To my parents
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A-2 Diagrams involving scattering within the second band. 122
In this dissertation, I present the results of theoretical investigations of the effect of fluctuations, disorder and inhomogeneity in unconventional superconductors. Copper oxide based and iron pnictide based high temperature superconductors are the systems of primary interest. Both the materials have been subject of massive experimental and theoretical investigations since their discovery. The mechanism of superconductivity is one of the most challenging problems of contemporary physics, and it is hoped that by comparing the two classes of materials one can gain insight into this question. Both materials have many similarities, yet they are different. Both the materials are layered compounds and have intimate relation with antiferromagnetism, but the electronic structure is fundamentally different. Copper oxide based superconductors have only one band near the Fermi surface, while iron pnictides are multiband systems.

Most of these materials are intrinsically dirty, since they become superconductors when doped with either electrons or holes. There is substantial evidence from experiments that these systems have extremely anisotropic order parameters in contrast with conventional superconductors like Sn or Hg. Such an anisotropy in the order parameter makes disorder a very important parameter in the problem. Additional complexity comes in iron pnictides due to the multiple bands and orbitals involved. In this dissertation, I discuss the results of our work on disorder in multiband systems in the context of iron pnictides. We calculate the low temperature transport properties and
spectral properties in the presence of disorder for models appropriate to various iron pnictides, and compare our results with experiments.

Another aspect of these materials is inhomogeneity. Especially in copper oxide based superconductors, scanning tunneling spectroscopy measurements have revealed nanoscale inhomogeneity in the order parameter. Some researchers have argued that these inhomogeneities may play a crucial role in mechanism of pairing. We study a simple toy model to gain some understanding about the correlation between inhomogeneity and superconductivity. The normal states of these materials represent an equally interesting and challenging problem as the superconducting state. The fluctuations of the order parameter above the transition temperature can significantly affect the normal state properties. In copper oxide based superconductors, disconnected Fermi surfaces have been observed in experiments. We study the effect of d-wave order parameter fluctuations above the critical temperature for model systems relevant to copper oxide materials, and try to relate them to the observed normal state electronic structure.
CHAPTER 1
INTRODUCTION

1.1 Historical Background

On April 08, 1911, Kamerlingh Onnes discovered that below 4.2K the electrical resistivity of pure mercury abruptly becomes unmeasurable. This effect, now known as “superconductivity”, has attracted the attention of many physicists for roughly a century [1–3]. Nearly four decades after the discovery, Ginzburg and Landau proposed a phenomenological theory based on Landau’s general theory of second order phase transitions. They introduced the density of superconducting electrons as an order parameter. Nearly 50 years after Onnes’s discovery, in 1957, Bardeen, Cooper and Schrieffer proposed the famous microscopic pairing theory of superconductivity (BCS theory) [4]. They showed that even a small attraction between electrons mediated by phonons makes the normal state unstable and this leads to formation of pairs of electrons with opposite spin and momentum (“Cooper pairs”). The key prediction of this model was the formation of an energy gap in the quasi-particle excitation spectrum. This theory also predicted that the ratio of this gap to the transition temperature \( T_c \) is 1.76 and the ratio of specific heat jump at the transition to the normal state value is 1.43, in agreement with experiments. The BCS model provided a basic framework to calculate different physical quantities. The quest for the superconductors with higher transition temperature continued for many years, and a major breakthrough came in 1986, when Bednorz and Mülller discovered superconductivity in La\(_{2-x}\)Ba\(_x\)CuO\(_4\) (“LBCO”) at 35K [5]. The parent compound La\(_2\)CuO\(_4\) is an insulator and becomes superconducting when doped either with holes or with electrons. Very quickly, other groups found superconductivity in YBa\(_2\)Cu\(_3\)O\(_{7-\delta}\) (“YBCO”), Ba\(_2\)Sr\(_2\)CaCu\(_2\)O\(_{8+\delta}\) (“BSCCO”) and Tl\(_2\)Sr\(_2\)CaCu\(_2\)O\(_{8+\delta}\) (“TBCCO”) and \( T_c \) crossed the value of 150K, much higher than the temperature of liquid nitrogen. The common ingredient in all these superconductors is the CuO\(_2\) plane and it is widely accepted that these planes are crucial for superconductivity.
Due to the presence of these CuO$_2$ planes, these materials are collectively known as cuprates. In 2008, a new class of iron based superconductors ("pnictides") was discovered, with a general formula ROFFePn (1111 family). Here R is a rare earth element and Pn is element from pnictogen group [6]. The Sm based superconductor shows an onset $T_c = 55$K, which is highest among non-cuprate superconductors. These systems also have layers of Fe with a pnictogen on top and bottom of it alternatively. Soon after the discovery of the of 1111 family, superconductivity was observed in a BaFe$_2$As$_2$ based compound (122 family) [7, 8], in FeSe [9, 10] and LiFeAs [11].

1.2 Cuprates: Overview

The parent compounds of all cuprates are antiferromagnetic insulators and become superconductors upon hole and electron doping. First $T_c$ increases with doping, attains a maximum value and then starts to decrease and eventually disappears. Figure 1-1 shows the schematic phase diagram for cuprates [12–14]. With doping of holes, the long range antiferromagnetic phase disappears and superconductivity emerges. Although there is no consensus regarding the pairing mechanism, it is well established that it is not phonon mediated. Cuprates are very different from conventional superconductors. The key difference is a momentum dependent superconducting order parameter. It is well established now that the order parameter, or Cooper pair wave function, has d-wave symmetry [12], which means the order parameter becomes zero at some points in k-space. These points are called “nodes”, and the points with maximum value of order parameters are known as “anti-nodes”. So the presence of these nodal points makes the minimum energy to excite a quasiparticle zero, hence the superconductors are “gapless”. This leads to completely different behavior of low temperature thermodynamic and transport properties. Apart from anisotropic order parameter, another difference is a large energy gap compared to the conventional superconductors. In cuprates, $\Delta / T_c$ is much larger than the weak coupling BCS value of 2.15 for a d-wave order parameter. The maximum $T_c$ occurs at doping of roughly 0.16 holes per CuO$_2$ plane.
This optimal value of doping separates the underdoped and overdoped regimes in the phase diagram. The normal state of the cuprate superconductors is also very interesting. The underdoped cuprates show a “pseudo-gap” phase in the normal state, where the Fermi surface is partially gapped even in the normal state. Angle resolved photo emission spectroscopy (ARPES) experiments have found disconnected Fermi surfaces, which are now known as “Fermi-arcs” [16–18]. The presence of an energy gap on the Fermi surface leads to poor metallic behavior in transport measurements [19, 20]. In different experimental probes this energy gap starts to appear at a slightly different temperatures. This temperature is usually denoted as $T^*$, and it is still not clear whether it is associated with a second order phase transition or not [20, 21]. A systematic doping
dependent study of the Nernst effect has revealed that fluctuations in superconducting channel are not related with this pseudo-gap temperature $T^*$ [22]. Recent polarized neutron scattering measurements [23, 24] and polar Kerr effect experiments [25] have found evidence for a novel magnetic phase and broken time reversal symmetry below a temperature scale similar to $T^*$. There are many models proposed for this phase. One school of thought believes in the presence of competing orders [26, 27], while some people think of this phase as a reflection of pair fluctuations. The idea of pair fluctuations is based on preformed pairs above $T_c$, which leads to reduction of the single particle density of states. Emery and Kivelson have argued that in the bad metals, fluctuations prevent long range order [28]. They proposed that the pseudogap is a phase with preformed pairs, but without phase coherence. Their theory correctly gives the linear relation between the superfluid density and $T_c$, which is observed in many experiments on underdoped cuprates [29]. For the phase coherence, they define a phase ordering temperature,

$$T_\theta = A \frac{\hbar^2 n_s \ell}{4m^*},$$

(1-1)

where $n_s$ is the superfluid density at zero temperature, $m^*$ is the effective mass, $\ell$ is a length scale and $A$ is a model dependent constant of order 1. If $T_\theta \approx T_c$ then phase fluctuations become very important. In underdoped cuprates, the superfluid density is very small. Table 1-1 shows the ratio of $T_\theta/T_c$ for some systems. For the unconventional superconductors it is close to 1, while in the conventional superconductors it is very large. In Chapter 6, I discuss the role of fluctuations in detail, and use $T_c/T_\theta$ as a perturbation parameter.

Next to this pseudo-gap phase is the “strange metal” phase, where resistivity is linear in temperature from temperatures of few Kelvin to a thousand Kelvin [20] and on the overdoped side normal state is apparently a conventional Fermi liquid. The crossover between the strange metal phase and Fermi liquid phase is illustrated by a dotted line with a question mark in Fig. 1-1. The question mark on the dotted line is
Table 1-1. Phase ordering temperature $T_\theta$ and penetration depth $\lambda_c$ in different superconductors.

<table>
<thead>
<tr>
<th>Material</th>
<th>$\lambda_c$ in nm</th>
<th>$T_c$ in K</th>
<th>$T_\theta / T_c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pb</td>
<td>39</td>
<td>7</td>
<td>$2 \times 10^5$</td>
</tr>
<tr>
<td>Nb$_3$Sn</td>
<td>64</td>
<td>18</td>
<td>$2 \times 10^3$</td>
</tr>
<tr>
<td>Tl$_2$Ba$<em>2$CuO$</em>{6+\delta}$</td>
<td>200</td>
<td>80</td>
<td>2</td>
</tr>
<tr>
<td>Bi$_2$Sr$_2$CaCu$_2$O$_8$</td>
<td>185</td>
<td>84</td>
<td>1.5</td>
</tr>
<tr>
<td>La$_{2-x}$Sr$<em>x$CaCuO$</em>{4+\delta}$</td>
<td>370</td>
<td>28</td>
<td>1</td>
</tr>
<tr>
<td>YBa$_2$Cu$_2$O$_8$</td>
<td>260</td>
<td>80</td>
<td>0.7</td>
</tr>
<tr>
<td>Ba$_{1-x}$K$_x$Fe$_2$As$_2$</td>
<td>$\sim 1350$</td>
<td>38</td>
<td>$\sim 0.5$</td>
</tr>
</tbody>
</table>

to indicate current experimental ambiguity about the crossover. The superconducting state on the overdoped side is qualitatively similar to a mean field $d$-wave, but the same physics in the underdoped regime deviates significantly from a mean field superconductor. The energy scale associated with the superconductivity is not homogeneous over a nanometer length scale at least in some systems. Tunneling experiments have revealed nanoscale inhomogeneity in these materials and observed stripe and checkerboard like patterns in tunneling conductance [30]; the origin of these inhomogeneities are not understood. Some researchers believe that these inhomogeneities are not intrinsic and caused by dopant atoms [31], but many have argued that this might play a important role in pairing and high transition temperature. We have considered a simple toy model to study the effect of inhomogeneity, which is discussed in chapter 2.

1.3 Pnictides: Overview

Despite many similarities with cuprates, Fe pnictides are fundamentally different. The phase diagrams of cuprates are qualitatively similar for all families, but for pnictides different families show very different phase diagrams. Some parent compounds are antiferromagnetic metals with $(\pi, 0)$ ordering, on doping the transition temperature to the antiferromagnetic phase ($T_{SDW}$) decreases. Some systems go through a structural
transition before the ($\pi, 0$) spin density wave (SDW) transition. In some systems, the SDW phase disappears before emergence of the superconductivity \cite{32, 33} and in some systems SDW and superconductivity co-exist up to some doping \cite{34, 35}. There are a few stoichiometric superconductors like LaFePO \cite{6} and LiFeAs \cite{11} with similar electronic structure to LaFeAsO. Unlike other pnictides, the normal state of these compounds is nonmagnetic. Figure 1-2 shows the phase diagrams for various materials.
In case of LaFeAsO, magnetic order abruptly disappears as the superconducting phase onsets. In CeFeAsO, the magnetic phase disappears smoothly before the emergence of the superconductivity. For SmFeAsO and Co doped BaFe$_2$As$_2$, SDW and superconductivity coexist in a small region of phase diagram. Another key difference between Fe-based superconductors and cuprates is the electronic structure. There is more than one band near the Fermi surface with both electron and hole like dispersions. There are two hole like Fermi sheets centered at the $\Gamma$ point and electron like Fermi sheets are located at the $M$ point. The electronic structure is very sensitive to the height of pnictogen atom above Fe plane and plays a very important role in the transition temperature [36, 37]. Figure 1-3 illustrates the Fermi surface of BaFe$_2$As$_2$. The outer hole sheet centered at the $\Gamma$ point shows significant dispersion along the ‘c’ axis. This three dimensional nature is unique to the 122 family. The 1111 family is more like the cuprates in terms of the dimensionality, but the 122 systems are more three dimensional [38–40]. This difference in the dimensionality is reflected in the transport properties of two families in the normal and the superconducting state [41–44]. Theoretical investigation of the superconducting state for the 1111 family predict a sign changing s-wave state between electron and hole pocket [45–47]. Some groups have found very anisotropic gap structures on the electron sheets, potentially leading to gap
nodes. These nodes are referred as “accidental” because they are due to the details of the pairing interaction rather than being required by symmetry. In addition, a three dimensional nodal gap structure has been suggested \[40, 48\]. In chapter 4 and 5, I discuss the phenomenological models of the gap structure to explain some of the experimental data. The symmetry of the order parameter is still an unsettled issue. Some experiments suggest a fully gapped system and some find signatures of low lying excitations. The presence of multiple bands makes data analysis more complicated, because in most of the experiments measured quantities represent sums over all bands.

Many of the materials are intrinsically dirty and sample quality has improved slowly. In multiband systems, disorder plays a very crucial role. Disorder can scatter between and within the bands, such that the relative strength of interband and intraband disorder is a very important parameter in such systems. According to the Anderson theorem, in an isotropic s-wave superconductor, nonmagnetic impurity scattering is not pairbreaking \[49\], but in a sign changing ± s-wave system the presence of finite interband nonmagnetic disorder can produce pairbreaking \[50–52\]. Allen has showed that an anisotropic superconductor is mathematically equivalent to a multiband superconductor, hence it is not violation of the Anderson’s theorem \[53, 54\]. The effect of impurity scattering has been included within the extended framework of Abrikosov-Gorkov theory \[55, 56\] in the same formalism used by Allen, where the momentum summation is performed over each individual band \[54\]. In chapter 3, I discuss the formalism of the multiband problem in detail. In pnictides, the role of disorder can not be ignored to understand the experimental data. In chapter 3, I focus on the effect of disorder on the critical temperature and spectral function, in chapter 4, I discuss the effect of disorder on the low temperature thermal conductivity for the models relevant to the 1111 and the 122 families of pnictides. In chapter 5, I present our study of low temperature penetration depth for the models introduced in chapter 4. Finally, in chapter 6, I discuss the effect of d wave superconducting fluctuation above the transition.
CHAPTER 2
INHOMOGENEOUS PAIRING

Most of this chapter has been published as “Sublattice model of atomic scale pairing inhomogeneity in a superconductor,” Vivek Mishra, P. J. Hirschfeld and Yu. S. Barash, Phys. Rev. B 78, 134525 (2008).

