV.} \]

\[ ^{10} \text{In the algebra of Eq. (4.22), we did not include any self energy contributions which would indeed be present according to our theory. But, we showed in the previous section that the self energy has a singularity only around the boson feature energy. Therefore, it is regular around the coherence peak and is consequently taken into account by the background term.} \]
We see that the fitting is *good* in this window. The results of the calibration are

\[
\begin{align*}
\alpha_{\text{cal}} &= 2245.1 \\
\eta_{\text{coh}} &= 9.5 \text{meV} \\
a_{\text{coh}} &= 0.0050 \text{meV}^{-2} \\
b_{\text{coh}} &= 0.66 \text{meV}^{-1}.
\end{align*}
\] (4.24)

From the coherence peak calibration above, we also get an estimate for the (inverse) lifetime of the *d*-wave BCS quasiparticles in an energy window around the coherence peak.\(^{11}\)

### 4.5.3 Fitting the Boson Feature

Now, we start with the fitting of the boson feature. We restrict our attention to an energy window of 80 – 140\text{meV} which contains the hump in Fig. 4.6. The fitting form for the boson feature is

\[
n(E) = \frac{2g^2(\alpha_{\text{cal}}a^2)}{(2\pi)^4 \sqrt{v_x'v_y'}} \text{Im} \left[ I(E + i\eta_{\text{feature}}) \times \log \left[ \frac{(E - \Omega_0 - E_{\text{coh}}) + i\eta_{\text{feature}}}{4(\sqrt{v_x'v_y'})K_xK_y} \right] \right] \\
+ (a_{\text{feature}}E + b_{\text{feature}}).
\] (4.25)

The salient features of the fitting form Eq. (4.25) are

1. The first term on the r.h.s - \text{Im}[..., etc. - is due to the singular part of the self...

---

\(^{11}\)The \(\eta_{\text{coh}} \approx 10\text{meV}\) (assumed to be constant over the Brillouin zone and the energy window 30 – 50\text{meV}) is not small compared to \(E_{\text{coh}} = 39.8\text{meV}\). This is not a good sign, but we note that we have used the value of \(\eta\) at the saddle point as representative of the inverse lifetime over the zone which might not be sensible. Also, \(\eta\) can have an energy dependence [9]. In Ref. [9], \(\eta_{\text{coh}} \approx 1\text{meV}\) for \(E_{\text{coh}} \approx 40\text{meV}\) which would imply that the *d*-wave BCS quasiparticle are nearly sharp.
energy $\Sigma(E)$ and it is this piece that gives the characteristic shape that will allow us to fit experimental data.

2. The second term on the r.h.s - \((a_{\text{feature}}E + b_{\text{feature}})\) - is a background term. It is representative of the regular contributions due to the self energy. Essentially, we are assuming that this regular contribution is not heavily dependent on energy and can be approximated by a polynomial of degree one.

3. From Eq. (4.26),

$$I(E) = \int_{B.Z.} \frac{a^2 d\vec{k}}{(2\pi)^2} \left( \frac{1}{E^2 - E(\vec{k})^2} \right)$$

(4.26)

4. $v_x' = d^2E(\vec{k})/dk_x^2$ and $v_y' = d^2E(\vec{k})/dk_y^2$ at the momentum $\vec{k}_{\text{saddle}}$ (See Eq. (4.10)). For our choice of dispersion and gap function, $v_x'v_y' = 8849.5meV^2 length^4$.

5. $K_x$ and $K_y$ are momenta cut-offs around the saddle point - See Fig. 4.2 - within which the \(d\)-wave BCS dispersion $E(\vec{k})$ is well approximated as Eq. (4.10). We choose them such that in Fig. 4.2, $K_x = 0.5$ and $K_y = 0.06$. Therefore, $K_xK_y = 0.03$.

6. We arrived at this form using Eq. (4.15) and Eq. (4.14).

7. We have included an imaginary part \(i\eta_{\text{feature}}\) to $E$ in $n(E)$ to control the logarithmic singularity. This $\eta_{\text{feature}}$ can be interpreted as the inverse lifetime of the \(d\)-wave BCS quasiparticles in the energy window 80 – 140meV. We are assuming that the lifetime is a constant (independent of both momentum and energy) over this window. As required for the quasiparticles to be well defined, in the end we have to check that $\eta_{\text{feature}} << 80meV$.

8. The fitting parameters in the above expression Eq. (4.25) are:

\[\text{Note that this background also takes into account the contribution to the LDOS due to the “free” part of the self energy corrected \(d\)-wave BCS propagator, i.e. the contribution that is obtained when \(g = 0\). This contribution is equal to } \int_{B.Z.} a^2 d\vec{k}(E + \epsilon(\vec{k}))/((2\pi)^2(E^2 - E(\vec{k})^2)). \text{ This is consistent with the argument that the shape of the boson feature is a result of the singular contribution of the self energy.}\]
(a) $\Omega_0$: the bosonic mode frequency.

(b) $g$: the electron-boson coupling strength.

(c) $\eta_{\text{feature}}$: the inverse lifetime of the $d$-wave BCS quasiparticles in the energy window 80 – 140meV.

(d) $a_{\text{feature}}$ and $b_{\text{feature}}$: parameters for the background contribution.

Now, we discuss the shape of the boson feature. The property of the logarithm $f(x) \propto \log(x + i\eta)$ is that $\text{Re}[f(x)] \propto \log(x^2 + \eta^2)$ (a rounded logarithmic-kink singularity) and $\text{Im}[f(x)] \propto \text{ArcTan}[x/\eta]$ (a rounded up-step edge). Looking at Eq. (4.25), if $I(E + i\eta_{\text{feature}})$ has both real and imaginary parts, then both the real and imaginary parts of the logarithmic term in the r.h.s of Eq. (4.25) would contribute to boson feature $\delta n(E)$. We numerically saw that the function $I(E + i\eta_{\text{feature}})$ had real and imaginary parts of comparable magnitude over the energy range 80 – 140meV and for $\eta_{\text{feature}} \in [1, 1000]meV$. Therefore, the boson feature according to our theory is a combination of a rounded logarithmic-kink (with the maxima sitting at $E = E_{\text{coh}} + \Omega_0$) and a rounded up-step (with the inflection point of the step sitting at $E = E_{\text{coh}} + \Omega_0$). This combination allows for a good fit of the boson hump (cf. Fig. 4.6) as will be shown next.

In Fig. 4.8, we show a fit of the experimental boson feature with our fitting form. As we see, the fit is pretty good over the energy window.

The fitting parameters as extracted from the fitting procedure (done using FindFit
function of Mathematica software package) are:

\[
\begin{align*}
\Omega_0 &= 72 \text{meV} \\
g &= 21.6 \text{meV} \\
\eta_{\text{feature}} &= 6.1 \text{meV} \\
a_{\text{feature}} &= 0.0024 \text{meV}^{-2} \\
b_{\text{feature}} &= 0.35 \text{meV}^{-1}
\end{align*}
\] (4.27)

Few remarks are in order:

1. Lee et al had concluded that the bosonic mode frequency was $52 \pm 8 \text{meV}$. Our conclusion of $72 \text{meV}$ from fitting one typical spectrum is significantly different from their estimate. They had extracted the boson frequency using the inflection point before the hump, while our estimate locates the boson feature after the hump. This is why we see a significant difference in the two estimates.
2. The strength of electron-boson coupling according to our scheme is estimated to be of the order of 20\,meV. Since our theory depends on $g$ being small, it needs to be checked whether our estimate is indeed small or not (more on this in the next section).