2.1 Motivation

Recently, scanning tunneling spectroscopy (STS) experiments have observed inhomogeneity in the local density of states (LDOS) of cuprates, which has been related to the presence of an inhomogeneous energy scale [30]. Inelastic neutron scattering measurements have also found signatures of spin and charge density waves [57]. The origin of these inhomogeneities is not yet clear. Some researchers believe that these inhomogeneities come from the process of self organization due to competing orders [58], while some others attribute this to disorder induced by random distribution of dopant atoms [31, 59, 60]. Many theoretical investigations have argued that these inhomogeneities can play a crucial role in the mechanism of pairing, which leads to such high critical temperature [61–63]. Martin et al. studied a Hubbard model with an effective inhomogeneous pairing potential in the weak coupling BCS framework. A one dimensional periodic modulation in pairing potential was included with modulation length scale \( \ell \gg a \), where \( a \) is the lattice spacing. They found enhancement of the critical temperature and the maximum increase in \( T_c \) was obtained for \( \ell \sim \zeta_0 \), where \( \zeta_0 \) is the coherence length for the homogeneous system. In a similar work by Loh et al. [64], a two dimensional XY model was studied, with nearest neighbor coupling and including inhomogeneity in the exchange term by adding a periodic modulation. They found a monotonic enhancement of the Berezinskii-Kosterlitz-Thouless transition temperature \( (T_{BKT}) \) [65, 66] with increasing modulation length scale, but at the cost of reduction in superfluid stiffness. \( T_{BKT} \) is the ordering temperature for pure two dimensional systems, where long range order in the thermodynamic limit is forbidden [67], but order can occur
at length scales much larger than the sample length scales. Aryanpour et al. [68, 69] studied an attractive Hubbard model on square lattice with checkerboard, stripe and random patterns of pairing potential for an order parameter with s wave symmetry, within a mean field approximation, and found superconducting and charge density wave ground states. They also found enhancement of $T_c$ for certain value of doping for inhomogeneous distribution of the pairing potential in comparison with homogeneous systems.

In connection with the STM experiments, Nunner et al.[31] considered a model for $d$ wave superconductor, with variation of the pairing potential induced by dopant atoms over a unit cell length scale and explained the correlation between measured local gap and many observables in $\text{Ba}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$. Maška et al. [70] have shown that a disorder induced shift of atomic levels also enhances the pairing potential for a single band Hubbard model. Recently, Foyevtsova et al. have found similar results for a three-band Hubbard model, which is appropriate for cuprates [71]. In complex materials such as layered HTSC or pnictides with large unit cells, the pairing interaction can vary within a unit cell. Hence understanding the correlation between inhomogeneity and superconductivity is very important. Real systems are very difficult to handle even numerically, so the study of simple model Hamiltonian is very useful to gain understanding of inhomogeneous pairing. Earlier studies [62, 64, 68, 69] were done using purely numerical methods, but in such methods it is sometimes difficult to draw simple qualitative conclusions. Here we consider a simple “toy” model on a bipartite lattice in two dimensions with two different values of effective coupling constant $g$ on two interpenetrating sublattices as shown in Figure 2-1. Montorsi and Campbell [72] have found a superconducting ground state on a bipartite lattice in arbitrary dimension with an attractive homogeneous pairing interaction. In our study, we calculate the ground state properties of this system for any values $(g_A, g_B)$, where $A$ and $B$ represent the two sublattices. We consider two possible cases, first when both the sublattices have
Figure 2-1. Unit cell of square lattice, where squares and circles denote sites of type 'A' and 'B', and the lattice spacing is denoted by 'a', which we have set to 1. The coordinate system used in the Fourier transformation is shown with two dashed lines.

attractive interaction \((g_A, g_B > 0)\) and a second case with a mixture of attractive and repulsive interactions \((g_A, -g_B > 0)\). This is reminiscent of calculations in the context of impurities in \(d\) wave superconductor, where models with abrupt sign change in the pairing interaction have been studied [73, 74]. In next section, I discuss the details of the various models and approaches.

2.2 Model

The Hamiltonian on the bipartite square lattice is given by Eq. (2–1), where \(c_i, c_i^\dagger\) are the electron annihilation and creation operators on site \(i\). We restrict ourselves to nearest neighbor hopping between the sites with hopping energy \(t\) and with only on site pairing \(\Delta_i\), which is the mean field order parameter at \(i^{th}\) site. The sum in the Eq. 2–1 is over all sites and spins denoted by \(\sigma\). We consider isotropic \(s\) wave pairing and the case of half-filling, for which the chemical potential \(\mu\) is set to zero.
\begin{equation}
H = \sum_{i,\delta,\sigma} -tc^\dagger_{i,\sigma}c_{i+\delta,\sigma} + (\Delta_i c^\dagger_{i,\sigma}c^\dagger_{i,-\sigma} + h.c.),
\end{equation}

The Hamiltonian can be expressed as a matrix in Fourier space spanned by the staggered Nambu basis \( \tilde{c}_k = (c^A_{-k\sigma}, c^B_{-k\sigma}, c^A_k, c^B_k) \),

\begin{equation}
H = \sum_k \tilde{c}^\dagger_k M \tilde{c}_k,
\end{equation}

with

\begin{equation}
M = \begin{bmatrix}
0 & \xi_k & \Delta^A & 0 \\
\xi_k & 0 & 0 & \Delta^B \\
\Delta^A & 0 & 0 & -\xi_k \\
0 & \Delta^B & -\xi_k & 0
\end{bmatrix},
\end{equation}

where the dispersion relation is given by,

\begin{equation}
\xi_k = -4t \cos\left(\frac{k_x}{\sqrt{2}}\right) \cos\left(\frac{k_y}{\sqrt{2}}\right)
\end{equation}
in the reduced Brillouin zone. After diagonalizing the Hamiltonian, we find the quasiparticle energies \( \pm E_{1,2} \),

\begin{equation}
E_{1,2} = \frac{\mp \Delta^A \pm \Delta^B + \sqrt{(\Delta^A + \Delta^B)^2 + 4\xi_k^2}}{2},
\end{equation}

which reduce to the usual \( E_k = \sqrt{\xi_k^2 + \Delta^2} \) for \( \Delta^\alpha \rightarrow \Delta \). Self-consistent gap equations for the gaps on each sublattice are

\begin{align}
\Delta^A &= g^A \sum_k \left\{ -\frac{x_1^2}{x_1^2 + 1} \tanh\left(\frac{\beta E_1}{2}\right) + \frac{x_2^2}{x_2^2 + 1} \tanh\left(\frac{\beta E_2}{2}\right) \right\}, \\
\Delta^B &= g^B \sum_k \left\{ \frac{1}{x_1^2 + 1} \tanh\left(\frac{\beta E_1}{2}\right) + \frac{-1}{x_2^2 + 1} \tanh\left(\frac{\beta E_2}{2}\right) \right\},
\end{align}

where \( x_{1/2} \) are the parameters, defined as

\begin{equation}
x_{1,2} = \frac{\mp (\Delta^A + \Delta^B) + \sqrt{(\Delta^A + \Delta^B)^2 + 4\xi_k^2}}{2\xi_k}.
\end{equation}
Figure 2-2. Critical temperature $T_c / t$ plotted vs. difference of sublattice coupling constants $\delta \equiv (g^A - g^B)$. Red curve: window density of states. The average value over the unit cell $\bar{g}$ is $t$. Blue curve: exact.

In our convention, a positive $g$ corresponds to an attractive on-site interaction. ‘$\beta$’ is $(k_B T)^{-1}$, where Boltzmann’s constant ‘$k_B$’ is set to 1. For obtaining the analytical results, we estimate the integrals involved using the approximate window density of states (wDOS).

$$\rho(\omega) = \begin{cases} 1/8 t & -4 t \leq \omega \leq 4 t, \\ 0 & \text{elsewhere} \end{cases}$$

which is a good approximation for the tight binding model for qualitative purposes [75, 76]. This problem is also equivalent to a two band superconductor with an electron and a hole band. Using the wDOS, we calculate many properties analytically and compare with full numerical calculation. The difference in the pairing potentials $(\delta \equiv g^A - g^B)$ of two sublattices is the parameter that controls the inhomogeneity. For a homogeneous system, $\delta$ is zero. The average value of pairing potential ($\bar{g}$) is kept constant in order to enable us to separate the effect of the inhomogeneity from the trivial effects arising from changing the overall pairing strength.
2.3 Critical Temperature

To calculate $T_c$, we linearize the gap equations in $\Delta^a$ and solve the system of two equations for the maximum eigenvalue. Within the window approximation,

$$k_B T_c \approx \left( \frac{8 t \gamma}{\pi} \right) \exp \left[ -\frac{8 t (g^A + g^B) - (8t)^2}{4 g^A g^B - 8 t (g^A + g^B)} \right]$$

$$= \left( \frac{8 t \gamma}{\pi} \right) \exp \left[ -\frac{16 t \bar{g} - 64 t^2}{4 \bar{g}^2 - \delta^2 - 16 t \bar{g}} \right],$$

(2–9)

(2–10)

where $\gamma (= 0.577)$ is Euler’s constant. Fig. 2-2 shows the critical temperature as a function of inhomogeneity parameter $\delta$, all energy scales are normalized to the hopping energy $t$. The qualitative behavior of the full numerical solution and the wDOS approximation is similar, but there is a big quantitative difference. This difference is due to the van Hove singularity at the Fermi energy for a simple 2D tightbinding dispersion, but the enhancement of the critical temperature with increasing inhomogeneity is in agreement with previous studies. For small inhomogeneity, we get

$$\frac{T_c}{T_{c \text{ homo}}} = 1 + \left( \frac{\delta}{2 \bar{g}} \right)^2 \left[ \ln \left( \frac{8 t \gamma}{\pi k_B T_{c \text{ homo}}} \right) \frac{1}{4 t / \bar{g} - 1} \right].$$

(2–11)

Here $T_{c \text{ homo}}$ is the transition temperature for the homogeneous case and in the physical range that we consider here the average value of interaction $\bar{g}$ is always smaller than the bandwidth $4t$, which is the largest energy scale in the problem.

2.4 Quasiparticle Spectrum and Phase Diagram

The quasiparticle dispersion in superconducting state with finite value of the order parameter $\Delta^a$ is given by Eq. (2–5), which is a function of $k_x$ and $k_y$. For various cases, we plot the quasiparticle energies as a function of $k_x$ for a fixed value of $k_y = 0$ in Fig. 2-3. Panel (a) shows the quasiparticle energy for the homogeneous case, when both the sublattice have equal value of the order parameter with normal state dispersion as dashed line. On the other hand, in the inhomogeneous case the bands splits and this leads to four distinct bands with gap on the Fermi level as shown in panel (b). When one of the sublattices has zero coupling constant, then two energy levels
Figure 2-3. The quasiparticle energy (in units of $4t$) in the momentum space along $k_x$ (on x-axis), with $k_y=0$ . (a) spectrum when both the gaps are zero (b) gaps have same sign and equal magnitude (c) gaps with same signs but different magnitudes (d) gaps with opposite signs and unequal magnitudes.

remain gapless, as shown in panel (c). Panel (d) shows the dispersion for the case, when one of the pairing interactions is repulsive. In this case, a level crossing occurs inside the Brillouin zone. This leads to a contour of zero energy excitations, which is equivalent to a superconductor with a line node. In Fig. 2-3(d), $E_2$ is always positive, but $E_1$ is positive except in a narrow range $-\sqrt{\Delta^A|\Delta^B|} \leq \xi \leq \sqrt{\Delta^A|\Delta^B|}$. The gapless phase in isotropic s wave superconductors in the presence of magnetic impurities was first found by Abrikosov and Gorkov [55]. A bound state is formed near the magnetic impurity and overlap of bound states from each randomly distributed impurity leads to formation of an impurity band [77, 78]. The residual DOS on the Fermi surface is
proportional to the bandwidth of impurity band. Similar gapless phases can appear due to inhomogeneous sign changing order parameter due to low energy Andreev bound states near off diagonal impurities \[73, 74\]. Gapless phases can also appear in a multiband superconductors with sign-changing order parameters due to interband nonmagnetic scattering \[50, 79\]. In multiband systems with sign changing isotropic s-wave states, pure intraband magnetic and off diagonal or phase impurities can also lead to impurity resonances. For the present case, one can imagine that such off diagonal phase impurities are densely distributed over the system, and interference of bound states due to these phase impurities leads to the gapless superconductivity. To observe the spectral features for each sublattice, we calculate the local density of states on A and B sites,

\[
\rho^A(\omega) = \sum_k \left[ \frac{x_1^2}{1 + x_1^2} \left[ \delta(\omega - E_1) + \delta(\omega + E_1) \right] + \frac{x_2^2}{1 + x_2^2} \left[ \delta(\omega - E_2) + \delta(\omega + E_2) \right] \right] \\
\rho^B(\omega) = \sum_k \left[ \frac{1}{1 + x_1^2} \left[ \delta(\omega - E_1) + \delta(\omega + E_1) \right] + \frac{1}{1 + x_2^2} \left[ \delta(\omega - E_2) + \delta(\omega + E_2) \right] \right].
\]

(2–12)

(2–13)

Fig. 2-4 exhibits the LDOS on the two sublattices. In panels (a) and (b), when both the couplings are positive, we clearly see a full spectral gap. But when one of the couplings becomes zero, as in (c), a sharp peak develops at the Fermi level on the associated sublattice. The system remains gapless as the coupling constant on this sublattice is made negative, as in (d). Within this two parameter \((g^A, g^B)\) model, we construct the phase diagram of the ground state of the model Hamiltonian, shown in Fig. 2-5.

### 2.5 Superfluid Density

When one of the coupling constants is zero or negative, the corresponding phase is gapless and has low energy excitations. These low energy excitations lead to novel
behavior in the transport and the thermodynamic properties of the system. The order parameter is constant, but due to a phase difference of $\pi$ between the two sublattices, one gets a gapless phase. As Aryanpour et al. have emphasized [69], models of inhomogeneous pairing can lead to a variety of ground states, including insulating ones. To show that the the states that we consider here are indeed superconducting, we use the criteria developed by Scalapino et. al. [80] for the lattice systems. We calculate the superfluid density $n_s$, which is the sum of the diamagnetic response of the system (kinetic energy density) and paramagnetic response (current-current correlation function)

$$\frac{n_s}{m} = \langle -k_x \rangle - \Lambda(\omega = 0, q \to 0).$$

(2–14)
Figure 2-5. Zero temperature mean field phase diagram in the space of the two coupling constants $g^A$ and $g^B$. The solid lines represent transitions between the normal metal defined by zero order parameter, gapped and gapless superconducting phases. The dashed-dotted line represents the line of constant average pairing $g = t$. The dashed line represents the homogeneous BCS case. Finally, the dotted line represents the normal-gapless superconducting transition line as calculated analytically using the window density of states.
The current-current correlation function is defined as,

$$\Lambda_{xx}(q, i\omega_m) = \int_0^\beta d\tau e^{i\omega_m\tau} \langle j^P_x(q, \tau)j^P_x(-q, 0) \rangle,$$  \hspace{1cm} (2–15)

where the current at the \(i^{th}\) site is given by,

$$j^P_x(i) = it \sum_\sigma \left( c_{i+x,\sigma}^\dagger c_{i,\sigma} - c_{i,\sigma} c_{i+x,\sigma} \right).$$ \hspace{1cm} (2–16)

After evaluating the expectation value, we find the following relatively simple expression for the analytic continuation of the static homogeneous response:

$$\Lambda_{xx}(\omega = 0, q \to 0) = 2 \sum_k \left[ 4t \sin(\frac{k_x}{\sqrt{2}}) \cos(\frac{k_y}{\sqrt{2}}) \right]^2 \frac{f(E_1) - f(E_2)}{E_1 - E_2}.$$ \hspace{1cm} (2–17)

If the \(E_i(k)\) do not change sign over the Brillouin zone, as is the case for the gapped phase \(g_A, g_B > 0\), it is clear that this expression vanishes as \(T \to 0\) as in the clean BCS case. This is no longer the case in the gapless regime \(g_B \leq 0\), where a finite value of \(\Lambda\), corresponding to a residual density of quasiparticles, is found at zero temperature.