3. Our estimate of $\eta_{\text{feature}} \approx 6\,\text{meV}$ is an order lower than 80\,meV. Thus, our assumption on the sharpness of the $d$-wave BCS quasiparticles is not violated.

### 4.5.4 Checking the Weak-Coupling Assumption

Now, we come to the issue of checking the weak-coupling assumption. The rigorous way to do this would be come up with a protocol to compare the magnitude of $\Sigma(E)$ using the extracted parameters with the magnitude of $G_0^{-1}(\vec{k}; E)$. If the magnitude of the self energy is small compared to the inverse of the free propagator, the perturbation theory is valid.

Instead, we take a short-cut and use the coherence peak calibration can help us to do this check. The argument runs as follows: the full LDOS has two contributions, $n_{\text{free}}(E)$ coming from the “free” part ($g = 0$) of the full $d$-wave BCS propagator (which we approximate as in Eq. (4.23)) and $\delta n(E)$ coming from the singular self energy contribution (which is approximated by the logarithmic term in Eq. (4.25)). For the perturbation theory to be valid, the self energy piece must be small compared to the “free” piece, i.e.

$$\delta n(E_{\text{feature}}) \ll n_{\text{free}}(E_{\text{coh}}). \quad (4.28)$$

In principle, we should do the comparison at the same energy. But, if we look at the experiment data in Fig. 4.6, we see that there is at most a factor of two difference in the LDOS values at the two energies. We ignore this at most factor of two for now.
In order to do the comparison required in Eq. (4.28), we need just take the ratio $r$ of the coefficients of the logarithms in the expressions of $n(E_{feature})$ and $n(E_{coh})$ and show that it is $<< 1$. From Eq. (4.23) and Eq. (4.25),

$$r \approx \frac{2g^2 |I(E_{feature} + i\eta_{feature})|}{(2\pi)^2}$$

(4.29)

Numerically, $|I(E_{feature} + i\eta_{feature})| = 0.0015$. Therefore, for our extracted values of $g$, we get $r = 0.034$. This value of $r$ gives us confidence in our weak-coupling assumption and the fitting scheme described here that is based on it.

We also give an indirect argument. In Ref. [10], a numerical calculation was done to investigate the bosonic features in BSCCO and it had the same assumption as ours’ : the mechanism of the $d$-wave superconductivity is independent of the bosonic mode. It was a lowest order perturbation theory in $g$ and thus also depended on $g$ being small. In their calculation, they used values of $g$ (See Table I of Ref. [10], $0.75 < g < 1.5$) of the same order of magnitude as that of the nearest-neighbor hopping strength (characteristic of the bandwidth of the bare dispersion, cf. Eq. (4.18). They call it by its usual name $t_1$ set to 1, see the text after Eq. (2) of Ref. [10]. Thus, they had $0.75 < g/t_1 < 1.5$. In our notation, $c_2$ represents the nearest-neighbor hopping strength and the relation between the two quantities is $t_1 = c_2/4$. Thus, $0.18 < g/c_2 < 0.38$). Given that their calculation is valid as a perturbation theory\(^{13}\), $g \approx 150 - 240meV$ in case of BSCCO ($c_2 \approx 600meV$) is not improbable as a small $g$. Our estimate of $g \approx 20meV$ is $< 150meV$ and is thus even smaller giving additional confidence on the weak-coupling assumption.

\(^{13}\)We believe in their calculation’s validity because of the following : their calculation had momentum dependent electron-boson couplings which were capable of renormalizing the $d$-wave gap. By comparing the location of the coherence peaks (Fig. 1 of their paper Ref. [10]) in the no mode coupling case with the boson coupled cases, it is reasonable to say that the gap is not renormalized significantly. If this is the case, then it is safe to say that $g$ is small enough. They have not commented on how much the gap gets renormalized or on any other checks done to verify the validity of their perturbation theory. In our theory with its simplifying assumptions of an Einstein Oscillator for the bosonic mode and momentum independent electron-boson coupling, the gap renormalization is exactly zero.
4.6 Conclusion

In summary, we have shown how a weak-coupling point of view can be used to analyze the high-energy features in the STM data of BSCCO. Our weak-coupling model was set up by coupling $d$-wave BCS quasiparticles to Einstein oscillators via a momentum independent electron-boson coupling. Using our theory, we predicted an analytic (logarithmic) form for the self energy of the $d$-wave BCS quasiparticle induced by the boson, and for the LDOS due to the (self energy corrected) $d$-wave BCS quasiparticle. We also proposed a fitting scheme based on the analytic form to analyze experimental data that allows us to 1) extract the frequency of the boson, 2) an estimate for the electron-boson coupling. Also, it allows us to extract an estimate of the inverse lifetime of the $d$-wave BCS quasiparticles at energies where the boson feature is located. Our estimate for the frequency of the bosonic mode in BSCCO is $72\,\text{meV}$. Our estimate of the electron-boson coupling strength in BSCCO is $20\,\text{meV}$.

4.6.1 Advantages and Disadvantages of the Proposed Fitting Scheme

The advantages of our scheme are

1. Having a simple functional form for the boson feature (cf. Eq. (4.25)) makes a numerical fit for vast number of STM spectra highly feasible computationally.\textsuperscript{14}

2. Since we also have a recipe to check whether the weak-coupling assumption is true or not, the logical consistency of the fitting scheme can be kept under scrutiny.

\textsuperscript{14}One would need to evaluate $I(E, \eta)$ (cf. Eq. (4.26)) for a range of $E$ and $\eta$, but this evaluation has to be done only once.
3. Our scheme also gives the inverse lifetimes of the $d$-wave quasiparticles $\eta$ which is additional information on the underlying electrons.

The disadvantages of our scheme are

1. We do not get any momentum dependent information. The estimated $g$ from our scheme would be representative of some form of momentum averaged $g(\vec{k})$.

2. It does not tell us anything positively about the mechanism in that 1) if the scheme succeeds and the fitting always respects the weak-coupling assumption, then it can be concluded that the boson observed in the STM is not part of the mechanism, and 2) if we see that the weak-coupling assumption is being violated, then we can only conclude that the boson perhaps plays a role in the mechanism. In case the weak-coupling assumption gets violated, in order to resolve the question of the observed boson as the mechanism, one would need to set up an Eliashberg calculation and compare the calculated gap magnitude to the observed one. If they compare well, then the boson can be said to be the mechanism. But as we remarked in a footnote(2) in the previous section, setting up an Eliashberg calculation for a $d$-wave superconductor is a challenging task.

3. The scheme is also presently incapable of pinpointing the nature of bosonic mode.

### 4.6.2 Relation to Previous Work

In light of our work, we should comment that our starting point is same as that of a previous numerical work, Ref. [10]. This previous work is silent on the aforesaid inversion issue of the bosonic mode’s frequency extraction which was one of the motivations for our work. It must also be mentioned that Zhu and Balatsky have taken the opposite
position and considered the case of the d-wave superconductivity arising out of an inhomogeneous bosonic mode leading to inhomogeneous gap magnitudes [11]. Nanoscale inhomogeneity in gap magnitude is a well-established fact and has been observed in all STM experiments on Cuprates [12, 13, 14, 15, 16, 17]. Also, Lee et al have observed nontrivial correlations between the spatially varying coherence gaps and spatially varying boson mode energies.