The other term we need to evaluate is the expectation value of the lattice kinetic energy density operator, which in the homogeneous BCS case is directly proportional to the superfluid weight \(n_s/m = \langle -k_x \rangle\) at \(T = 0\). The kinetic energy operator \(k_x\) is defined as,

$$k_x(i) = -t \sum_\sigma \left( c_{i+x,\sigma}^\dagger c_{i,\sigma} + c_{i,\sigma} c_{i+x,\sigma} \right).$$ \hspace{1cm} (2–18)

The expectation value of the x-kinetic energy density is given as,

$$\langle k_x(i) \rangle = 2 \sum_k \xi_k \left[ \frac{x_1}{1 + x_1^2} \tanh(\frac{\beta E_1}{2}) + \frac{x_2}{1 + x_2^2} \tanh(\frac{\beta E_2}{2}) \right].$$ \hspace{1cm} (2–19)

For the case when \(g_A, g_B > 0\) at \(T = 0\), we can simplify this expression as,

$$\langle -k_x(i) \rangle = 2 \sum_k \frac{\xi_k^2}{\sqrt{(\Delta_0^A + \Delta_0^B)^2 + 4\xi_k^2}},$$ \hspace{1cm} (2–20)

which is always positive; hence, the system is a superconductor and displays a conventional Meissner effect at \(T = 0\). The expression also shows explicitly that
the superfluid density on each site corresponds to that of the average superconducting order parameter over the system.

Fig. 2-6 shows the variation in the superfluid weight as a function of inhomogeneity.

At $T = 0$, $n_s$ for this model is a constant and equal to the value for the homogeneous system, whenever the system is fully gapped, since the average gap remains the same. The superfluid density is independent of inhomogeneity in the gapped phase, but the transition temperature increases monotonically with inhomogeneity (see Fig. 2-2). As one increases the inhomogeneity further with fixed average coupling, there is a critical value $\delta_1$ for which the system enters the gapless phase, at which the superfluid density drops abruptly. The temperature dependence of such a case is shown, along with other cases, in Fig. 2-7, and we see that this discontinuity corresponds to the creation of a
finite residual DOS at the Fermi surface. There is then a second critical value $\delta_2$, beyond which the superfluid density vanishes, identical to the value beyond which no solution with $\Delta_{AB} \neq 0$ is found. These considerations determine the labeling of the phase diagram shown in Fig. 2-5.

### 2.6 Optimal Inhomogeneity

When inhomogeneity is increased further in the gapless phase while keeping the average pairing potential $\bar{g}$ fixed, the transition temperature monotonically increases, but the zero temperature superfluid density continuously goes down with larger inhomogeneity. In such situations, large phase fluctuations due to low superfluid density
Figure 2-8. Mean field critical temperature $T_c/t$ (dashed-dotted line) and the phase-ordering temperature $T_\theta/t$ (dashed line) vs inhomogeneity $\delta/t$ for a fixed average interaction $\bar{g}=t$. The solid line is the minimum of the two curves at any $\delta/t$.

prohibit the long range order [28]. To estimate the temperature when long range order is destroyed by phase fluctuations, we use the criterion proposed by Emery and Kivelson [28] and define a characteristic phase ordering temperature,

$$T_\theta = \frac{\hbar^2 n_s \ell}{4m^*} \quad (2–21)$$

which decreases in the gapless phase following the reduction in zero temperature superfluid density. For quasi two-dimensional superconductors, the length scale $\ell$ is the larger of the two lengths, the average spacing between layers ‘$d$’ and $\xi_c$, where $\xi_c$ is the superconducting coherence length perpendicular to the layers. An exact determination of $\ell$ is beyond our simple mean field model, but it is qualitatively irrelevant in the presence of the abrupt drop of the superfluid density. Taking simply $\ell$
\[\sim a\], which is within a factor of 2–3 of both \(d\) and \(\xi_c\) in the cuprates, we may now obtain a crude measure of the optimal inhomogeneity needed to maximize the true ordering temperature in this model. We have set the value of \('A'\) to unity. In Fig. 2-8, we now plot both the mean field \(T_c\) and the phase-ordering temperature \(T_\theta\) as functions of inhomogeneity \(\delta/t\). We see that the two curves cross very close to the phase boundary \(\delta_c\) at \(\delta=2t\) in the figure due to the steep drop in superfluid density there. It therefore appears that the optimal inhomogeneity within the this model occurs for a checkerboard like pairing interaction with attractive interaction on one sublattice and zero interaction on the other.

### 2.7 Conclusion

We have considered a simple mean field model on a square bipartite lattice with inhomogeneous pairing interaction. We studied the physical properties of this system by keeping the average pairing interaction fixed over a unit cell and changing the local pairing interaction on each sublattice. We find two distinct kinds of superconducting phases fully gapped for attractive interactions on both sublattices, and gapless phase in other cases. The critical temperature monotonically increases with inhomogeneity, which is consistent with earlier numerical work by several groups. We find that as the superconducting state becomes gapless, the zero temperature superfluid density starts to decrease with inhomogeneity and phase fluctuations start to determine the true transition temperature. This gives an optimal value of inhomogeneity for maximum \(T_c\). We find that this optimal value of \(T_c\) for the model considered here corresponds to a checkerboard like pattern, when one of the sublattice has zero pairing interaction and the corresponding superconducting state is gapless. While our results have been obtained within the mean field approximation, we do not expect fluctuations to change them significantly because the length scale associated with inhomogeneity is small and the system is homogeneous over unit cell length scales. Our results suggest
that modulated pairing interaction at the atomic scale may provide a route to high temperature superconductivity.
CHAPTER 3
DISORDER IN MULTIBAND SYSTEMS


3.1 Introduction

Real materials always carry randomly located defects, which gives rise to an effective disorder potential. Electrons and holes are inelastically scattered from these defects, hence disorder plays a very important role in the physical properties of materials at lower temperatures. Even in the ordered phases of matter like superconductors or magnets, disorder cannot be ignored. The simplest model of disorder treats impurities as point like scattering centers randomly distributed over the sample. This can be done by treating them as delta function potentials which could be magnetic and/or nonmagnetic. Physical properties can be calculated by doing an ensemble averaging over all configurations of impurities. The effect of disorder is studied in superconductors in the framework of Abrikosov-Gorkov theory [55], which can be generalized to a multiband systems like pnictides or MgB$_2$. In such systems, impurities can scatter the electrons/holes within a same band or in between two different bands. A simple model Hamiltonian for disorder potential is,

$$ H_{\text{disorder}} = \sum_n \int dr \sum_{ij} U_{ij}(r-R_n) \psi^\dagger_{i\sigma}(r) \psi_{j\sigma}(r). $$ (3–1)

Here $i,j$ denote bands and $\bar{R}_n$ is the impurity position. In the Fourier space for a delta function kind of impurity potential,

$$ H_{\text{disorder}} = \sum_{ij,k,k'} U_{ij} \psi^\dagger_{i,k\sigma} \psi_{j,k'\sigma}. $$ (3–2)
The relative strength of the inter and intra band disorder potentials is a very important parameter, which is taken as phenomenological input in the rest of the discussion. Both pure intraband scattering and completely isotropic scattering are discussed. In the next section, I discuss the basic formalism of the disorder problem in a two band superconductor.

3.2 Formalism

We used the following model Hamiltonian first proposed by Suhl et al. [81],

\[ \mathcal{H} = \sum_{k,\sigma,i} \xi_{i,k} c_{i,k,\sigma}^\dagger c_{i,k,\sigma} + \sum_{k,k',\sigma,i,j} V_{i,k,k',j}^j c_{i,k,\sigma}^\dagger c_{j,-k',-\sigma}^\dagger c_{j,-k,\sigma} c_{j,k',\sigma} \] (3–3)

Here \( c^\dagger, c \) are the creation and the annihilation operators. \( i, j \) are the band index, \( k \) is the momentum and \( \sigma \) is the spin. \( \xi_{k,\sigma,i} \) is band dispersion for \( i^{th} \) band and \( V_{i,k,k',j}^j \) is the pairing potential. Since only the form of the order parameter is important for understanding the properties of superconductors, we use a simple separable form of the pairing potential for generating the desired momentum dependence of the order parameter, which is given as,

\[ V_{i,k,k',j} = V_0 \mathcal{Y}(k) \mathcal{Y}(k') \] (3–4)

where \( V_0 \) is strength of pairing and \( \mathcal{Y}(k) \) is the function which defines the momentum dependence of the order parameter. Within the mean field approximation, the Matsubara Green’s function is diagonal in the band basis and written as,

\[ \mathcal{G} = \begin{bmatrix} G_1 & 0 \\ 0 & G_2 \end{bmatrix} = \begin{bmatrix} \frac{-\omega_n^1 + \Delta_1 \gamma + \xi_1 \beta_1}{\omega_n^1 + \xi_1^2 + \Delta_1^2} & 0 \\ 0 & \frac{-\omega_n^2 + \Delta_2 \gamma + \xi_2 \beta_2}{\omega_n^2 + \xi_2^2 + \Delta_2^2} \end{bmatrix} \] (3–5)

Here \( \omega_n \equiv (2n + 1)\pi T \) is the fermionic Matsubara frequency, \( \Delta_{1/2} \) is mean field order parameter and \( \mathbb{1} \) is 2×2 identity matrix in the Nambu basis of each individual band. The self-consistent equation for the order parameter is,

\[ \Delta_i(k) = 2T \sum_{k' \sigma} V_{i,k,k',j}^j \frac{\Delta_j(k')}{\omega_n^2 + \xi_j^2 + \Delta_j^2} \] (3–6)
Here $\omega_c$ is the cut-off energy scale. The effect of disorder is included by calculating the disorder self energy. For low impurity concentrations, one can ignore the processes which involve scattering from multiple impurity sites [82]. Within this single site approximation, we sum all possible scattering events to calculate the $T$-matrix, which is related to the self energy as

$$\Sigma = n_{\text{imp}} T,$$

with $n_{\text{imp}}$ the impurity concentration. For a two-band superconductor, another channel of scattering comes through scattering between the bands by the impurities. Fig. 3-1 shows the impurity averaged diagrams up to third order. Any process which involves an odd number of interband scatterings does not contribute to the self energy, because at the end the final state belongs to the other band. In the context of pnictides, we focus on nonmagnetic impurity potentials. A microscopic calculation of the impurity potential induced by a dopant atom suggests strong intraband scattering potential, while interband scattering and magnetic scattering is relatively weak [83]. Doping is one source of disorder, but the doping concentration may not really be proportional to impurity concentration, since doping can also modify the band structure and modify the pairing interaction. Therefore we consider two limiting cases, the strong scattering unitary limit when $U_{ij} N_j \gg 1$ and the weak scattering Born limit with $U_{ij} N_j \ll 1$. $N_j$ is the density of states at the Fermi level for the $i^{th}$ band. In this chapter, I focus primarily on the Born limit to understand the effect of disorder on the spectral function and critical temperature. Some details of the problem for arbitrary impurity potential strength are given in the appendix A. In the Born limit, only the lowest order diagrams contribute to
Figure 3-1. These are the impurity averaged diagrams, which contribute to the self energy of the first band Green’s function. Here the interband contribution comes through processes, which involve an even number of interband scatterings. The diagrams also take into account the order of inter and intraband scatterings. \( U_{ij} \) is the impurity potential strength. \( i=j \) denotes intraband and \( i \neq j \) denotes interband scattering.

The self energy and all kinds of scattering are important. The self energy is written as,

\[
\Sigma_{1,0} = n_{\text{imp}} \left[ (U_{11}^2 + \bar{U}_{11}^2) g_{1,0} + (U_{12}^2 + \bar{U}_{12}^2) g_{2,0} \right], \quad (3-8)
\]
\[
\Sigma_{1,1} = -n_{\text{imp}} \left[ (U_{11}^2 - \bar{U}_{11}^2) g_{1,1} + (U_{12}^2 - \bar{U}_{12}^2) g_{2,2} \right], \quad (3-9)
\]
\[
\Sigma_{2,0} = n_{\text{imp}} \left[ (U_{22}^2 + \bar{U}_{22}^2) g_{2,0} + (U_{21}^2 + \bar{U}_{21}^2) g_{1,0} \right], \quad (3-10)
\]
\[
\Sigma_{2,1} = -n_{\text{imp}} \left[ (U_{22}^2 - \bar{U}_{22}^2) g_{2,2} + (U_{21}^2 - \bar{U}_{21}^2) g_{1,2} \right]. \quad (3-11)
\]

Here in quantities \( \Sigma_{i,\alpha} \) and \( g_{i,\alpha} \), the first subscript \( i \) is for bands and the second subscript \( \alpha \) denotes the Nambu component of the Green’s function. \( g_{i,\alpha} \) is the energy integrated
Green’s function, defined as

\[ g_{i,0} = -\int d\xi \frac{i\omega_n}{\omega_n^2 + \xi_i^2 + \Delta_i^2}, \]

\[ g_{i,1} = -\int d\xi \frac{\Delta_i}{\omega_n^2 + \xi_i^2 + \Delta_i^2}. \]  

(3–12)  

(3–13)

In a particle hole symmetric system \( g_{i,3} \) is zero. The full Green’s function is evaluated selfconsistently with disorder self energies

\[
\left[ G(i\tilde{\omega}_n, \tilde{\Delta}_n) \right]^{-1} = \left[ G^0(i\omega_n, \Delta) \right]^{-1} - \Sigma(i\tilde{\omega}_n, \tilde{\Delta}_n).
\]

(3–14)

Here \( G^0 \) is the bare Green’s function and \( G \) is the full Green’s function, defined in terms of renormalized energy \( \tilde{\omega}_n \) and renormalized order parameter \( \tilde{\Delta}_n \) as,

\[
G = -\frac{i\tilde{\omega}_n \hat{1} + \hat{\Delta}_1 + \hat{\xi}_3}{\tilde{\omega}_n^2 + \xi^2 + \Delta^2}.
\]

(3–15)

The self consistency condition can be rewritten as,

\[
\tilde{\omega}_i(\omega_n) = \omega_n - \Sigma_{i,0}(\omega_n),
\]

(3–16)

\[
\tilde{\Delta}_i(\omega_n) = \Delta_i + \Sigma_{i,1}(\omega_n),
\]

(3–17)

\[
\Delta_i = 2T \sum_{k', j, \omega_n=0} V^\omega_{k'j} \frac{\tilde{\Delta}_j(k')}{\omega_j^2 + \xi_j^2 + \Delta_j^2}.
\]

(3–18)

Here the subscripts \( i, j \) denote the bands. Once the full Green’s function is known, any one particle physical quantity can be calculated easily. In next section, I discuss the effect of disorder on the spectral function for order parameters relevant for the iron pnictides.

### 3.3 Node Lifting Phenomenon

Knowledge of the symmetry of the order parameter of a superconductor is crucial to understand the mechanism of superconductivity and to design devices using that particular material. The symmetry of the newly discovered Fe pnictides is still a controversial issue, and there are contradictory results from experiments. Some of
Figure 3-2. Schematic picture of order parameter. Red and Blue denote different signs of the order parameter over Fe-pnictide Fermi surface. There is a phase difference of $\pi$ between the order parameters of two electron pockets ($\beta$) located at $(\pi,0)$ and $(0,\pi)$. The full system has $A_{1g}$ symmetry. The order parameter on hole pockets ($\alpha$) at $(0,0)$ is very isotropic [45].

The transport measurements suggest the presence of low energy excitations [84–94]. Theoretical investigations have found that sign changing $\pm s$ wave state appears to be most stable in these materials [45–47, 95–98]. Some researchers have found nearly isotropic order parameter on the Fermi surface, while some others have found strong anisotropy on electron like Fermi surface sheets. For some set of parameters, order parameters with accidental nodes on the electron sheets have been reported. Some of the experimental results can be then explained with isotropic $\pm s$ wave states by including strong interband scattering [50, 51, 99, 100], which can create a low energy
impurity band in the gap. From the earlier work on the effect of disorder on two band superconductors, it is known that nonmagnetic impurity scattering between the bands is pairbreaking for superconductors with sign changing order parameter \([50, 51]\).