Another recent work, Ref. [18], done in 2010 asked the same inversion question of the bosonic mode’s frequency extraction from the LDOS of BSCCO. What they did was to set up an elaborate Eliashberg calculation for a \( d \)-wave superconductor with a dominant mode with a much higher mode energy (\( \approx 6 \) times that of the boson’s) which was responsible for the establishment of the superconductivity. They also included another mode with smaller electron-boson coupling which modeled the mode observed in the experiment. After solving the Eliashberg equations numerically, they found that the bosonic mode’s frequency lay at the minimum of the dip of the dip-hump feature and that is the criterion they suggested for the frequency extraction. Their work was primarily numerical and it was hard to tell what was physical/mathematical reason behind their conclusion. In comparison, we feel our work, though simplistic, has the merit of transparency.

Another response to the Lee et al was by Hwang et al, Ref. [19]. The abstract of their response said:

“Using atomic-resolution scanning-tunneling microscopy (STM) to extract the spectrum of these modes in the high-temperature superconductor BSCCO, Lee et al. [1] find a mode whose frequency does not depend on doping but that it changes on isotopic substitution of \( O_{16} \) with \( O_{18} \). From this, they infer a role for lattice modes (phonons). However, examination of their data reveals a weaker, but distinct, feature that has all
the characteristics of the magnetic excitation identified as the bosonic mode in other competing experiments. We therefore suggest that the lattice mode seen by Lee et al. is not relevant to superconductivity and is due to inelastic tunneling through the insulating oxide layer.”

This response reveals two other general stories in the phenomenology of Cuprates. One is the issue of the magnetic modes (perhaps even important for the mechanism) which we are not going into here. The other is the issue of inelastic tunneling through the oxide layer. BSCCO does not cleave at the $CuO_2$ layer which is believed to contain the key physics leading to high temperature superconductivity. It cleaves at the Bismuth oxide layer and there is another intervening oxide layer in between the STM tip and the nearest $CuO_2$ layer. Thus, there is a belief that the intervening layers might contribute to the STM signal. Another work which has tried to model this into a calculation to identify signatures in STM spectra due to the inelastic tunneling processes is by Pilgram, Rice and Sigrist [20], which the reader should go for more details and the related literature. We would comment that our calculation is agnostic as to whether there are these extra modes in the Lee et al. experiment. But our work is pertinent in that i) we can say how many humps/dips can be engendered by just one boson, and ii) if there is a weakly coupled magnetic mode, our theory can be applied to this case too.
BIBLIOGRAPHY


APPENDIX A

APPENDICES FOR CHAPTER 2

A.1 The Recursion Method

In this appendix, we outline the steps involved in the implementation of the Recursion
method (Ref. [1]) to calculate the local density of states (LDOS) of a (quadratic) Hamiltonian
on a discrete lattice. Let us say the given Hermitian Hamiltonian is of the form

\[ \hat{H} = \begin{pmatrix}
    \ddots & & & \\
    \vdots & a & b & c & \ddots \\
    \vdots & b^* & d & e & \ddots \\
    \vdots & c^* & e^* & f & \ddots \\
    \ddots & & & \ddots
\end{pmatrix} \tag{A.1} \]

in some basis. For normal electrons, the basis could be the position basis, and for superconducting quasiparticles, the basis could be a doubled position basis where to each site is associated an “electron” and a “hole” amplitude, \(à la\) a lattice formulation of the Bogoliubov Hamiltonian for a superconductor (See Ref. [2]).

Now, let us say we want to calculate the electronic LDOS at a site \(|n = 0\rangle\). We start the Recursion method by tridiagonalizing the Hamiltonian starting with \(|n = 0\rangle\). For superconducting case, \(|n = 0\rangle\) might mean the electronic amplitude on site 0 if we are interested in the LDOS of the electrons. There is a recursive way in which we can achieve the basis transformation required for the desired tridiagonalization of the (hermitian) Hamiltonian. The recursion is

\[ \hat{H}|n\rangle = a_n|n\rangle + b_{n+1}|n + 1\rangle + b_n^*|n - 1\rangle \tag{A.2} \]
where the recursion is started at \( |\mu = 0 \rangle \). After the basis transformation, the Hamiltonian in the new basis looks like

\[
\hat{H} = \begin{pmatrix}
\vdots & \vdots & \vdots & \vdots \\
\cdots & a_0 & b_1 & 0 & \cdots \\
\cdots & b_1^* & a_1 & b_2 & \cdots \\
\cdots & 0 & b_2^* & a_3 & \cdots \\
\vdots & \vdots & \vdots & \vdots
\end{pmatrix}.
\] (A.3)

Some features of the basis states of the new basis are: 1) Each basis state is a linear combination of many sites, but it has the same point symmetry around the site 0 as the initial orbital. 2) After \( n \) steps of the Recursion, the \( n^{th} \) basis state is confined to an area \( A \) such that any point in \( A \) is at most \( n \) distant in space from the site 0 using the Manhattan metric, i.e. there is zero amplitude outside this area \( A \). Most of the amplitude of the \( n^{th} \) basis state lies on the perimeter of this area \( A \), but there is a tail extending inwards to the site 0.

Once the \( a_n, b_n \) (also called the Recursion coefficients) are calculated, the local Green’s function is arrived at by inverting the tridiagonal matrix and is given by a continued fraction expansion \(^1\) as follows

\[
G(0, 0; E) = \langle 0| \frac{1}{E - \hat{H}} |0 \rangle = \frac{1}{E - a_0 - \frac{|b_1|^2}{E - a_1 - \frac{|b_2|^2}{E - a_2 - \cdots}}}.
\] (A.4)

To get the LDOS, we take the imaginary part of the Green’s function, i.e.

\[
n_0(E) = -\frac{1}{\pi} G(0, 0; E).
\] (A.5)

As only a finite number of Recursion coefficients (RCs) can be computed on a computer, some form of extrapolation is generally used in practice and a lot has been said on this topic (See Ref. [1]). For us, it was sufficient to calculate around a thousand Recursion coefficients.

\(^1\)The tridiagonal form makes it easy to write the inverse as a continued fraction expansion.
coefficients and then set the remaining coefficients equal to the last calculated Recursion coefficient.

What determined that calculating around thousand RCs using the Recursion method was enough? The criterion that we used was to check whether in the uniform (i.e. without impurity for either normal or superconducting system) case, whether the LDOS is smooth without any spurious oscillations. The spurious oscillations come about because of our extrapolation scheme: “set remaining RCs equal to the last calculated RC”. When we do this, we are artificially making the system non-uniform from the last calculated RC onwards precisely because of the inexactness of our extrapolation. This is equivalent to having a boundary which gives rise to scattering and consequent “Friedel”-like oscillations. Another check that these oscillations were due to the artificially introduced boundary was by checking that the frequency of these oscillations were consistent with the echo times (See Chapter 2) of a quasiparticle starting at site 0 and echoing back from the artificial boundary. Our aim was to make sure that the amplitude of these spurious “Friedel”-like oscillations was small enough compared to the desired numerical accuracy and we found around a thousand RCs was sufficient for this purpose.