Such scattering leads to formation of mid-gap impurity bands, which affects the low temperature properties. This explains some experiments, but there are some nuclear magnetic relaxation (NMR) and specific heat data which cannot be explained. Kobayashi et al. have measured NMR relaxation rate \(1/T_1\) for \(\LaFeAsO_{1-x}F_x\) for various values of \(x\) and they found \(T^n\) behavior with \(n \leq 3\) for some dopings \([101]\). \(T^3\) behavior of NMR relaxation rate is expected for a superconductor with line node and linear, if the system is dirty. Mu et al. measured magnetic field dependent specific heat coefficient for \(\LaFeAsO_{1-x}F_x\), and they reported \(\sqrt{H}\) behavior, which is an indication of nodal gap\([102]\). These NMR and field dependent specific heat data for \(\LaFeAsO_{1-x}F_x\) favors the presence of nodal gap and can not be explained by isotropic \(s_\pm\) order parameters with disorder. One of the stoichiometric compounds \(\LaFePO\) clear evidence of shows a linear term in the penetration depth, which can only be explained by nodes in the order parameters \([103, 104]\). Angle resolved photoemission spectroscopy (ARPES) experiments don’t find order parameter nodes on the Fermi surface \([105–113]\), but this may be a surface effect. We consider a different model here, where we start with a system with accidental nodes and by adding disorder to it, we show that the the nodes disappear. This physics is simple to understand: intraband scattering will average the nodal gap over the Fermi surface with finite average \(\langle \Delta_k \rangle\), leading to an isotropic gap at sufficiently large disorder.

The order parameters for our simple model are,

\[
\Delta_{\text{hole}} = \Delta_1, \quad (3-19)
\]

\[
\Delta_{\text{electron}} = \Delta_2(1 \pm r \cos 2\phi). \quad (3-20)
\]
Here ‘$\phi$’ is the angle on each Fermi surface sheet, measured from the center of that sheet and ‘$r$’ is the parameter, which controls anisotropy. A value of larger than unity yields an order parameter with nodes. For gaining qualitative understanding, we consider only one hole sheet and one electron sheet. Figure 3-2 shows a schematic picture of order parameter found by Graser et al. [45] for 1111 family. The effect of disorder on the transport properties is discussed in detail in next two chapters. Here we look at the spectral function, which is measured in ARPES measurements. The spectral function is directly related to the retarded Green’s function as,

$$A(k, \omega) = -\frac{1}{\pi} \text{Im} \left[ G(\omega_n \rightarrow \omega + i0^+, k) \right]. \quad (3–21)$$

Here $\omega$ is a real frequency. We look at the spectral gap, which is defined to be the energy between the peak and the Fermi level where $A(k, \omega)$ falls to half its peak value. The spectral gap contains full information about the momentum dependence and for an order parameter $\Delta_k$, it is proportional to the absolute value $|\Delta_k|$. To model the order parameter of 1111 family pnictides, we use following pairing potential,

$$V_{11}(k, k') = -V_1, \quad (3–22)$$
$$V_{12}(k, k') = V', \quad (3–23)$$
$$V_{22}(k, k') = -V_2 (1 + r \cos 2\phi) (1 + r \cos 2\phi'). \quad (3–24)$$

Using this set of pairing potentials, we calculate the full Green’s function with the self consistency conditions 3–16, 3–17 and 3–18. Pairing potentials with negative signs are attractive, and positive interband pairing potentials are repulsive. A repulsive interband potential is necessary to get a set of order parameters with opposite signs. We first look at the spectral function in the presence of only intraband scattering. For isotropic $\pm$ s wave superconductors, pure intraband scattering is not pair breaking. Such a system is equivalent to a s wave superconductor with nonmagnetic impurities and obeys Anderson’s theorem [49]. But in the presence of anisotropy (nonzero $r$), impurity
scattering causes suppression of the anisotropic component, within this type of theory, which neglects the localization effects [52]. For large values of disorder, the anisotropic component of order parameter becomes very small, but there is no critical value of disorder which can kill the superconductivity, within this theory where localization effects are neglected. Figure 3-3 shows the spectral gap ($\Omega^{\alpha/\beta}_G(\phi)$) for the hole ($\alpha$) and the electron ($\beta$) sheets. We can see that the change in the order parameter of the hole pocket is very weak. The small suppression shown in figure 3-3 is due to the interband pairing potential, which couples the two bands. Another very important quantity which

Figure 3-3. Spectral gap as function of angle for the hole pocket $\Omega^{\alpha}_G(\phi)$ and for the electron pocket $\Omega^{\beta}_G(\phi)$. The parameter $\Gamma$ is the normal state average impurity scattering rate measured in units of the clean limit critical temperature $T_{c0}$. The anisotropy parameter ‘$r$’ is 1.3 for this figure and the ratio of density of states ($N_\alpha/N_\beta$) for the two bands is 1.25.
Figure 3-4. Density of states is shown for two different anisotropies. The upper panel shows DOS for $r=1.3$ and lower panel show DOS for $r=1.1$. For the same amount of disorder the gap in DOS is larger for the less anisotropic ($r=1.1$) system.
Figure 3-5. Spectral gap as function of angle for the hole pocket $\Omega_G^\alpha(\phi)$ and for the electron pocket $\Omega_G^\beta(\phi)$ in presence of magnetic intraband impurities. The anisotropy parameter ‘$r$’ is 1.3 for this figure and the ratio of density of states ($N_\alpha/N_\beta$) for the two bands is 1.25.

clearly shows the node lifting is the density of states (DOS), which is

$$N(\omega) = \int d\mathbf{k} A(\mathbf{k}, \omega).$$  \hspace{1cm} (3–25)

Fig. 3-4 shows the DOS for two different anisotropies as a function of energy for various disorder. A finite gap appears in the DOS as soon as the nodes disappear. The critical value of disorder that lifts the nodes depends on the anisotropy of the order parameter. For larger anisotropy ($r \gg 1$) nodes vanish more slowly, while accidental nodes ($r \geq 1$) vanish for very small concentrations of impurities.

The presence of weak magnetic impurities cannot be ruled out in these systems. We have also looked at the effect of magnetic impurities. In an ordinary s wave superconductors magnetic impurities can create a gapless phase where the spectral
gap is zero \[55\], they are pair breakers in both isotropic and anisotropic superconductors. As we expect, for the two band superconductor under consideration here, both isotropic and anisotropic components get suppressed. As shown in figure 3-5, magnetic impurities suppress the order parameter on the hole pocket and on the electron pocket significantly. Since the isotropic and anisotropic components are suppressed equally, the nodes don’t disappear. For very large values of disorder, superconductivity eventually disappears. Another important question is, what is the effect of general nonmagnetic impurities? The size of the interband impurity potential is still an unanswered problem. If we think of an impurity as a screened Coulomb potential, we would expect the interband scattering to be smaller due to large momentum transfer in the process. Orbital physics may however play a vital role in producing large interband scattering \[114\], so we consider the effect qualitatively here. Figure 3-6 shows the DOS in the presence of interband scattering. In the presence of weak interband scattering, nodes get lifted more slowly compare to the pure intraband case. For larger interband scattering, nodes do not vanish at all, and the isotropic limit (interband=intraband) is strongly pair breaking. Weak interband scattering leads to formation of midgap impurity states, which for strong interband scattering move towards the Fermi level. For isotropic scattering the impurity band is formed on the Fermi level. I discuss the formation of impurity bands in the next chapter 4, where I use full T matrix which captures the physics of bound states accurately. In the next section, I discuss the effect of disorder on the critical temperature.

### 3.4 Effect On Critical Temperature

The effect of the disorder on critical temperature strongly depends on the symmetry of the order parameter. In isotropic s wave superconductors, \(T_c\) does not change with nonmagnetic impurities \[49\], but \(T_c\) goes to zero for a critical value of disorder for nonmagnetic impurities \[55\]. In anisotropic superconductors, \(T_c\) decreases even with nonmagnetic impurities. When a isotropic component is also present in order parameter, then \(T_c\) goes down with disorder till the anisotropic component goes to zero.
Figure 3-6. DOS in the presence of the interband scattering. The black curve shows the DOS for a nodal state with $r=1.3$ and pure intraband scattering rate $\Gamma=2.5 \ T_{c0}$. The nodes have disappeared due to pure intraband scattering and interband scattering is added to the state corresponding to the black curve. Legends show the strength of the interband scattering, which changes from 0–100% of intraband scattering.

and after that it saturates to its value at this critical scattering rate because the system again obeys the Anderson’s theorem [52]. Here we look at the effect of anisotropy and additional bands. To calculate $T_c$, we linearize the self consistent equations 3–16, 3–17 and 3–18 in $\Delta$ near $T_c$. Near $T_c$,

$$
 g_{j,0} = \int d\mathbf{k} \frac{i\tilde{\omega}_n}{\tilde{\omega}_n^2 + \xi_j^2},
$$

$$(3-26)$$

$$
 g_{j,1} = \int d\mathbf{k} \frac{\tilde{\Delta}_j}{\tilde{\omega}_n^2 + \xi_j^2}.
$$

$$(3-27)$$

Since the disorder self energy depends only on energy, not on momentum, the anisotropic component of the order parameter does not depend on energy. The change
in the anisotropic component comes through the gap equations, which near $T_c$ read as

$$\Delta_i = 2T \sum_{k', j, \omega_n=0} V_{kk'}^{ij} \frac{\tilde{\Delta}_i(k')}{\xi_j^2 + \xi_j^2}. \quad (3–28)$$

In the basis $\hat{\Delta} \equiv (\Delta_\alpha, \Delta_\beta^{iso}, \Delta_\beta^{ani})$, we can write the gap equations in the compact form

$$\hat{\Delta} = \ln \left( \frac{1.13 \omega_c}{T_c} \right) \left( \hat{1} + \hat{\mathcal{V}} \hat{\mathcal{R}}^{-1} \hat{\mathcal{X}} \hat{\mathcal{R}} \right)^{-1} \hat{\mathcal{V}} \hat{\Delta} = \ln \left( \frac{1.13 \omega_c}{T_c} \right) \mathcal{M} \hat{\Delta}. \quad (3–29)$$

Here $\hat{\mathcal{V}}$ is the interaction matrix in $\hat{\Delta}$ basis, which can be obtained by writing the gap equations in $\hat{\Delta}$ and $\hat{1}$ is $3 \times 3$ identity matrix. $\hat{\mathcal{R}}$ is the orthogonal matrix, which diagonalizes the matrix $\hat{\Lambda}$,

$$\hat{\Lambda} = \frac{\pi n_{imp}}{4} \begin{bmatrix} N_\beta U_{\alpha\beta}^2 & N_\beta U_{\alpha\beta}^2 & 0 \\ N_\alpha U_{\beta\alpha}^2 & N_\alpha U_{\beta\alpha}^2 & 0 \\ 0 & 0 & -N_\beta U_{\beta\beta}^2 \end{bmatrix}. \quad (3–30)$$

The concentration of impurities is denoted by $n_{imp}$, and $\hat{\mathcal{X}}$ is a diagonal matrix whose elements are

$$\hat{\mathcal{X}}_{ij} = \delta_{ij} \left[ \Psi \left( \frac{1}{2} + \frac{\omega_c}{2\pi T_c} \right) - \Psi \left( \frac{1}{2} + \frac{\omega_c}{2\pi T_c} + \frac{\lambda_i}{2\pi T_c} \right) \right], \quad (3–31)$$

where $\Psi$ is the digamma function and $\delta_{ij}$ is the Kronecker delta function. The $\lambda_i$'s are the eigenvalues of the matrix $\hat{\Lambda}$. The maximum eigenvalue ($\lambda_{max}(T_c)$) of the matrix $\mathcal{M}$ is related to $T_c$,

$$T_c = 1.13 \omega_c \exp \left( -\frac{1}{\lambda_{max}(T_c)} \right). \quad (3–32)$$

The solution of Eq. 3–32 gives the value of $T_c$. We look at the effect of disorder and its correlation with the anisotropy, which can provide some understanding about the order parameter. Systematic disorder in a system can be introduced by irradiation or by doping. Suppression of $T_c$ in the LaFeAsO$_{0.9}$F$_{0.1}$ irradiated by neutrons shows suppression of $T_c$, which is weaker than d-wave superconductor YBC0 $^{115}$. Similar results have been found for NdFeAsO$_{0.7}$F$_{0.3}$, which suggest a $T_c$ suppression weaker than theoretical model of $\pm s$ wave with interband disorder $^{116}$. Another experiment on
LaFe$_{1-y}$Zn$_y$AsO$_{1-x}$F$_x$ with different dopings (x), where Zn doping (y) is used to introduce disorder, provides a doping dependent information about the order parameters. Underdoped and optimally doped samples show very little variation; on the other hand overdoped samples show very rapid suppression of $T_c$ [117]. This indicates that the order parameter is not universal like the cuprates but it changes across the phase diagram. Similar substitution experiments on optimally doped K doped 122 systems, find very contrasting results, Zn does not changes $T_c$ while Mn doping suppresses $T_c$ rapidly [118]. There is some evidence that impurities do not fully substitute in the melt, so $T_c$ should be carefully correlated with residual resistivity. Taken at face value, however, these experiments suggest that the anisotropy is a minimum at optimal doping. Doping dependent irradiation experiments on electron doped 122 family also shows very weak $T_c$ suppression for optimal doping and stronger suppression for overdoped samples.

We first look at the effect of anisotropy on $T_c$ suppression in presence of nonmagnetic impurities. Figure 3-7 shows the effect of disorder on $T_c$ for different anisotropy. For isotropic order parameters ($r = 0$), pure intraband scattering doesn’t make any change. Once the interband channel of scattering opens up, $T_c$ goes down and eventually becomes zero. On the other hand, for anisotropic systems pure intraband scattering leads to $T_c$ suppression and the rate of suppression increases with larger anisotropy.

Next, we look at $T_c$ suppression in the context of node lifting. Figure 3-8 shows the minimum spectral gap as a function of $T_c$ suppression. The nodes for a system with $r = 1.3$ disappear for roughly 10% $T_c$ reduction. Microscopic calculations often find $r \geq 1$ and for smaller $r$ nodes go away much faster. The presence of additional bands increase the rate, because $T_c$ decreases slowly with more bands in presence of intraband disorder. The DOS of each band also plays a role, which is illustrated in fig. 3-8. This effect on microscopically obtained order parameter by Graser et al. [45] with all bands is shown in figure 3-9, where nodes are lifted for approximately 5% suppression.
Figure 3-7. $T_c$ suppression as a function of total normal state scattering rate $\Gamma$. $T_{c0}$ is clean limit critical temperature, which is used as an energy scale. Four different panels show the effect of interband scattering, where panel (a) pure intraband, (b) 25%, (c) 50%, (d) 100% of the intraband scattering.

of $T_c$. Once the nodes are lifted, the system shows fully gapped behavior below the minimum spectral gap.

### 3.5 Conclusion

We considered an alternate scenario to explain the experimental results on pnictides, where we started with a clean nodal system. In such systems, intraband impurity nonmagnetic scattering can lift the nodes and create a gap in DOS. The presence of interband scattering acts against this process, hence a more realistic model of impurities should provide more understanding. Low temperature thermal conductivity puts further constraints on the nature of disorder in these systems, which I discuss in detail in the next chapter. Systematic introduction of disorder by irradiation or by doping also suggests that the order parameter has anisotropy, and structure of the order
Figure 3-8. Spectral gap as a function of $T_c$ reduction.