We will end with some remarks regarding what we found useful in our studies on the extrapolation of RCs:

1. Extrapolation is needed to obtain a smooth LDOS. If we have a small number of RCs, we then have a spiky LDOS within the bandwidth, with the number of spikes/delta functions equaling the number of RCs. As is usual, one includes a

\[\text{To better understand the effect of finite number of RCs, one ought to compare the LDOS calculated from the Recursion method with that from Exact Diagonalization and from the formula in Eq. (2.4). This would also inform on how the Van Hove singularities (logarithmic in two dimensions) get cut off while using the various methods to calculate LDOS.}\]
small imaginary part to the energy to round the delta functions. Thus, to obtain a smooth LDOS, one needs a good number of RCs.

2. To obtain a good number of RCs, what we did was to calculate around a thousand Recursion coefficients and then set remaining RCs equal to the last calculated RC. This was good enough to make the amplitude of the spurious “Friedel”-like oscillations - as mentioned above - small enough compared to the desired numerical accuracy and we found around a thousand RCs was sufficient for this purpose.

3. For the normal electron case, we saw that even around 400 RCs was sufficient to have a smooth LDOS without any spurious oscillations. For the superconducting case, we saw that we needed around 1000 RCs. We calculated 1600 RCs for our calculations.
BIBLIOGRAPHY


A.2 Dimensional Reduction of Certain Integrals from $2d$ to $1d$

In this appendix, we describe how certain two dimensional integrals with diverging integrands can be converted to one dimensional integrals with regular integrands. The kind of integral we are interested in are of the form

$$I(\vec{R}; E) = \frac{1}{(2\pi)^2} \int\limits_{-\pi}^{\pi} dk_x \int\limits_{-\pi}^{\pi} dk_y \frac{e^{i\vec{k} \cdot \vec{R}}}{E + i\delta - \epsilon(k)}. \quad (A.6)$$

in the limit $\delta \to 0$. These kinds of integrals are encountered while calculating Green’s functions of electrons in two dimensional square lattices.

Let us look at the $k_y$ integral for a particular $k_x$. The denominator vanishes for certain values of $k_y$ thus motivating the conversion of the $k_y$ integral to a contour integral. The mapping $z = e^{ik_y}$ achieves the conversion which also maps the integral from $-\pi$ to $\pi$ to a contour integral over the unit circle. The periodicity of the integrand over the zone ensures the analyticity of the resulting complex integrand. Thus,

$$I(\vec{R}; E) = \frac{1}{(2\pi)^2} \int\limits_{-\pi}^{\pi} dk_x e^{i k_x R_x} \oint \frac{dz}{iz} \frac{z^{R_y}}{E + i\delta - \epsilon(k_x, z)}. \quad (A.7)$$

For a particular $E$ energy contour and $k_x$, we get an even number of poles (there are two poles if the contour is convex). Expanding the denominator around the poles gives us

$$E + i\delta - \epsilon(k_x, z) = -\frac{\hbar \nu_y(E, k_x)}{iz_p} (z - z_p (1 - \frac{\delta}{\hbar \nu_y(E, k_x)})). \quad (A.8)$$

The poles $z_p$s are defined by $\epsilon(k_x, z_p) = E$ and $\hbar \nu_y(E, k_x) \equiv \partial \epsilon(\vec{k})/\partial k_y$ is the group velocity along $y$ direction. We need only worry about the $(z - z_p)$ term in the expansion of the denominator since other expansion terms will yield zero residues. Because of the $(1 - \delta/\hbar \nu_y(E, k_x))$ factor in the expansion Eq. (A.8), we realize that the pole where the sign of the $\hbar \nu_y$ is same as the positive $\delta$ will be “pulled” inside the unit circle while the other pole will be “pushed” out of the unit circle. Thus, when we do the $k_x$ integral, only one half of the $E$ energy contour (not to be confused with the complex contour; to
distinguish we will call $E$ contours as energy contours) will contribute to the integral. In
the process, we have converted the 2D integral over the zone into an integral over part
of the energy contour. Filling in the steps,

$$I(\vec{R}, E) = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} dk_x e^{i k_x R_x} \oint_{U.C.} \frac{dz}{i z} \frac{z R_y}{\hbar v_{g_y}(E, k_x)} (z - z_p (1 - \frac{\delta}{\hbar v_{g_y}(E, k_x)}))$$

$$= -\frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} dk_x e^{i k_x R_x} 2\pi i \frac{z_p}{\hbar v_{g_y}(E, k_x)}$$

$$= -\frac{1}{(2\pi)^2} 2\pi i \int dk_x \frac{e^{i k_x R_x} e^{i k_y p(E, k_x) R_y}}{\hbar v_{g_y}(E, k_x)}$$

$$= \frac{1}{2\pi i} \oint_{\text{sgn}(\delta) = \text{sgn}(v_{g_y}(E, s))} ds \frac{e^{i \vec{k}(s, E) \cdot \vec{R}}}{|\nabla \epsilon(\vec{k}(s, E))|} \quad (A.9)$$

where the last step was achieved by converting the element $dk_x$ to a variable $s$ parametrizing the contour of constant $E$ energy, and we integrate over that part of the energy contour where the sign of $\delta$ is same as $v_{g_y}$.

In this way, we have converted the initial two dimensional integral to a one dimen-
sional integral with a regular integrand. This one dimensional form can be used in numerics as well, thereby considerably lowering computing time.

An unresolved point in the above dimensional reduction of the integral is that we started out in Eq. (A.6) with an expression that is manifestly invariant to ninety degree rotations. But, we ended up in Eq. (A.9) with an expression that is not manifestly invariant to ninety degree rotations, i.e. the portion of the energy contour we integrate over depends on the order of the $k_x$ and $k_y$ integrations, and yet the result is the same \(^3\).

\(^3\)There is enough symmetry in the square lattice case to explicitly show that doing the dimensional reduction in either order gives the same result.
APPENDIX B
APPENDICES FOR CHAPTER 3

B.1 Limit on the Error introduced by Kramers-Kronig Integration

The Kramers-Kronig relation relates the real part of a Green’s function to the imaginary part as follows

\[ \text{Re}[G(r, \omega)] = -\frac{1}{\pi} P \int_{-\infty}^{\infty} dx \frac{\text{Im}[G(r, \omega, x)]}{(\omega - x)} = P \int_{-\infty}^{\infty} dx \frac{n(r, x)}{(\omega - x)}. \]  

(B.1)

If we limit the integral by cut-offs \( \Lambda_+ \) and \( \Lambda_- \), then the error \( E \) introduced is

\[ E = \int_{-\infty}^{\Lambda_-} dx \frac{n(r, x)}{(\omega - x)} + \int_{\Lambda_+}^{\infty} dx \frac{n(r, x)}{(\omega - x)}. \]  

(B.2)

Let us say that the fraction of the total spectral weight (= 1 if we have a one-band model which we have assumed in the main text) being measured in the experiment be \( x \). Therefore,

\[ n_{\text{avg}}(r) = \frac{1}{|\Lambda_+ - \Lambda_-|} \int_{\Lambda_-}^{\Lambda_+} dx n(r, x), \]

\[ n_{\text{avg}}(r)|\Lambda_+ - \Lambda_-| = x \]

\[ n_{\text{avg}}(r)W(r) = 1. \]  

(B.3)

In Eq. (B.3), the first equation defines \( n_{\text{avg}}(r) \) and the third equation defines a “bandwidth” \( W(r) \). To estimate error using Eq. (B.2), we note that the maximum positive error happens when the (un-measured) LDOS is such that all of the un-measured spectral weight \( (1 - x) \) is located at \( \Lambda_- \) and the maximum negative error happens when the (un-measured) LDOS is such that all of the un-measured spectral weight \( (1 - x) \) is located at \( \Lambda_+ \). Therefore, the error is bounded as
Agreeing with our intuition, the error bounds are decreased if more of the total spectral weight is measured, and - more importantly - when \( \omega \) moves away from the cut-offs.

### B.1.1 Digression: Estimating the Fractional Error

To estimate the fractional error, we need an estimate of the value of \( \text{Re}[G(r, r; \omega)] \). If we estimate \( \text{Re}[G(r, r; \omega)] \) by approximating \( n(r; \omega) \approx n_{\text{avg}}(r) \), then we get

\[
\text{Re}[G(r, r; \omega)] = n_{\text{avg}}(r) \log \left| \frac{\omega - \Lambda_+}{\omega - \Lambda_-} \right| \tag{B.5}
\]

From Eq. (B.4) and Eq. (B.5), an estimate on the maximum fractional error is

\[
E_{\text{frac}} = \frac{(x^{-1} - 1)}{1 + \frac{|\omega - \Lambda_i|}{|\Lambda_+ - \Lambda_-|} \log \left| \frac{\omega - \Lambda_+}{\omega - \Lambda_-} \right|} \tag{B.6}
\]

where \( \Lambda_i \) is such that \( |\Lambda_i - \omega| < |\Lambda_- - \omega| \).

For an energy \( \omega \) well within the measured energy range, i.e. \( \omega = (\Lambda_+ + \Lambda_-)/2 + y \) where \( |y| << |\Lambda_+ - \Lambda_-| \), we have \( \frac{|\omega - \Lambda_i|}{|\Lambda_+ - \Lambda_-|} = \frac{1}{2} + \frac{|y|}{|\Lambda_+ - \Lambda_-|} \) and \( \log \left| \frac{\omega - \Lambda_+}{\omega - \Lambda_-} \right| = \frac{4y}{|\Lambda_+ - \Lambda_-|} \). Therefore to lowest order in \( y \), we get for the maximum fractional error

\[
E_{\text{frac}} = \frac{1}{1 + \frac{2y}{(x^{-1} - 1) |\Lambda_+ - \Lambda_-|}} \tag{B.7}
\]

Thus from Eq. (B.7), for a low maximum fractional error we desire

\[
x^{-1} - 1 << \frac{2y}{|\Lambda_+ - \Lambda_-|}. \tag{B.8}
\]
From the above Eq. (B.8), it appears that for \( y = 0 \), we can never have a low maximum fractional error. One might think that this comes from the approximation 

\[
n(r; \omega) \approx n_{\text{avg}}(r) \text{ over the measured energy range which leads to the } \log \left| \frac{\omega - \Lambda}{\omega - \Lambda'} \right|,
\]

we note that this is more of a pathology. We will always have an energy value \( \omega' \) for which the calculated \( \text{Re}[G(r; r; \omega')] \) will equal zero, given by

\[
P\left[ \int_{\Lambda}^{\omega'} dx \frac{n(r; x)}{(\omega' - x)} + \int_{\omega'}^{\Lambda'} dx \frac{n(r; x)}{(\omega' - x)} \right] = 0 \quad \text{(B.9)}
\]

since \( n(r; x) \) is a positive definite function of energy \( x \), and \((\omega' - x)^{-1}\) changes sign at \( \omega' \). For such cases, the fractional error will always be large pathologically from any estimating procedure.

We also note that our approximation for the un-measured LDOS was quite drastic (all of the un-measured spectral weight at \( \Lambda_i \)). In a real experiment, we would expect the un-measured LDOS to have the un-measured spectral weight spread out over a bandwidth \( \approx W(r) \). Thus, for the pathological case mentioned above, the correct \( \text{Re}[G(r; r; \omega)] \) will also be close to zero. In a real application of the lifetime extraction scheme to an experiment, one might want to avoid such pathologies and only restrict the application of the scheme to energy ranges where the extracted \( \text{Re}[G(r; r; \omega)] \) is not close to zero.
B.2 Proof of Monotonic decay of $G_0(\vec{R}; \omega)$ for large $\vec{R}$

The proof uses the dimensional reduction described in Appendix A.2. In two dimensions, $G_0(\vec{R})$ on a lattice is given by the formula

$$G_0(\vec{R}; \omega) = \lim_{\delta \to 0^+} \frac{1}{(2\pi)^2} \int_{B.Z.} d\vec{k} e^{i\vec{k} \cdot \vec{R}} \frac{e^{i\delta - \epsilon(\vec{k})}}{\omega + i\delta - \epsilon(\vec{k})}$$

(B.10)

Let us look at the $k_y$ integral for a particular $k_x$. The denominator vanishes for certain values of $k_y$ thus motivating the conversion of the $k_y$ integral to a contour integral. The mapping $z = e^{ik_y}$ achieves the conversion which also maps the integral from $-\pi$ to $\pi$ to a contour integral over the unit circle. The periodicity of the integrand over the zone ensures the analyticity of the resulting complex integrand. Thus,

$$G_0(\vec{R}; \omega) = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} dk_x e^{i k_x R_x} \int_{-\pi}^{\pi} dk_y \frac{e^{i k_y R_y}}{\omega + i\delta - \epsilon(k_x, z)}$$

(B.11)

For a particular $\omega$ energy contour and $k_x$, we get an even number of poles (there are two poles if the contour is convex). Expanding the denominator around the poles gives us

$$\omega + i\delta - \epsilon(k_x, z) = -\frac{\hbar v_g(\omega, k_x)}{iz_p} (z - z_p (1 - \frac{\delta}{\hbar v_g(\omega, k_x)})).$$

(B.12)

The poles $z_p$s are defined by $\epsilon(k_x, z_p) = \omega$ and $\hbar v_g(\omega, k_x) \equiv \frac{\partial \epsilon(\vec{k})}{\partial k_y}$ is the group velocity along $y$ direction. We need only worry about the $(z - z_p)$ term in the expansion of the denominator since other expansion terms will yield zero residues. From the $(1 - \delta/\hbar v_g(\omega, k_x))$ factor in the expansion Eq. (B.12), we realize that the pole where the sign of the $\hbar v_g$, is same as the positive $\delta$ will be “pulled” inside the unit circle while the other pole will be “pushed” out of the unit circle. Thus, when we do $k_x$ integral, only one half of the $\omega$ energy contour (not to be confused with the complex contour; to distinguish we
will call $\omega$ contours as energy contours) will contribute to the integral. In the process, we have converted the 2D integral over the zone into an integral over part of the energy contour. Filling in the steps,

$$G_0(\vec{R}; \omega) = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} dk_x e^{ik_x R_x} \int_{U.C.} \frac{dz}{iz} \frac{z R_y}{iz_p} \left( z - z_p \left( 1 - \frac{\delta}{hv_g(\omega, k_x)} \right) \right)$$

$$= -\frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} dk_x e^{ik_x R_x} 2\pi i \frac{z R_y}{hv_g(\omega, k_x)}$$

$$= -\frac{1}{(2\pi)^2} 2\pi i \int dk_x e^{ik_x R_x} e^{ik_p(\omega, k_x) R_y}$$

$$= \frac{1}{2\pi i} \int_{\text{sgn}(\delta) = \text{sgn}(v_{gy}(\omega, s))} ds \frac{e^{i\tilde{k}(\omega, \vec{R})}}{|\nabla \epsilon(\tilde{k}(s, \omega))|}$$

(B.13)

where the last step was achieved by converting the element $dk_x$ to a variable $s$ parameterizing the contour of constant $\omega$, and we integrate over that part of the energy contour where the sign of $\delta$ is same as $v_{gy}$.