Figure 3-9. Spectral gap for microscopic order parameter as a function of $T_c$ reduction.
parameter is not universal in the Fe pnictides. Kuroki et al. [36] have pointed out the importance of structural parameters in these materials. In a more realistic treatment of disorder, one must take care of any structural change caused by irradiation or doping, and its effect on the pair interaction.
CHAPTER 4  
TRANSPORT I - THERMAL CONDUCTIVITY

4.1 Introduction

Thermal conductivity is a very useful bulk probe which has played an important role in identifying the symmetry of the order parameter in unconventional superconductors [119, 120]. Low temperature thermal conductivity \( T < 5K \) provides vital information about the low energy electronic excitations in the system; at higher temperatures, phonons also make a significant contribution. Thermal conductivity is very sensitive to nodes and shows a strong response to the magnetic field. Thermal conductivity measurements in the presence of an in-plane magnetic field have also been used to identify the location of nodes in unconventional superconductors [119, 120]. In nodal superconductors, thermal conductivity is linear at low temperatures and is associated with residual quasiparticles induced by disorder or the magnetic field. Recently, many low T thermal conductivity measurements have been performed on the BaFe\(_2\)As\(_2\) based 122 family and on the stoichiometric 1111 compound LaFePO.

In LaFePO, a huge linear term \( (3000 \mu Wcm^{-1}K^{-2}) \) has been detected, which is much larger than cuprates (e. g. in YBCO \( 190 \mu Wcm^{-1}K^{-2} \) [122]). In BaFe\(_2\)(As\(_{1-x}\)P\(_x\))\(_2\) the linear term is \( 250 \mu Wcm^{-1}K^{-2} \) [123], which clearly suggests the presence of nodes in these systems. In hole doped Ba\(_{1-x}\)K\(_x\)Fe\(_2\)As\(_2\), a very weak linear term has been detected, while field dependence of the linear term suggests strong anisotropy in the order parameters [124]. In Ni doped 122, no linear term has been detected and the field dependence is also very weak, which indicates the presence of an energy gap [125]. On the other hand, in another electron doped material Ba(Fe\(_{1-x}\)Co\(_x\))\(_2\)As\(_2\), a linear term order of \( 1 \mu Wcm^{-1}K^{-2} \) has been found in ab plane measurements and similar size terms have been detected for the thermal conductivity along the c axis [42, 126]. Another group claims a linear term of order \( 100 \mu Wcm^{-1}K^{-2} \) for the same material [127]. The magnetic field dependence is similar to nodal superconductors in these...
samples. In next section, I briefly review the theory of thermal conductivity and then
discuss the results for 122 and 1111 families in subsequent sections.

4.2 Basic Formalism

4.2.1 Thermal Conductivity

The thermal conductivity is calculated using Kubo’s formula for the heat current as
originally proposed by Ambegaokar and Griffin in the context of s wave superconductors
[128]. The heat current operator for an anisotropic superconductor derived by Durst and
Lee [129] is,

\[ j_h(q, \Omega) = \sum_{\mathbf{k}, \omega} \left( \omega + \frac{\Omega}{2} \right) \left[ \mathbf{v}_F \mathbf{c}^{\dagger}_{\mathbf{k}+\mathbf{q}} \mathbf{c}_{\mathbf{k}} - \frac{d\Delta}{d\mathbf{k}} \mathbf{c}^{\dagger}_{\mathbf{k}} \mathbf{c}_{\mathbf{k}+\mathbf{q}} \right]. \] (4–1)

This is generalization of the heat current obtained by Ambegaokar and Griffin [128]. The
thermal conductivity is given as,

\[ \frac{\kappa}{T} = -\lim_{\Omega \to 0} \frac{\text{Im}P(q, \Omega)}{\Omega}. \] (4–2)

Here \( \kappa \) is the thermal conductivity and \( P(q, \Omega) \) is heat current-current correlation
function, which is a bubble diagram with heat current vertex. After a straightforward
calculation, we can write,

\[ \frac{\kappa_\alpha}{T} = n \frac{k_B^2}{16\pi \hbar d} \sum_i \int_0^\infty d\omega \text{sech}^2 \left( \frac{\omega}{2T} \right) \langle \left| m_i \frac{1}{\text{Re}[\sqrt{\Delta_i^2 - \tilde{\omega}^2}]} \left( \mathbf{v}_{i-}^2 + \frac{|\tilde{\omega}|^2 \mathbf{v}_{i+}^2}{|\tilde{\omega}^2 - \Delta_i^2|} \mathbf{v}_{i-}^2 \right) \right|_{\phi, k_z} \rangle. \] (4–3)

Here we have accounted for the layered two dimensional structure of the system for
which DOS for the \( i^{th} \) band is \( m_i/2\pi \hbar^2 d \), where ‘\( m_i \)’ is the band mass of the \( i^{th} \) band and
‘\( d \)’ is the c axis unit cell length. In Eq. 4–4, \( \langle f(k_z, \phi) \rangle_{k_z, \phi} \) denotes the average over the
Fermi surface, ‘\( n \)’ is number of layers, \( \alpha = a, c \) is the direction of the thermal conductivity,
\( \mathbf{v}_{Fi} \) is the Fermi velocity on the \( i^{th} \) band, and \( \mathbf{v}_{i\pm}^2 \equiv \mathbf{v}_{Fi}^2 \pm (\partial_\alpha \Delta_{k,i})^2 \). \( \tilde{\omega} \) and \( \tilde{\Delta} \) are the energy
and the order parameter respectively renormalized by impurity scattering. In the limit
\( \Delta \ll E_F \), we can ignore the gap velocity term; the expression then simplifies to,

\[
\frac{\kappa_\alpha}{T} \approx n \frac{k_B^2}{16\pi \hbar d} \sum_i \int_0^{\infty} \frac{d\omega}{T} \frac{\omega^2 \text{sech}^2 \left( \frac{\omega}{2T} \right)}{\text{Re} \sqrt{\Delta_i^2 - \tilde{\Delta}_i^2}} \left[ 1 + \frac{\left| \tilde{\omega}_i \right|^2 - \left| \Delta_i \right|^2}{\left| \tilde{\Delta}_i^2 - \Delta_i^2 \right|} \right].
\]

In the zero temperature limit, the integrand in Eq. 4–4 is sharply peaked at \( \omega = 0 \) due to the \( \text{sech}^2 \) term. So we can approximate the integral by substituting the rest of the integrand by its \( \omega = 0 \) value and integrate the rest to get

\[
\lim_{T \to 0} \frac{\kappa_\alpha}{T} \approx n \frac{k_B^2}{16\pi \hbar d} \frac{4\pi^2}{3} \sum_i \left< m_i (v_{Fi} \cdot \hat{\alpha})^2 \frac{\Gamma_0^2}{(\tilde{\Delta}_i^2 + \Gamma_0^2)^{3/2}} \right>_{k_\alpha, \phi}.
\]

Here we used \( \tilde{\omega}(\omega = 0) = i\Gamma_0 \), where \( \Gamma_0 \) is the residual scattering rate due to impurities as \( \omega \to 0 \). In the zero temperature limit, the major contribution to the integrand in Eq. 4–5 comes from the regions close to the nodes. We linearize the order parameter near the nodes as

\[
\Delta(k) = \left. \frac{d\Delta}{dk} \right|_{k = k_m} (k - k_m) \equiv v_\Delta (k - k_m),
\]

where \( k_m \) is the position of the node and \( v_\Delta \) is the nodal gap velocity. Using this nodal approximation, we can perform the Fermi surface averaging of the integrand in Eq. 4–5 and get,

\[
\frac{\kappa_\alpha}{T} \approx n \frac{k_B^2}{16\pi \hbar d} \frac{4\pi^2}{3} \sum_{i, k_m} m_i (v_{Fi} \cdot \hat{\alpha})^2_{\text{nodal}} v_\Delta.
\]

This is a very good approximation as long as the Fermi velocity is not changing rapidly near the nodes. One thing to note here is the absence of single particle scattering rate \( \Gamma_0 \) in this zero temperature limit. The effect of disorder enters only through renormalization of the gap velocity. In the case of d wave superconductors, the gap velocity doesn’t get renormalized by disorder, hence this residual thermal conductivity is independent of disorder (“universal”), which is confirmed by experiments [121]. In the previous chapter 3, I discussed the effect of disorder within the Born approximation in
the context of the spectral function, but from the point of view of transport properties, bound states formed by impurities play a very important role as well. In the next section 4.2.2, I review the T-Matrix approximation, which captures the physics of impurity bound states exactly in the limit of weak impurity concentration in 3D.

4.2.2 T-Matrix And Impurity Bound States

The T-Matrix approximation involves all the diagrams which contributes to scattering from a single impurity (see Fig. 3-1). For low impurity concentrations \( n_{\text{imp}} \ll 1 \), the scattering processes which involve more than one impurity are very small in 3D. The general expression for the T-Matrix self energies in presence of both intraband and interband scattering are,

\[
\Sigma_{1,0} = n_{\text{imp}} \frac{U_{12}^2 g_{1,0} + U_{12}^2 g_{2,0} - g_{1,0} (U_{12}^2 - U_{11} U_{22})^2 (g_{2,0}^2 - g_{2,1}^2)}{D},
\]

(4–8)

\[
\Sigma_{1,1} = -n_{\text{imp}} \frac{U_{11}^2 g_{1,1} + U_{12}^2 g_{2,1} - g_{1,1} (U_{12}^2 - U_{11} U_{22})^2 (g_{2,0}^2 - g_{2,1}^2)}{D},
\]

(4–9)

\[
\Sigma_{2,0} = \Sigma_{1,0}(1, 2 \rightarrow 2, 1),
\]

(4–10)

\[
\Sigma_{2,1} = \Sigma_{1,1}(1, 2 \rightarrow 2, 1).
\]

(4–11)

Here \( U_{12} \) is the interband scattering and \( U_{11}, U_{22} \) are the intraband scattering potentials for band 1 and 2 respectively, the \( g \)'s are energy integrated Green's function defined by Eq. 3–12 and 3–13 and the denominator of the T-Matrix \( D \) is,

\[
D = 1 - 2 U_{12}^2 (g_{1,0} g_{2,0} - g_{1,1} g_{2,1}) - U_{22}^2 (g_{2,0}^2 - g_{2,1}^2) - U_{11}^2 (g_{1,0}^2 - g_{1,1}^2) + (U_{12}^2 - U_{11} U_{22})^2 (g_{2,0}^2 - g_{2,1}^2) (g_{1,0}^2 - g_{1,1}^2).
\]

(4–12)

We focus on the strong scattering unitary limit, where the impurity potential is much larger than the Fermi energy. There are two interesting limiting cases for the unitary limit. The first case is when the interband scattering is smaller than the intraband scattering and the second case is the isotropic case when these two kinds of scatterings have equal magnitude. In the first case, it turns out that in the unitary limit the intraband
scattering completely dominates and no scattering occurs between the bands. For nonmagnetic impurities the self energy is given as,

\[ \Sigma_{1,0} = n_{imp} \frac{-g_{1,0}}{(g_{1,0}^2 - g_{1,1}^2)}, \tag{4–13} \]

\[ \Sigma_{1,1} = n_{imp} \frac{g_{1,1}}{(g_{1,0}^2 - g_{1,1}^2)}, \tag{4–14} \]

\[ \Sigma_{2,0} = n_{imp} \frac{-g_{2,0}}{(g_{2,0}^2 - g_{2,1}^2)}, \tag{4–15} \]

\[ \Sigma_{2,1} = n_{imp} \frac{g_{2,1}}{(g_{2,0}^2 - g_{2,1}^2)}. \tag{4–16} \]

These self energies are the same as originally obtained by Hirschfeld et al. for a single band \[82\]. The energy of the bound state formed by impurity is given by the pole of the T-Matrix for a single impurity. Superposition of bound states from many isolated impurities leads to formation of an impurity band, whose bandwidth is given by the imaginary part of the impurity averaged T-matrix. Such impurity bands can be seen clearly in the DOS. For a realistic impurity, interband and intraband scattering are unlikely to be equal and therefore we restrict our discussion to nonmagnetic impurities.

For magnetic impurities, the exact nature of the magnetic impurity potential becomes important. The quantum mechanical nature of impurity spin and kondo screening can not be ignored \[130\]. On the other hand, in the limit of isotropic nonmagnetic scattering the self energies become the same for all bands and are written as,

\[ \Sigma_{1,0} = -n_{imp} \frac{g_{1,0} + g_{2,0}}{(g_{1,0} + g_{2,0})^2 + (g_{1,1} - g_{2,1})^2}, \tag{4–17} \]

\[ \Sigma_{1,1} = n_{imp} \frac{g_{1,1} + g_{2,1}}{(g_{1,0} + g_{2,0})^2 - (g_{1,1} + g_{2,1})^2}, \tag{4–18} \]

\[ \Sigma_{2,0} = \Sigma_{1,0}, \tag{4–19} \]

\[ \Sigma_{2,1} = \Sigma_{1,1}. \tag{4–20} \]
Figure 4-1. Impurity resonance position as a function of scattering phase shift \( c = 1/N\pi U \) for different ratios of inter and intraband scatterings. Black curves represent symmetric \( \pm s \) wave state, with \( \Delta_1 = -\Delta_2 = \Delta_0 \) and red curves presents asymmetric \( \pm s \) wave state with \( \Delta_1 = \Delta_0, \Delta_2 = -1.4\Delta_0 \). The solid line represents isotropic scattering limit.

To gain some understanding into the impurity bound states, I start with equation for the pole \( (D = 0) \) for the single impurity T-Matrix,

\[
0 = 1 - 2U_{12}^2(g_{1,0}g_{2,0} - g_{1,1}g_{2,1}) - U_{22}^2(g_{2,0}^2 - g_{2,1}^2) - U_{11}^2(g_{1,0}^2 - g_{1,1}^2) + (U_{12}^2 - U_{11}U_{22})^2(g_{2,0}^2 - g_{2,1}^2)(g_{1,0}^2 - g_{1,1}^2).
\]

In our simple model, we take \( \pi U_{11}N_1 = \pi U_{22}N_2 = U \) and \( \pi U_{12}N_{1/2} = V \). First we consider the popular model for 1111 family, the \( s_\pm \) wave state, where the two bands have isotropic but opposite sign gaps \( (\Delta_1 = \Delta_0, \Delta_2 = -y\Delta_0) \) and we take equal DOS \( (N_1 = N_2) \) for both the bands, which doesn’t affect the results qualitatively. The
parameter $y$ is a dimensionless constant, which controls the relative magnitudes of the order parameters in the two bands. For this case, we can solve Eq. 4–22 to get the resonance energy,

$$\frac{\omega_0}{\Delta_0} = \sqrt{\frac{[\theta(y+1)^2 + (y-1)^2] - \sqrt{[\theta(y+1)^2 + (y-1)^2]^2 - 16y^2}}{4}},$$  \hspace{1cm} (4–22)$$

where $\theta$ is,

$$\theta = \frac{(1 + 2U^2 + (U^2 - V^2)^2)^2 + 4V^2}{(1 + 2U^2 + (U^2 - V^2)^2)^2 - 4V^2}.$$

(4–23)

For the special case of equal magnitude and opposite sign gaps, we can simplify the resonance energy $\omega_0$ as,

$$\frac{\omega_0}{\Delta} = \pm \sqrt{\frac{1 + 2(U^2 - V^2) + (U^2 - V^2)^2}{1 + 2(U^2 + V^2) + (U^2 - V^2)^2}}.$$  \hspace{1cm} (4–24)$$

Here we can clearly see that with intraband scattering ($V = 0$), the resonance energy is equal to the gap energy and only in the isotropic scattering unitary limit ($V \to \infty$ with $U = V$), the resonance occurs at the Fermi level. Figure 4-1, shows the resonance energy as a function of disorder for various interband and intraband scatterings for symmetric ($y = 1$) and asymmetric ($y = 1.4$) $s_\pm$ wave states. Only in the isotropic limit the impurity resonance state formed at the Fermi level, and in case of intermediate interband scattering the bound state energy is close to the gap edge and above the Fermi level; in fact it is found to move to the gap edge in the unitary limit. This behavior does not depend on the relative magnitudes of the two gaps. In the case of an anisotropic state with deep minima in one of the bands, these results are qualitatively valid, because at low temperatures only the deep minimum energy scale matters and the problem is equivalent to a state with deep minima on the anisotropic band. The states at the Fermi level are important in the context of the residual linear term in thermal conductivity. In the next section, I discuss the results on in-plane thermal
conductivity for the 1111 family. The strength of disorder is measured with average normal state scattering rate $\Gamma$, which is defined as

$$\Gamma = \frac{n_{\text{imp}}}{\pi N_{\text{ave}}}, \quad \text{(4–25)}$$

where $N_{\text{ave}}$ is the average DOS and the strength of disorder potential is measured with scattering phase shift $c_i = 1/N_i U_{ii}$, where the subscript denotes the bands. In the unitary limit, the parameter $c_i$ is zero, and for the following discussion for 1111 systems, we take $c_i = 0.07$.