For large $\vec{R}$, i.e. far from impurity, we notice that the phase $e^{i\tilde{k}(\omega, \vec{R})}$ varies rapidly and thus the stationary phase approximation can be applied. The phase factor is stationary at points on the energy contour where the group velocity is along the $\vec{R}$ direction since $d(\vec{k}(s, \omega), \vec{R})/ds = \vec{R}.d\vec{k}(s, \omega)/ds = 0$ only when $\vec{R}$ is perpendicular to $d\vec{k}(s, \omega)/ds$ and $d\vec{k}(s, \omega)/ds$, being the tangent to the energy contour, is perpendicular to the group velocity. Therefore,

$$G_0(\vec{R}; \omega) = \frac{e^{i\pi/4}}{2\pi i} \frac{1}{|\nabla \epsilon(\tilde{k}_{\text{dom}}(\vec{R}, \omega))|} \sqrt{\frac{2\pi}{|\vec{R}||d^2 \tilde{k}(s, \omega)/ds^2|_{\tilde{k}_{\text{dom}}(\vec{R}, \omega)}}} e^{i\tilde{k}_{\text{dom}}(\vec{R}, \omega) \cdot \vec{R}}$$

(B.14)

where $\tilde{k}_{\text{dom}}(\vec{R}, \omega)$ is the $\tilde{k}$ corresponding to which the group velocity at energy $\omega$ is along $\vec{R}$ and, thus, is a function of $\vec{R}$ (only through $\hat{R}$) and $\omega$. For a convex dispersion function $\epsilon(\tilde{k})$, we will have only one $\tilde{k}_{\text{dom}}$ and thus

$$|G_0(\vec{R}; \omega)| \propto \frac{1}{\sqrt{|\vec{R}|}}$$

(B.15)
for large $\vec{R}$. This proves the monotonic decrease of $G_0(\vec{R}; \omega)$ when the lifetime is infinitesimal. When we have a finite lifetime due to self-energy processes, the propagator in momentum space looks like $\tilde{G}_0(\vec{k}; \omega) = (\omega + i\delta - (\epsilon(\vec{k}) + i\eta(\vec{k}, \omega)))^{-1}$ where the $\omega$ might have undergone a chemical potential shift, and the whole algebra in the above will go through similarly and we will get

$$|G_0(\vec{R}; \omega)| \propto \frac{1}{\sqrt{|\vec{R}|}} e^{-\frac{\eta(\vec{k}_{\text{dom}}(\vec{R}, \omega))}{\sqrt{\epsilon(\vec{k}_{\text{dom}}(\vec{R}, \omega))}}}$$

(B.16)

In one dimension, we only get the monotonic exponential decay for large $\vec{R}$. 

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B.3 Implementation of Cost Function for finding $G_0(R = 0; \omega)$

In this appendix, we show one example of the implementation of the Cost function defined in the main text. We show the profile of this Cost function as a function of $G_0(R = 0; \omega)$ guesses for the no-error case (which includes the numerical error incurred during two-dimensional Numerical Integration in Mathematica) and error-full cases in Fig. B.1. We show it as a matrix where the center point(6,6) corresponds to the correct $G_0(R = 0; \omega)$ and the (7,7)-entry corresponds to average over the $G(r, r; \omega)$ set (see next section). From point to point, we change the guess by $\text{Re}[\text{Avg}(G(r, r; \omega)) - G_0(R = 0; \omega)]$ along x-direction and $\text{Im}[\text{Avg}(G(R; \omega)) - G_0(R = 0; \omega)]$ along y direction. We see that in the no-error case, the Cost function has minimum at the correct value of $G_0(R = 0; \omega)$ (i.e., the (6,6)-entry in Fig. B.1a). In case of 0.1%, it does well to within $\text{Avg}(G(r, r; \omega)) - G_0(R = 0; \omega)$ (minima at (row 6, column 7)-entry in Fig. B.1b). In case of 0.5%, it starts to seriously deviate and the best guess then would be $\text{Avg}(G(r, r; \omega))$ (See Appendix B.4).
We recall that the T-matrix equation for scattering of point impurity is

\[
G(r, r'; \omega) = G_0(r, r'; \omega) + G_0(r, r_{\text{imp}}; \omega) \cdot T(\omega) \cdot G_0(r_{\text{imp}}, r'; \omega).
\]  

(B.17)

When we take the average of Eq. B.17 with \( r' = r \) over a window around the impurity, the data set is imagined to be taken on a spatial window around a point impurity,
the two terms on the right hand side average to (in two dimensions)

\[ \frac{1}{L^2} \sum_{r} G_0(0; \omega) = \left( \frac{2\pi}{L} \right)^2 \sum_{k} G_0(k; \omega) \]  

(B.18)

\[ \frac{1}{L^2} \sum_{r} G_0(r, 0; \omega) T(\omega) G_0(0, r; \omega) = \left( \frac{2\pi}{L} \right)^4 T(\omega) \sum_{k} G_0(k; \omega)^2 \]  

(B.19)

Thus, we see from the right hand sides above that the second term in Eq. (B.17) is \(1/L^2(1/L^d\) in \(d\) dimensions) suppressed compared to the first term, and if the window were infinite, the spatial average of \(G(r, r; \omega)\) would exactly equal \(G_0(0; \omega)\). For a finite but large enough window, it is a good guess for \(G_0(0; \omega)\).
B.5 Remark on Smoothness of Phase of $G_0(\vec{R}; \omega)$

We want to fix the phase of $G_0(\vec{R}; \omega)$ which we get by taking the square root of the equation

$$G_0(\vec{R}; \omega)^2 = \frac{G(r, r; \omega) - G_0(\vec{R} = 0; \omega)}{G(r = 0, r = 0; \omega) - G_0(\vec{R} = 0; \omega)} \ast G_0(\vec{R} = 0; \omega)^2. \quad (B.20)$$

Upon taking the square root, we get $G_0(\vec{R}; \omega)$ up to a phase of $e^{i\pi}$. To fix this phase, we note that the propagator in the continuum $G_0(\vec{R}; \omega)$ has to be a smooth well-behaved function for $\vec{R} \neq 0$. This is because it satisfies a differential equation, i.e. the Green’s function equations of motion for the Hamiltonian operator. Therefore its phase should also be a smooth and well-behaved as a function of $\vec{R}$. To see this, we start with the equation of motion for the non-interacting case in the continuum:

$$(i\partial/\partial t + \nabla^2/2m)G_{\text{non}}(x, t; x', t') = \delta(x - x')\delta(t - t') \quad (B.21)$$

which upon Fourier transforming with respect to time gives

$$(\zeta + \nabla^2/2m)G_{\text{non}}(x, x'; \zeta) = \delta(x - x') \quad (B.22)$$

For $x \neq x'$, the above differential equation has no ill-behaved term and thus $G_{\text{non}}(x, x'; \zeta)$ has to be a well-behaved differentiable function.