4.3 Model for 1111 Systems

For 1111 systems, we consider three different set of order parameters and attempt to put a constraint on the possible order parameter for these systems by comparing them to experiments. The first case we consider is the popular symmetric $s$-wave state \cite{46}, which I discuss first.

4.3.1 The $s_\pm$ Wave State

The order parameter for $s_\pm$ wave state is,

$$\Delta_1 = -\Delta_2 = \Delta_0. \quad \text{(4–26)}$$

We first take equal DOS at Fermi energy and equal Fermi velocity for two bands. We take equal intraband scattering $'U_d'$ for both the bands and look at the effect of different interband scattering $'U_{12}'$. From the numerical solution of the BCS gap equations, the value of $\Delta_0$ is $1.76 T_{c0}$ in the clean limit, where $T_{c0}$ is the critical temperature for the clean system. With $s_\pm$ wave superconductor with only nonmagnetic intraband disorder, the thermal conductivity is exponentially small ($\exp(-\Delta_0/ T)$) in the low temperature range, the same as a conventional fully gapped s wave superconductor. The lower panel of Fig. 4-2, shows $\kappa/ T$ as a function of temperature. A more interesting situation arises with the presence of interband scattering. With finite interband scattering, the residual linear term remains zero in the zero temperature limit, because the impurity band is
Figure 4-2. The DOS (top) and thermal conductivity (bottom) as a function of temperature for an isotropic $s_\pm$ state with $\Delta_1=-\Delta_2=1.7 \, T_{c0}$, shown for $U_d=U_{11}=U_{22}$ (intraband scattering) and scattering rate parameter $\Gamma=0.3 \, T_{c0}$ in cases (i) weak intraband scattering only, $U_d/U_{12}=0$ (solid line); (ii) pairbreaking scattering with the midgap impurity band, $U_{12}/U_d=0.98$ (dashed line); (iii) pairbreaking scattering with impurity band overlapping the Fermi level, $U_{12}/U_d=1.0$ (dotted line). The temperature is measured in units of the critical temperature $T_c$. 
Figure 4-3. Density of states (insert) and thermal conductivity for an isotropic $s_{\pm}$ state with isotropic scattering and same impurity potential as Fig. 4-2 but with different impurity concentration which gives $\Gamma = 0.2, 0.25, \text{and } 0.3 T_{c0}$.

...formed away from the Fermi level. Only the limit of isotropic impurity scattering leads to the impurity band at the Fermi level, as shown in the top panel Fig. 4-2. The finite DOS at the Fermi level gives rise to a finite linear term in the zero temperature limit. We next look at the linear term in case of isotropic disorder. Here we increase the impurity concentration ($n_{imp}$), which increases the quasiparticle DOS at the Fermi level. This increase in the Fermi level DOS is directly reflected in the zero $T$ limit of the residual linear term shown in Fig. 4-3. There is a finite linear term in case of isotropic impurity scattering, but it is very small compared to the normal state linear term.
Figure 4-4. (Top) Normalized thermal conductivity \( \frac{\kappa(T)}{\kappa_0} \) vs. \( \frac{T}{T_c} \) for the deep minima state on the second band (Eq. (4–27)). Results are shown for various values of intraband scattering rate \( \nu / T_c \). (Bottom) The density of states for the corresponding cases. The order parameters are \( \Delta_1 = -1.1 T_c \) and \( \Delta_2 = 1.3 T_c (1+0.9 \cos 2\phi) \).

4.3.2 State with Deep Minima

In this section, I look a state with deep minima on one of the bands. Spin fluctuation calculations have found state with deep minima or with accidental nodes on the electron sheet. The order parameter for one of the bands is taken to be isotropic and for the other band is,

\[ \Delta_2 = (\Delta_{iso} + \Delta_{ani} \cos 2\phi), \quad (4–27) \]
where \( \Delta_{\text{ani}} \leq \Delta_{\text{iso}} \). We take \( \Delta_1 = -1.1 T_{c0}, \Delta_{\text{iso}} = 1.3 T_{c0} \) and \( \Delta_{\text{ani}}/\Delta_{\text{iso}} = 0.9 \) in the clean limit, where \( T_{c0} \) is the clean limit transition temperature. In such systems, the deep gap minima energy scale \( \Delta_{\text{min}}(\equiv \Delta_{\text{iso}} - \Delta_{\text{ani}}) \) plays a very important role in low temperature transport. For the temperatures \( T < \Delta_{\text{min}} \), the system shows the behavior of a fully gapped superconductor and in the temperature range \( \Delta_{\text{min}} < T < \Delta_1 \), we see a different behavior dominated purely by the anisotropic band. First we examine the effect of pure intraband scattering. As shown in the Fig. 4.3.2, pure intraband scattering leads to averaging of anisotropic component of the order parameter and increase in \( \Delta_{\text{min}} \) energy scale. Due to this fully gapped behavior, \( \kappa/T \) remains exponentially small at very low temperatures. Next we consider the isotropic limit, which allows formation of impurity bound states at the Fermi level. As soon as the presence of interband disorder induces quasiparticles at the Fermi level, the residual term rises rapidly. Fig. 4-5, shows the effect of disorder for various values of \( \Gamma \). Here disorder causes a linear term, which is much stronger than \( s_{\pm} \) wave states. Unlike d wave superconductors, the zero temperature limit of the residual linear term is not independent of disorder. We can estimate the effect of disorder from Eq. 4–7,

\[
\frac{\kappa}{T} \approx \frac{N_2 V_{F2}^2 \pi}{6} \frac{\Gamma_2^2}{\Gamma_2^2 + (\Delta_{\text{iso}} + \Sigma_{2,1} - \Delta_{\text{ani}})^2} \frac{1}{\Delta_{\text{ani}}(\Delta_{\text{iso}} + \Sigma_{2,1} - \Delta_{\text{ani}})} + \frac{N_1 V_{F1}^2 \pi^2}{6} \frac{\Gamma_1^2}{\Gamma_1^2 + (\Delta + \Sigma_{1,1})^2}^{3/2}.
\]

(4–28)

To get Eq. 4–28, we use the fact that integrand in Eq. 4–7 is sharply peaked at deep minima (\( \phi = \pi/2 \)), so we do series expansion of the order parameter near the minima as,

\[
\Delta_2 = -(\Delta_{\text{iso}} + \Delta_{\text{ani}} \cos 2\phi),
\]

(4–29)

\[
= -(\Delta_{\text{min}} + 2\Delta_{\text{ani}} (\phi - \phi_0)^2),
\]

(4–30)

where \( \phi_0 = \pi/2, 3\pi/2 \) are the locations of the minima. Fig. 4-6, shows both the estimated and the full numerical value of the residual linear term as a function of
Figure 4-5. Density of states $N(\omega)/N_0$ (top) and normalized thermal conductivity $\kappa(T)/\kappa_n(T)$ vs. $T/T_c$ for two band anisotropic model with deep gap minima on one band. The order parameters are $\Delta_1=-1.1 T_{c0}$ and $\Delta_2=1.3 T_{c0}(1+0.9\cos 2\phi)$. 
Figure 4-6. $\kappa / T$ in $T \to 0$ limit, for the state with deep gap minima. $\kappa_{00}$ is thermal conductivity for pure d-wave state. This figure shows the total thermal conductivity for the two bands.

disorder. The size of the linear term is measured in $\kappa_{00} / T$, which is the linear term for a d wave superconductor with order parameter $\Delta_{ani} \cos 2\phi$ given as,

$$\frac{\kappa_{00}}{T} \approx \frac{N v_F^2 \pi^2}{3\pi} \frac{1}{\Delta_{ani}},$$

(4–31)

Obtaining a finite linear term requires large interband scattering for the isotropic $s_\pm$ case. Such strong interband scattering causes a huge suppression of $T_c$, which is shown in Fig. 4-7. This doesn’t seem to be consistent with results on the material LaFePO, which is stoichiometric and therefore very clean [104]. This material also exhibits a linear $T$ penetration depth, which cannot be produced by disorder [103]. So
Figure 4-7. Effect of intraband and isotropic (equal strength inter and intra band impurity scattering) on $T_c$ in the unitary limit, for the case with deep minima on one of the bands.

we look to another picture, where one band has accidental nodes, which I discuss in the next section.

### 4.3.3 Nodal State

An A1g state with accidental nodes similar to Fig. 3-2 is achieved by the same order parameter described by Eq. 4–27, but with the condition $\Delta_{\text{ani}} > \Delta_{\text{iso}}$. This gives a set of twin nodes around $\phi = \pi/2, 3\pi/2$. For the following discussion, we set $\Delta_{\text{ani}}/\Delta_{\text{iso}} = 1.3$ and in the clean limit $\Delta_1 = -1.1 T_{c0}$, $\Delta_{\text{iso}} = 1.2 T_{c0}$, where $T_{c0}$ is the critical temperature for the clean system. The effect of disorder on the order parameters is included by solving the gap equations self consistently with renormalized Green’s function. We
Figure 4-8. Density of states normalized to total normal state DOS \( N(\omega)/N_0 \) for the nodal case. Results are shown for various values of intraband scattering rate \( \Gamma/T_c \). \( \Gamma = 0.4 T_c \) corresponds to node lifted state and shows a gap of \( 0.03 T_c \) in DOS. The order parameters are \( \Delta_1 = -1.1 T_c \) and \( \Delta_2 = 1.2 T_c(1+1.3\cos 2\phi) \).

only consider pure intraband scattering for the nodal state, keeping in mind LaFePO, which is a stoichiometric compound and estimated mean free path for the samples are \( \sim 94 \text{nm} \). In the clean limit, there is finite linear term, which increases with disorder and then abruptly goes away as soon as the nodes are lifted by disorder. Fig. 4-8 shows the DOS for various values of disorder, and Fig. 4-9 shows the residual linear thermal conductivity as a function of temperature for various values of disorder. The residual linear term depends on disorder for systems with accidental nodes and
is not universal like d wave superconductors. The break down of universality is due to
the renormalization of the gap velocity $v_\Delta$. The form of the linear term is otherwise still
independent of single particle scattering rate $\Gamma$, as in the d wave case. Fig. 4-10, shows
the linear term as a function of disorder. We can estimate the linear term using Eq. 4–7.
In this case, most of the contribution to the linear term comes from nodes, hence we can
linearize the order parameter near the nodes as

$$\Delta_2 = -(\Delta_{iso} + \Delta_{ani} \cos 2\phi), \quad (4–32)$$

$$\Delta_2 = (v_\Delta (\phi - \phi_0)^2), \quad (4–33)$$
where $\nu_\Delta$ is

$$\nu_\Delta = \sqrt{\Delta_{ani}^2 - \Delta_{iso}^2},$$

and with this nodal approximation we can get an estimate for $T = 0$ limit of $\kappa / T$,

$$\frac{\kappa}{T} \approx k_B^2 h \frac{2\pi^2}{3} \frac{N_0 v_F^2}{\sqrt{\Delta_{ani}^2 - \Delta_{iso}^2}} = k_B^2 \frac{\pi}{h^d} \frac{m_e v_F^2}{3 \sqrt{\Delta_{ani}^2 - \Delta_{iso}^2}}.$$
Here we have taken into account the layered structure of LaFePO by taking DOS \( N_0 = m/2\pi h^2 d \), where \( d = 0.85 \text{nm} \) is c axis unit cell length and \( m_e \) is the electron mass. To estimate the Fermi velocity, we use the coherence length \( (\xi_0 \sim \hbar v_F/2\pi T_c) \), which is \( 18 \text{nm} \) estimated from the upper critical field \([104]\). This gives \( v_F = 10^5 \text{m/s} \) and for the order parameter we take \( \Delta_{\text{iso}} = T_c = 7K \) and \( \Delta_{\text{ani}} = 1.3\Delta_{\text{iso}} \). These numbers give \( \kappa/T = 0.25W/K^2m \), which is very close to the experimentally measured value of \( \kappa/T = 0.3W/K^2m \). In the next section, I will discuss the model used for studying the 122 systems.

### 4.4 Model For 122 Systems

The 122 family based on the parent compound BaFe\(_2\)As\(_2\) has attracted many researchers because good single crystals with reasonably good surfaces can be grown easily. Many groups have measured low T transport and thermodynamic properties for both the hole doped Ba\(_{1-x}\)K\(_x\)Fe\(_2\)As\(_2\) systems and electron doped Ba(Fe\(_{1-x}\)Co\(_x\))\(_2\)As\(_2\), Ba(Fe\(_{1-x}\)Ni\(_x\))\(_2\)As\(_2\). The major difference between these 122 compounds and 1111 compounds is dimensionality. The 122 family seem to be much more three dimensional, while on the other hand the 1111 is very two dimensional like cuprates \([42, 44]\). Band structure calculations have found significant c axis dispersion for both the hole doped and the electron doped systems \([132–135]\). There is a significant quantitative discrepancy between different band structure groups, but the qualitative nature of 3D character for hole pockets have been found by all. ARPES measurements on Ba(Fe\(_{1-x}\)Co\(_x\))\(_2\)As\(_2\) have also reported strong 3D character of hole pockets \([136–139]\), and both the ARPES measurements and band structure calculation suggests that 3D character of hole sheets increases with electron doping. Microscopic spin fluctuation calculations of gap symmetry have found 3D nodal states on hole pockets \([40, 48]\) for the 122 family. Inelastic neutron scattering experiments on electron doped Ba(Fe\(_{1-x}\)Ni\(_x\))\(_2\)As\(_2\) also suggest three dimensional nodal structure \([140]\). Further evidence of 3D nodal states come from penetration depth and thermal conductivity...
Figure 4-11. Zero temperature limit of normalized residual linear term as a function of Co doping for Ba\((\text{Co}_x\text{Fe}_{1-x})_2\text{As}_2\) in \(H=0\) and in \(H=H_{c2}/4\). \(H_{c2}\) is the upper critical field for respective dopings [42].
measurements [42, 44]. Reid et al. have performed a systematic doping dependent measurement of the zero temperature limit residual linear term on Ba(Co$_x$Fe$_{1-x}$)$_2$As$_2$ [42]. In the absence of a magnetic field, they reported zero residual linear term for in-plane heat current within experimental resolution, but along the c axis for some dopings they found a residual linear term of order 1 $\mu W/K^2 cm$. In the presence of magnetic field both directions show similar values when normalized to their respective normal state values. Fig. 4-11 illustrates the normalized linear term as a function of doping with and without the presence of the magnetic field. To model these systems, we consider three different possible kinds of Fermi surfaces, keeping in mind the quantitative disagreement between different groups regarding the amount of c axis dispersion. We need the Fermi velocities and Fermi momentum for calculating the transport properties and we used the Fermi surfaces calculated using density functional theory (DFT) shown in Fig. 4-12. For the electron sheet ($S_2$ in Fig. 4-13), we consider an anisotropic state with deep minima,

$$\Delta_{S_2} = \Delta_0 (1 + r \cos 2\phi).$$  \hfill (4–36)

The gap values are taken as phenomenological input here to match our results with experiments. We set $\Delta_2 = 1.5 meV$ and $r = 0.9$ for all the cases. For the hole sheets, we consider two different kinds of order parameters,

$$\Delta^1_{S_1} = \Delta_0 [1 + r \cos 4\phi (1 - \cos k_z)].$$  \hfill (4–37)

which is qualitatively similar to the order parameter obtained by Graser et al. [40], in their spin fluctuation calculations. The other order parameter considered here for the hole sheet is,

$$\Delta^2_{S_1} = \Delta_0 [1 + r \cos k_z].$$  \hfill (4–38)
Figure 4-12. The root mean square in plane and out of plane Fermi velocities $v_{F,xy}$ and $v_{F,z}$ respectively are plotted vs. $ck_z/2$ for the five different cases, we consider. Fermi velocities used in calculations are renormalized by a factor of 4 to take into account the effective mass.
Figure 4-13. Fermi surfaces $S_1$ for the hole pocket for cases 1-5 with their respective nodal structures indicated by dark blue line. The electron sheet $S_2$ considered for all cases, with location of gap minima (dark blue dashed lines) shown by dashed blue line.

Fig. 4-13 shows different Fermi surfaces and the nodal structure of the theoretically proposed order parameters. We consider five cases: The first two cases are with Fermi surface with weak $k_z$ dispersion and order parameter for the hole sheet with V shaped nodes $\Delta_{S_1}^1$ and $\Delta_{S_1}^2$ respectively. The next two cases are combinations of more flared Fermi surface with $\Delta_{S_1}^1$ and $\Delta_{S_1}^2$ respectively. The last case is with the closed hole pocket and horizontal line node $\Delta_{S_1}^2$. Experiments on Co doped BaFe$_2$As$_2$ have found a finite linear term along c axis, but no linear term for the in-plane direction. Keeping this in mind, we choose the locations of horizontal line nodes to get maximum c axis transport. This is possible if the nodes are located in a place where the c axis Fermi velocity is large (See Table 4-2). For all the cases, we use same electron pocket $S_2$, with the order parameter given by Eq. 4–36. Table 4-1 summarizes the basic parameters used for
Table 4-1. Basic parameters used for different models in calculations for case 1 to 5. $\Delta_0$ is the magnitude of order parameter in meV, $r$ is the anisotropy parameter, $v_{F,xy,\text{ave/nodal}}$ are the average and nodal unrenormalized Fermi velocities for in the plane ($v_{F,xy}$) and out of the plane ($v_{F,z}$) directions in the unit of $10^4$ m/s.

<table>
<thead>
<tr>
<th></th>
<th>$S_1$ (Case 1)</th>
<th>$S_1$ (Case 2)</th>
<th>$S_1$ (Case 3)</th>
<th>$S_1$ (Case 4)</th>
<th>$S_1$ (Case 5)</th>
<th>$S_2$ (For all)</th>
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<td>$\Delta_0$ (meV)</td>
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<td>-8.6</td>
<td>-9.4</td>
<td>-8.4</td>
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<td>$r$</td>
<td>0.9</td>
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<td>0.9</td>
<td>1.2</td>
<td>1.1</td>
<td>0.9</td>
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<td>$v_{F,xy,\text{ave}}$</td>
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<td>3.15</td>
<td>2.90</td>
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<td>0.69</td>
<td>0.23</td>
<td>4.13</td>
<td>1.26</td>
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calculation of the linear thermal conductivity. We focus on the zero temperature limit of the residual linear term $\kappa / T$ with only intraband impurity scattering in the unitary limit.

4.4.1 Zero Temperature Residual Term

The $T = 0$ limit of the linear $T$ thermal conductivity term is evaluated using

$$\frac{\kappa_\alpha}{T} \simeq n \frac{k_B^2}{16 \pi \hbar^2} \frac{4 \pi^2}{3} \sum_i \left( k_{Fi,\perp} (v_{Fi,\perp} \cdot \hat{\alpha})^2 \frac{\Gamma_{0i}^2}{(\tilde{\Delta}_i^2 + \Gamma_{0i}^2)^{3/2}} \right)_{k_2,\phi}. \quad (4-39)$$

Here $k_{Fi,\perp}$ and $v_{Fi,\perp}$ are the in plane components of the Fermi momentum and the Fermi velocity respectively for the $i^{th}$ band, $k_{Fi,\perp}/v_{Fi,\perp}$ is the effective mass term for an anisotropic layered system. The renormalized order parameters and the scattering rates are

$$\tilde{\Delta}_i = \Delta_i(\mathbf{k}) + \Sigma_{i,1}(\omega = 0), \quad (4-40)$$

$$\Gamma_i = -\text{Im} \Sigma_{i,0}(\omega = 0), \quad (4-41)$$

where self energies are calculated using the equations 4–13, 4–14, 4–15 and 4–16.

We first calculate the linear term in absence of an external magnetic field and in the next section 4.4.2, I discuss the effect of the magnetic field in detail. We first look at cases 1 and 2, for which the Fermi surface has weak dispersion along the c axis. Fig. 4-14 shows the residual thermal conductivity both in absolute units and the normalized values. The latter are obtained by taking the ratio of absolute values with respective
Table 4-2. Residual linear term in low T thermal conductivity in $\mu W/K^2 cm$ for various pnictide compounds.

<table>
<thead>
<tr>
<th>Material</th>
<th>In plane</th>
<th>c axis</th>
<th>References</th>
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<td>LaFePO</td>
<td>1900</td>
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<td>[104]</td>
</tr>
<tr>
<td>BaFe$<em>{2}$$(\text{As}</em>{1-x}\text{P}_x)_2$</td>
<td>250</td>
<td></td>
<td>[123]</td>
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<tr>
<td>FeSe$_{0.82}$</td>
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<td>[141]</td>
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<tr>
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<td>2.3</td>
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<td>0.9</td>
<td></td>
</tr>
<tr>
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<td>0.9</td>
<td>[42]</td>
</tr>
<tr>
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<td>3.8</td>
<td></td>
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<tr>
<td>BaFe$<em>{1.746}\text{Co}</em>{0.254}\text{As}_2$</td>
<td>17</td>
<td>5.6</td>
<td></td>
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</tbody>
</table>

Figure 4-14. Residual linear term in $T \rightarrow 0$ limit as a function of total normal state scattering rate $\Gamma$ in meV, for case 1 (a,b) and case 2 (c,d). The solid line shows the in plane direction and dashed line shows c axis. Panels a and c show absolute value of the linear term in $\mu W K^{-2} cm^{-1}$ for case 1 and 2 respectively and panels b and d show linear term normalized to normal state thermal conductivity $\kappa_N / T_c$ for case 1 and 2.
Figure 4-15. Residual linear term in $T \to 0$ limit as a function of total normal state scattering rate $\Gamma$ in meV, for case 3 (a,b) and case 4 (c,d). The solid line shows the in plane direction and dashed line shows c axis. Panels a and c show absolute value of the linear term in $\mu W K^{-2} cm^{-1}$ for case 3 and 4 respectively and panels b and d show linear term normalized to normal state thermal conductivity $\kappa_N / T_c$ for case 3 and 4.

normal state values ($\kappa_N$) at $T_c$ given as

$$\kappa_N = \frac{\pi}{12} \frac{n k_B^2 T_c}{\hbar d} \sum_i \left\langle \frac{k_{Fi,\perp}}{v_{Fi,\perp}} (\mathbf{v}_{iF} \cdot \mathbf{\hat{a}})^2 / \Gamma_i \right\rangle_{\phi, k_z}, \quad (4-42)$$

where $\sum_i$ is sum over all the bands. We see qualitatively different behavior of the in-plane linear term for V shaped and horizontal line nodes. For V shaped line nodes, the linear term $\kappa / T$ is roughly constant up to a critical value of disorder ($\Gamma_{NL}$) and then rapidly goes to zero as shown in panel (a) of Fig. 4-14. This critical value of disorder is the node lifting point. In presence of pure intraband scattering, the anisotropic
component of the order parameter goes down and eventually the system becomes fully gapped, as discussed in the last chapter in detail. For horizontal line nodes, $\kappa / T$ increases with disorder and then goes to zero at $\Gamma_{NL}$. On the other hand, c axis values monotonically decrease with disorder. The c axis values are extremely small for these cases compared to in-plane values, and normalized value for both directions are very small. In this case, “small” means both small compared to the value expected for the universal result with fully developed line nodes, and comparable or smaller than experimental resolution. We next consider case 3 and 4, of Fig. 4-13 which have much stronger dispersion along c axis compare to cases 1 and 2. The qualitative behavior for in-plane $\kappa / T$ is same as the earlier two cases, but we see a huge difference in the magnitudes of absolute and normalized values. In these cases, the c axis transport is comparable with in-plane transport and normalized values for c axis are larger than in-plane normalized values, as seen in the experiments by Reid et al. The c axis $\kappa / T$ increases with disorder, before going to zero at $\Gamma_{NL}$. The horizontal line nodes produces more quasiparticles than the V shaped nodes, but they go away at a faster rate than V shaped node in the presence of intraband scattering. In case 5, where we consider horizontal line nodes on a closed Fermi surface, the in-plane linear term decreases with disorder because the node move towards the zone face and the in-plane Fermi velocity near the nodes goes down. In this case, the linear term in both directions is comparable but the normalized values for c axis are very large compare to in plane normalized values. The main problem with case 5 is that the $\Gamma$ estimated for experimental samples can easily lift the nodes and create a fully gapped system. The presence of finite interband scattering in the unitary limit does not make any difference, but for isotropic scattering when both intraband and interband are equally strong, the impurity bound states will be on the Fermi level. In such situation, the residual linear term will be large and anisotropy between the in-plane and the c axis direction will be same as in the normal state, but this picture is against the experimental results [42]. Another quantity
Figure 4-16. Residual linear term in $T \rightarrow 0$ limit as a function of total normal state scattering rate $\Gamma$ in meV, for case 5. The solid line shows the in plane direction and dashed line shows c axis. Panel a and b shows absolute value of the linear term in $\mu W K^{-2} cm^{-1}$ and linear term normalized to normal state thermal conductivity $\kappa_N / T_c$ for case 5 respectively.

which the experimentalists have stressed is the normalized anisotropy of thermal conductivity $\gamma_\kappa$,

$$\gamma_\kappa = \frac{\kappa_c / \kappa_{CN}}{\kappa_{ab} / \kappa_{abN}}.$$  \hfill (4-43)

For c axis currents, the normal state thermal conductivity is small compared to the ab-plane, so the normalized conductivity $\kappa / \kappa_N$ is large for the c axis even when the absolute values for the c axis are small. So the value of $\gamma_\kappa$ is close to 10 for 122 systems. Fig. 4-17 shows thermal conductivity anisotropy as a function of disorder for all cases in consideration. Next we consider the effect of external magnetic field.

4.4.2 Magnetic Field Dependence

The effect of magnetic field is studied within the Doppler shift approximation, which is qualitatively a good approximation at low temperature and low fields[142–144]. This is a semiclassical approach, where the energy of the quasiparticle moving in the superfluid velocity field $\mathbf{v}_s(\mathbf{r})$ of the vortex lattice experiences a shift of energy $\delta \omega$ given by,

$$\delta \omega = m \mathbf{v}_F \cdot \mathbf{v}_s,$$  \hfill (4-44)
Figure 4-17. Thermal conductivity anisotropy $\gamma_n$ for all cases as a function of normalized disorder. $\Gamma_{NL}$ is critical value of disorder, which lifts the nodes.

where $v_F$ is the Fermi velocity and $v_s$ is the supercurrent velocity around the vortex core, which is given as,

$$v_s = \frac{\hbar}{2mr} \hat{\theta}. \quad (4-45)$$

Here $r$ is the distance from the vortex core and $\hat{\theta}$ is the circular direction perpendicular to the direction of applied field $H$ and tangential to the circle of radius $r$ from the vortex core. For a magnetic field along the c axis, the Doppler shift energy becomes,

$$\delta \omega = \frac{\hbar}{2r} v_F \sin(\theta - \phi) = \frac{E_H}{\rho} \sin(\theta - \phi), \quad (4-46)$$
where $\theta$ is the vortex winding angle, $\phi$ is the angle of $\mathbf{v}_F$ in momentum space and the energy scale $E_H$ is $\hbar v_F/2R_H$. $R_H$ is the magnetic scale defined as

$$R_H = \sqrt{\frac{\Phi_0}{\eta H}}, \quad (4–47)$$

where $\Phi_0$ is the magnetic flux quantum and $H$ is the external field. $\eta$ is a constant of order unity and depends on structure of the vortex lattice. We have taken a triangular vortex lattice for which $\eta$ is 0.433. This Doppler shift approximation is valid as long as the applied field is much smaller than the upper critical field ($H_{c2}$) (see [145] for a comparative study of various semiclassical methods). The Green’s function in the presence of the magnetic field becomes

$$G = \frac{(\tilde{\omega} - \delta \omega) \mathbf{i} + \tilde{\Delta}_k \mathbf{\hat{r}}_1 + \xi_k \mathbf{\hat{r}}_3}{(\tilde{\omega} - \delta \omega)^2 - \tilde{\Delta}_k^2 + \xi_k^2}. \quad (4–48)$$

All local physical quantities are now calculated by using the Doppler shifted Green’s function and then local quantities are averaged over the vortex lattice. The exact way of averaging depends on the nature of the physical quantity [143]. For specific heat or density of states the averaging is done in following way,

$$\langle F(H, T) \rangle = \frac{1}{\pi R_H^2} \int_0^{R_H} dr \int_0^{2\pi} d\theta F(r, \theta; H, T). \quad (4–49)$$

This particular way of averaging is appropriate for the c axis thermal conductivity, when the field is along the c axis (heat current $\parallel$ to the field). For thermal currents in-plane with field along the c axis, different regions of vortex do not contribute equally, but they may be considered to form an effective series combination. For such situations the following average is more appropriate,

$$\langle F^{-1}(H, T) \rangle = \frac{1}{\pi R_H^2} \int_0^{R_H} dr \int_0^{2\pi} d\theta \frac{1}{F(r, \theta; H, T)}. \quad (4–50)$$

For systems with three dimensional nodes and strong 3 dimensional Fermi surface, the actual situation is more complicated and is combination of both series and parallel
Figure 4-18. Residual linear term in T→0 limit as a function of applied magnetic field \( H \) in Tesla, for case 1 (a,b) and case 2 (c,d). The solid black line shows series averaging and dashed black lines shows parallel averaging for the in plane direction and solid red line shows \( \kappa / T \) axis. Panels a and c show the absolute value of the linear term in \( \mu W K^{-2} cm^{-1} \) for case 1 and 2 respectively and panels b and d show the linear term normalized to normal state thermal conductivity \( \kappa_N / T_c \) for case 1 and 2.

combinations. Hence here we consider both the series \( \langle \kappa^{-1} \rangle \) and the parallel averaging \( \langle \kappa \rangle \) as limits to a more sophisticated averaging procedure. We note that the parallel average appears to be closer to the results of the Brandt, Pesch and Tewordt (BPT) approach, valid at higher fields [79, 146–149]. We focus on the qualitative aspects of the field dependence in low magnetic field in the zero temperature limit, hence use the Doppler shift method, with the further assumption that the field does not change the order parameter much, and keep the upper critical field \( H_{c2} \approx 40T \). The value of
the disorder scattering rate is chosen to fix the normal state value of $\kappa_N/T_c$ close to experimental values. For the cases 1 and 2 $\Gamma$ is 0.1meV, for case 3 and 4 $\Gamma$ is 0.3meV and for case 5 $\Gamma$ is 0.01meV. For case 5, such a small value of disorder is chosen to keep the nodes. Any experimentally relevant value is sufficient to remove the nodes. For the first two cases, the in-plane direction has a stronger response to the magnetic field than the out of plane direction. On the other hand, the c axis shows a strong response in normalized plots as shown in Fig. 4-18; this is due to the smaller normal state value
Figure 4-20. Residual linear term in $T \to 0$ limit as a function of applied magnetic field $H$ in Tesla for case 5. Panel (a) and panel (b) show the absolute value of the linear term in $\mu W K^{-2} \text{cm}$ and the linear term normalized to normal state thermal conductivity $\kappa_N/T_c$ respectively. The solid black line shows series averaging and dashed black lines shows parallel averaging for the in plane direction and solid red line shows $\kappa/T$ c axis.