For the interacting case, the equations of motion are an infinite hierarchy of differential equations with the successive equations involving higher order Green’s functions (See Ref. [1]). It is not clear to the author, how one could extend the non-interacting argument to the interacting case. Instead, we argue as follows. As is usual in perturbation theory, the full propagator in momentum space satisfies a Dyson’s equation and is given by

$$\tilde{G}(\vec{p}, \zeta) = (\zeta - p^2/2m - \Sigma(\vec{p}; \zeta))^{-1}$$

where $\Sigma(\vec{p}; \zeta)$ is called the Self-energy and captures the effect of interactions. If this self-energy doesn’t change the analytic structure of $\tilde{G}(\vec{p}, \zeta)$ when compared to $\tilde{G}_0(\vec{p}, \zeta)$ (More precisely, the pole at $\zeta = p^2/2m$ from
the non-interacting case survives, though it will get shifted off the real axis), then upon Fourier transforming to real space, the differentiability of $G(x, x'; \zeta)$ will be preserved. Looking at Eq. (B.10)'s continuum version,

$$\nabla^2 G(\vec{R}; \omega) = \lim_{\delta \to 0^+} \frac{1}{(2\pi)^2} \int_{B.Z.} d\vec{k} \frac{|\vec{k}|^2 e^{i\vec{k}.\vec{R}}}{\omega + i\delta - |\vec{k}|^2/2m - \Sigma(\vec{k}; \omega)}$$  \hspace{1cm} (B.23)

and if the pole structure of the integrand is same with and without $\Sigma$, then the differentiability of $G_0(x, x'; \zeta)$ implies differentiability of $G(x, x'; \zeta)$. In the case of a lattice, $G_0(\vec{R}; \zeta)$ is well-behaved for $\vec{R} \neq 0$ and at $\vec{R} = 0$ there is a kink in its phase.

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B.6 Proof of Self-Energy Relation

In this section we prove that the relation between the electron and hole lifetimes,
\[
\eta_{\text{hole}}(-\omega) = -\eta_{\text{electron}}(\omega), \quad (B.24)
\]
where \( \eta(\omega) = \text{Im}[\Sigma(\omega)] \) (we have suppressed a possible momentum index).

We will do this using the 2x2 Matsubara formalism. In this formalism, the Green’s function for the non-lifetime broadened system in the normal state (i.e. no superconductivity) looks like
\[
G_0(k; i\omega_n)^{-1} = \begin{pmatrix}
  i\omega_n - \epsilon(k) & 0 \\
  0 & i\omega_n + \epsilon(k)
\end{pmatrix} \quad (B.25)
\]
where \( \omega_n = (2n + 1)\pi T \) is the fermionic Matsubara frequency.

We will first prove Eq. B.24 in the case of the normal electrons coupled to phonons. The self-energy in this case looks like
\[
\Sigma(\vec{k}; i\omega_n) = -\frac{T}{N_L} \sum_{\vec{p},\Omega_m} g(\vec{k} - \vec{q}, \vec{q}) g(\vec{k}, -\vec{q}) D(\vec{q}; i\Omega_m) \tau_3 G_0(\vec{k} - i\vec{q}; i\omega_n - i\Omega_m) \tau_3 \quad (B.26)
\]
where \( \Omega_m = 2m\pi T \) is the bosonic Matsubara frequency, \( \tau_3 \) is the third component of Pauli matrices in the Nambu space, \( D(\vec{q}; i\Omega_m) \) is the fourier-transform of the phonon’s Green’s function \( D(\vec{q}; \tau) = -< T_r[A(\vec{q}; \tau)A(-\vec{q}; 0)] \) (\( T_r \) is the usual time ordering operator) and evaluates
\[
D(\vec{q}; i\Omega_m) = \frac{1}{2} \left( \frac{1}{i\Omega_m - \Omega(\vec{q})} - \frac{1}{i\Omega_m + \Omega(\vec{q})} \right) \quad (B.27)
\]
where \( \Omega(\vec{q}) \) is the phonon dispersion. It has the following property : \( D(\vec{q}; i\Omega_m) = D(\vec{q}; -i\Omega_m) \). The \( g(\vec{k}, \vec{q}) \) is the electron-phonon coupling strength coming from the electron-phonon interaction term
\[
H_{\text{el-ph}} = \frac{1}{N_L} \sum_{\vec{k},\vec{q},\sigma} g(\vec{k}, \vec{q}) c^\dagger_{\vec{k}+\vec{q},\sigma} c_{\vec{k},\sigma} A_{\vec{q}}. \quad (B.28)
\]
Using the property $D(\vec{q}; i\Omega_m) = D(\vec{q}; -i\Omega_m)$ and $\Omega_{-m} = -\Omega_m$, we can show that (suppressing momenta indices)

\[
\Sigma_{22}(-i\omega_n) \propto \sum_{\Omega_m} \frac{D(\Omega_m)}{-i\omega_n - i\Omega_m + \epsilon} = \ldots + \frac{D(\Omega_{-1})}{-i\omega_n - i\Omega_{-1} + \epsilon} + \frac{D(\Omega_0)}{-i\omega_n + \epsilon} + \frac{D(\Omega_1)}{-i\omega_n - i\Omega_1 + \epsilon} + \ldots
\]

\[
= \ldots + \frac{-D(\Omega_{-1})}{i\omega_n + i\Omega_{-1} - \epsilon} + \frac{i\omega_n - \epsilon}{i\omega_n + i\Omega_1 - \epsilon} + \frac{-D(\Omega_0)}{i\omega_n - \epsilon} + \frac{-D(\Omega_1)}{i\omega_n - i\Omega_1 - \epsilon} + \ldots
\]

\[
= \ldots + \frac{-D(\Omega_{-1})}{i\omega_n - i\Omega_1 - \epsilon} + \frac{i\omega_n - \epsilon}{i\omega_n - i\Omega_1 - \epsilon} + \frac{-D(\Omega_0)}{i\omega_n - \epsilon} + \frac{-D(\Omega_1)}{i\omega_n - i\Omega_1 - \epsilon} + \ldots
\]

\[
= -\sum_{\Omega_m} \frac{D(\Omega_m)}{i\omega_n - i\Omega_m - \epsilon} \propto -\Sigma_{11}(i\omega_n) \tag{B.29}
\]

Thus, by analytic continuation, $\Sigma_{22}(z) = -\Sigma_{11}(z)$ where $\Sigma_{22}$ and $\Sigma_{11}$ are the hole and electron self-energies respectively. Thus when we analytically continue till $z = \omega + i\delta$ where $\omega$ is real, we see that $\Sigma_{22}(-\omega - i\delta) = -\Sigma_{11}(\omega + i\delta)$. From the analytic properties of Self-energy $\Sigma(\vec{p}; \omega \pm i\delta) = \delta\mu(\vec{p}; \omega) \mp \frac{i}{\epsilon} \eta(\vec{p}; \omega)$ (see e.g., Eqn. 82 in Ref. [1]), we conclude that

\[
\eta_{\text{hole}}(-\omega) = -\eta_{\text{electron}}(\omega) \ldots \text{QED} \tag{B.30}
\]

Also, the chemical potential shift is equal for both holes and electrons. This proof can be extended to higher orders in the electron-phonon coupling by noticing that all higher order terms contributing to self-energy contain odd number of fermion propagators, thus allowing the same kind of manipulation done above to go through analogously. This proof extends to other bosonic modes (e.g., spin wave modes) too since their propagators also satisfy $D(\vec{q}; i\Omega_m) = D(\vec{q}; -i\Omega_m)$. This proof also extends to the case of lifetime broadening induced by electron-electron interaction by the same token that the self-energy terms always have odd number of fermion propagators.
BIBLIOGRAPHY

APPENDIX C
APPENDICES FOR CHAPTER 4

C.1 Matsubara Sum for the Self Energy

In this appendix, we explicitly show the algebra behind the Matsubara summation that leads from Eq. 4.5 to Eq. 4.6 in the main chapter.

We start with Eq. 4.5,

$$
\Sigma(\vec{k}; i\omega_n) = -\frac{T}{N_L} \sum_{\vec{q}, m} g^2 D(i\Omega_m)\tau_3 G_0(\vec{k} - \vec{q}; i\omega_n - i\Omega_m)\tau_3
$$

$$
= -\frac{g^2}{N_L} \sum_{\vec{q}, m} \frac{1}{2} \left( \frac{1}{i\omega_n - i\Omega_m - \Omega_0} - \frac{1}{i\omega_n - i\Omega_m + \Omega_0} \right) \times \left( \frac{1}{(i\omega_n - i\Omega_m)^2 - E(\vec{q})^2} \right)
$$

$$
\times \begin{pmatrix}
i\omega_n - i\Omega_m + \epsilon(\vec{q}) & -\Delta(\vec{q}) \\
-\Delta(\vec{q})^* & i\omega_n - i\Omega_m - \epsilon(\vec{q})
\end{pmatrix}
$$

(C.1)

The Matsubara summation trick involves re-writing the above as

$$
\Sigma(\vec{k}; i\omega_n) = -\frac{g^2}{N_L} \sum_{\vec{q}, m} \frac{1}{2\pi} \oint dz \frac{1}{2} \left( \frac{1}{z - \Omega_0} - \frac{1}{z + \Omega_0} \right) \times \left( \frac{1}{(i\omega_n - z)^2 - E(\vec{q})^2} \right)
$$

$$
\times \begin{pmatrix}
i\omega_n - z + \epsilon(\vec{q}) & -\Delta(\vec{q}) \\
-\Delta(\vec{q})^* & i\omega_n - z - \epsilon(\vec{q})
\end{pmatrix} \times \frac{1}{e^{\frac{\epsilon(\vec{q})}{T}} - 1}.
$$

(C.2)

Since, the poles of $1/(e^{\epsilon(\vec{q})/T} - 1)$ are located at the bosonic Matsubara frequencies $\Omega_m = 2\pi m T$, therefore the contour integral in Eq. C.2 over the contour shown in the Fig. C.1 a) is the same as the summation in Eq. C.1. Now, the contour in Fig. C.1 a) can be deformed continuously into the contour shown in Fig. C.1 c) without crossing any poles via Fig. C.1 b). The poles enclosed by the new contour are at $z = \pm \Omega_0$ and $z = (i\omega_n \pm E(\vec{q}))$ where $E(\vec{q}) = \sqrt{\epsilon(\vec{q})^2 + \Delta(\vec{q})^2} > 0$. Therefore, the contour integral over
Figure C.1: a) The contour is composed of the small circles enclosing the poles of $1/(e^{\Omega/T} - 1)$ situated at the bosonic Matsubara frequencies $\Omega_m = 2\pi m T$. The un-circled pole represents pole/s due to the rest of the integrand in Eq. C.2. b) The contour in a) can be continuously deformed to the contour shown in b) without crossing any poles, since the contribution at infinity is zero. c) The contour in b) can further be trivially deformed now to enclose the previously un-circled pole in a).

the new contour now captures the residues of these poles and in the limit $T \rightarrow 0$, we get

$$\Sigma(\vec{k}; i\omega_n) = -\frac{ig^2}{2N_L} \sum_{\vec{q}} \frac{1}{(i\omega_n + \Omega)^2 - E(\vec{q})^2} \begin{pmatrix} i\omega_n + \Omega + \epsilon(\vec{q}) & -\Delta(\vec{q}) \\ -\Delta(\vec{q}) & i\omega_n + \Omega - \epsilon(\vec{q}) \end{pmatrix}$$

$$+ \frac{\Omega}{(i\omega_n - E(\vec{q}))^2 - \Omega^2} \begin{pmatrix} 1 + \frac{\epsilon(\vec{q})}{E(\vec{q})} & -\frac{\Delta(\vec{q})}{E(\vec{q})} \\ -\frac{\Delta(\vec{q})}{E(\vec{q})} & 1 - \frac{\epsilon(\vec{q})}{E(\vec{q})} \end{pmatrix}. \quad \text{(C.3)}$$

Upon analytically continuing to the real axis, we get to the desired Eq. 4.6.
C.2 Calculation of $g(E')$

In this appendix, we calculate the density of states $g(E')$ or the number of states between $E'$ and $E' + dE'$ divided by $dE'$. The constant-$E'$ curves are given by $E' = x^2 - y^2$. To calculate $g(E')$, we start by calculating the number of states $N(E')$ from 0 to $E'$ and then differentiate it with respect to $E'$. $N(E')$ is equal to the area enclosed by the “hyperbola” as shown in fig. C.2.  

Figure C.2: In this schematic, the shaded area represents the number of states from 0 to $E'$

---

1 It is in this calculation of the area that a different choice of cut-offs would lead to messiness. With unequal cut-offs, one would no longer have a square region of integration (see Fig. C.2) with the zero contour passing through the diagonal. Instead, one would have a rectangular region of integration with the zero contour not passing through the diagonal. Even with this choice of rectangular region, one can convince that for energies close enough to zero contour, the error in the area calculated systematically goes down to zero.
Therefore, the area enclosed is

\[
N(E') = 4\left[\frac{(v'_x + v'_y)K^2}{2} - \int_{E'} \sqrt{v'_x + v'_yK} \sqrt{x^2 - E'dx}\right]
\]

\[
= -E'\log\left[\frac{E'}{4(v'_x + v'_y)K^2}\right] + \text{terms regular at } E' = 0
\]

\[
= -E'\log\left[\frac{E'}{4(\sqrt{v'_x v'_y})K_xK_y}\right] + \text{terms regular at } E' = 0 \quad (C.4)
\]

which implies that

\[
g(E') = -\log\left[\frac{E'}{4(\sqrt{v'_x v'_y})K_xK_y}\right] + \text{terms regular at } E' = 0. \quad (C.5)
\]