The big difference between the series and the parallel averaging is also evident from Fig. 4-18. The series averaging has a curvature at low $H$, but the parallel averaging gives very linear behavior. Next we look at cases 3 and 4, which have more flared Fermi surfaces; the results are shown in Fig. 4-19. In zero field, the linear terms are comparable for both directions, but in the presence of a magnetic field, the ab plane direction has a strong field response. This is due to a order parameter with deep minima on the electron sheet. As soon as the Doppler shift energy becomes comparable to the deep minima energy scale, electron sheets make significant contribution due to large Fermi velocities. For these cases, both kinds of averaging show curvature at low field which is observed in experiments. For these cases, normalized linear terms are comparable, which is also consistent with the experiments. For case 5, as shown in Fig. 4-20, the magnetic field response of the ab plane is weaker than the c axis, because the nodes move to very close to the top of the Fermi surface, where the ab plane Fermi velocity is very small but the c axis component of the Fermi velocity is large. Again
in this case, there is significant difference between the series and parallel averaging. These two averaging procedures give two limits of the actual situation.

It appears that experimental results favor a flared Fermi surface and the flaring is increasing towards higher doping. To model this, we assume that the Fermi surface is changing linearly and the Fermi surfaces used in cases 1 and 2 and case 3 and 4 are two end points to this “line”. We calculate other Fermi surfaces by using this equation for the Fermi momentum and the Fermi velocities. The equation for this line is,

\[ \chi_n(\mathbf{k}) = \chi_1(\mathbf{k}) + \frac{t}{0.15} (\chi_2(\mathbf{k}) - \chi_1(\mathbf{k})) \]  

(4–51)
Here \( \lambda \) denotes the various Fermi momenta or velocities, and \( t \) is the parameter to generate the evolution. This is a very crude approach, but we can gain some understanding about the doping dependence this way. Fig. 4-21, shows some of the Fermi surfaces along this line. We calculate the residual linear term in zero field and in 10 Tesla field, shown in Fig. 4-22. We define \( \nu_{Fc}^{max} / \nu_{Fc}^{ave} \) as a parameter of flaring. This is not a monotonic function of parameter \( t \). The flaring parameter is 1.49 (\( t = 0 \)) for the Fermi surface used in case 1 and 2.44 for the Fermi surface used in case 3. We use the same V shaped order parameter used in case 1 and 3. Disorder is chosen to keep the in plane normal state linear term \( \sim 240 \mu W K^{-2} cm^{-1} \). Fig. 4-22 shows
the normalized linear term as function of flaring. The comparison to Fig. 4-11 is quite compelling, and suggests that doping increases the flaring. It shows very clearly that a flared Fermi surface is consistent with experimental results. At \( H = 10 \, T \), for flared surface normalized linear terms are comparable in two directions.

The magnetic field can be used to find the locations of nodes on the Fermi surface \([119, 120]\). In the next section, we propose a method to find the nodal structure of in such three dimensional systems.

### 4.5 Three Dimensional Field Rotation

The magnetic field angle dependence measurement of the thermal conductivity or specific heat is a very powerful method of locating the nodes in unconventional superconductors and has been used extensively by many research groups \([144, 150]\). Recently, angle dependent specific heat measurements have been made by Zeng et al. \([151]\) on FeSe\(_{0.45}\)Te\(_{0.55}\), which has minima in specific heat along the \( \Gamma M \) direction at low temperatures. These minima get inverted at higher temperatures \([152, 153]\). Here we propose a generalization of this method to find the structure of the order parameter by rotating the magnetic field with respect to the crystal axes. We consider the c axis thermal conductivity and calculate it as a function of field direction. Measurement of c axis thermal conductivity is practically very difficult for a general direction of magnetic field, but measurement of the specific heat coefficient at low temperature is a relatively easier task. For a magnetic field which makes an angle \( \Theta_Z \) with the c axis and \( \Phi \) from a axis, the Doppler energy is given by,

\[
E_H(k_z, \phi) = \frac{1}{2 R_H} \left[ v_F^{ab}(k_z) \left[ -\sin \theta \cos \Theta_Z \cos(\phi - \Phi) + \cos \theta \sin(\phi - \Phi) \right] + v_F^c(k_z) \sin \theta \sin \Theta_Z \right].
\] (4–52)

Here \( \theta \) is the vortex winding angle and \( \phi \) is the angle of the quasiparticle momentum from \( k_x \) axis. For this section, we take \( \Delta_{0,\text{hole}} = 0.3 \, meV \) and \( \Delta_{0,\text{electron}} = 1.3 \, meV \), which is appropriate for highly overdoped systems at \( H = 10 \, T \). We take two electron pockets
Figure 4-23. Normalized linear term as a function of magnetic field’s polar angle $\Theta_Z$ and azimuthal angle $\Phi$.

To restore the fourfold symmetry with $r = 0.9$. The minimum of the order parameter is located along the $(0, 0)$ to $(\pi, 0)$ and $(0, 0)$ to $(0, \pi)$ lines. The hole pocket V shaped nodes are rotated by $\pi/4$ compare to our previous calculations to bring the nodal V shapes along the Fe-Fe bond direction in the real space [40]. This rotation does not affect any of the earlier results. Fig. 4-23 shows the c axis residual linear term as a function of polar ($\Theta_Z$) and azimuthal angle ($\Phi$) from the crystal axes. We perform this calculation in the clean limit, since disorder tends to suppress the anisotropy. $\Phi = 45^0$ is location of the hole sheet nodes in the real space with respect to crystal axis a.

The thermal conductivity along the c axis does not show much variation as a function
azimuthal angle but along polar angle there is a minimum at $\Theta_Z = 0^\circ$. We have used in case 1. For a cylindrical Fermi surface, the direction of the nodes clearly show up in the magnetic field rotation; but for three dimensional flared Fermi surface, the momentum dependence of the c axis Fermi velocity and the band mass strongly affects the linear term. This happens because the thermal conductivity is proportional to the square of the Fermi velocity. We next consider the specific heat at low temperature, which is calculated by evaluating the following integral,

$$C(H, T) = -\frac{1}{2} \int_{-\infty}^{\infty} d\omega \frac{\omega^2}{T^2} sech^2 \left( \frac{\omega}{2T} \right) \int d\mathbf{k} \frac{1}{\pi} < \text{Im} G(\mathbf{k}, H) >_{\text{vortex}}.$$  

(4–53)
Here $<>_{\text{vortex}}$ is the average over the vortex unit cell. Fig. 4-24 shows the specific heat coefficient $C/T$ in the zero temperature limit normalized to its normal state value. This figure shows a weaker effect of the anisotropic Fermi surface and clearly shows minima at $\Phi = 45^\circ$ near $\theta_z = 90^\circ$. At high fields, the contributions from two electron pockets, dominate the specific heat. Only with very high experimental resolution can these small features in the specific heat be observed.

### 4.6 Conclusion

In this chapter, we considered models for explaining the thermal conductivity measurements on the 1111 and 122 families of pnictides. For the 1111 family compound LaFePO, we find that an order parameter with accidental nodes on electron pockets can be used to explain the experimental data. On the other hand, we considered nodes with three dimensional structure on the hole sheet and found that the V shaped nodes suggested by microscopic theory are consistent with the experiments, but the structure of the Fermi surface is equally important. It appears that the hole pockets are three dimensional and they change with doping. We also propose a method to detect the three dimensional nodal structure by using an angle dependent specific heat and thermal conductivity measurement. Although these methods are quite difficult experimentally, with recent advances in experimental techniques they may be possible. Further investigation is required to understand and use this 3D rotation methods. In the next chapter, I discuss the penetration depth for the models considered in this chapter and compare them with experimental measurements.
CHAPTER 5
TRANSPORT II - PENETRATION DEPTH

5.1 Introduction

Low temperature penetration depth is another bulk probe like thermal conductivity which provides information about low energy quasiparticles. Typically the absolute value of penetration depth ($\lambda$) is not measured, but the change in its value $\Delta \lambda$ from the zero temperature value $\lambda_0$ is measured as a function of temperature [154]. Theoretically, the absolute value of penetration depth depends on the details of band structure for all occupied states, but the relative change $\Delta \lambda$ with temperature depends only on the low energy quasiparticles and is proportional to quasiparticle density of states at low temperatures ($T \ll T_c$). For conventional fully gapped s wave superconductors, $\Delta \lambda$ is exponentially small in the low temperature regime. On the other hand for d wave superconductors it is linear in temperature in the clean limit and shows a $T^2$ behavior in dirty limit [155]. For multiband systems, like pnictides or MgB$_2$, experiments measure the overall contribution of all Fermi surface sheets, so analysis of such systems is more complicated. In these systems, multiple bands can lead to some kind of effective power law in a specific temperature range. Bands with large isotropic gap do not affect the low temperature $\Delta \lambda$. The penetration depth is related to the current response of the system to an external field as,

$$\frac{1}{\lambda^2} = \mu_0 K(q = 0, \omega = 0).$$  \hspace{1cm} (5–1)

Here $\mu_0$ is the permeability of free space and $K$ is total electromagnetic response of the system, defined as,

$$j(q, \omega) = K(q, \omega)A(q, \omega),$$  \hspace{1cm} (5–2)

where $A$ is the external vector potential and $j$ is the current. The current operator is given as,

$$j(q) = e \sum_{k, \sigma} v_{k-q, \sigma}^c c_{k, \sigma}.$$

\hspace{1cm} (5–3)
Here $\psi^\dagger, \psi$ are the creation and annihilation operators, respectively, and $\mathbf{v}$ is the quasiparticle velocity. A general derivation for any system is given in Appendix B.

For the models, we are interested in one can replace $\mathbf{v}$ by the Fermi velocity, since only the low energy quasiparticle close to the Fermi surface contribute to $\Delta \lambda$. The electromagnetic response is written as,

$$K^\alpha(q, i\nu) = -T \sum_{\omega_n, k} \frac{d^2 \xi_k}{dk^2} \text{Tr} \left[ (\hat{\tau}_0 + \hat{\tau}_3) G(k, i\omega_m) \right] + \mathbf{v}_\alpha^2 \text{Tr} \left[ G(k+q, i\omega_m) G(k, i\omega_m - i\nu) \right].$$

(5–4)

Here $\omega_n$ and $\nu$ are the Matsubara frequencies, $\hat{\tau}_0, \hat{\tau}$ are the identity and the Pauli matrix respectively, and $\alpha$ denotes the direction of the current assuming that the response tensor is diagonal. $G$ in Eq. 5–4 is impurity dressed Green’s function within the T-Matrix approximation. For multiband systems, the total penetration depth is is sum of contributions from each band,

$$\frac{1}{\lambda^2} = \sum_i \frac{1}{\lambda_i^2}. \tag{5–5}$$

For a layered system, after evaluating the expression given by Eq. 5–4 and taking the analytic continuation to real frequencies, we find for the penetration depth,

$$\frac{1}{\lambda^2} = \sum_i \frac{1}{\lambda_i^2}. \tag{5–6}$$

This expression includes self energy corrections due to disorder but not the vertex corrections. These have been shown to vanish for isotropic scatterers and a spin singlet order parameter [82], and are therefore not expected to be important here. In Eq. 5–7, $\alpha$ is the direction of the current, $i$ is the band index, $m_i$ is the band mass, $n$ is number of layers, $d$ is the c axis unit cell length and $\mathbf{v}_\Delta$ is the gap slope $d\Delta_k/dk_\alpha$. In the limit $T_c \ll E_F$, the contribution of the second term in Eq. 5–7 can be ignored. We are interested in the relative change of the penetration depth $\Delta \lambda$ and not in the zero
temperature value of $\lambda_0$, which requires an integration over the entire Brillouin zone, which is numerically very expensive task. In the next section, I consider a model for 1111 systems.

### 5.2 Model for 1111 Systems

The low temperature penetration depth results are not universal for the RFeAsO$_{1-x}$F$_x$ 1111 family. For $R = Sm, Pr$ based materials an exponential behavior has been reported, which is an indication of fully gapped system [156, 157]. On the other hand, for $R = La, Nd$, an nonexponential power law $T^n$ has been found, with $n \sim 2$ [43].

In another material LaFePO, a linear penetration depth is measured [88, 103], which is a clear evidence of line nodes. From the theoretical point of view, the isotropic $s\pm$ wave model with strong interband disorder has been proposed by Vorontsov et al. [158]. This model can give power laws $T^n$ with $n > 1$, but can not explain the linear behavior observed in LaFePO. It is also inconsistent with the c axis transport observed for the 122 family. An order parameter with a state with deep minima is qualitatively similar to the $s\pm$ model, because it also has a gap. Here we consider a state with accidental nodes on the electron pocket and an isotropic gap on the hole pocket, as discussed in Sec. 4.3. For the order parameter, we take $\Delta_{\text{hole}} = -1.1 T_{c0}$ for the hole sheet and $\Delta_{\text{electron}} = 1.5 T_{c0} (1 + 1.3 \cos 2\phi)$ for the electron sheet. First we look at the effect of pure intraband scattering, shown in Fig. 5-1. For simplicity, we take equal DOS and Fermi velocity for both the bands. In the clean limit, $\Delta\lambda$ is not linear but has a slight curvature. A power law fit gives $T^{1.19}$, and this happens due to a change of slope caused by the low energy scale $\Delta_{\text{ani}} - \Delta_{\text{iso}}$. The addition of a little disorder makes the curve more linear and the power law becomes $T^{1.04}$, as the disorder increases nodes disappear and we see an exponential behavior at very low temperature as an indication of full gap, with an a effective power law of $T^{1.77}$. We give exponents here which fit over a finite low temperature range ($0 - 0.2 T_c$), not because they are in any sense universal, but to compare with the exponents which have been reported by experiments.
Figure 5-1. Normalized change in penetration depth as a function of normalized temperature. $\lambda_0$ is zero temperature penetration depth and $T_c$ is the critical temperature. $\Gamma$ is impurity lifetime, measured in clean limit critical temperature. The order parameters are $\Delta_1 = -1.1 T_{c0}$ and $\Delta_2 = 1.5 T_{c0}(1 + 1.3 \cos 2\phi)$.

over this range. On further increasing disorder, the effective power increases and for $\Gamma = 1.5 T_{c0}$, the power becomes 2.6. Next we consider the state with deep minima on the electron pocket. For this case we use the same order parameter for the hole band as in nodal case, but for electron pocket we take $\Delta_{\text{electron}} = 1.5 T_{c0}(1 + 0.8 \cos 2\phi)$.

Fig. 5-2 shows results for this anisotropic $s_{\pm}$ state with deep minima. For this case, in the clean limit we find an effective power law $T^{-2.59}$ in the low temperature range. The addition of pure intraband disorder increases this power to 3.34, because pure intraband scattering lowers the anisotropic component of order parameter and increases the
Figure 5-2. Normalized change in penetration depth as a function of normalized temperature for the anisotropic $\pm s$ wave state with deep minima. $\lambda_0$ is zero temperature penetration depth and $T_c$ is the critical temperature. $\Gamma=0.1 T_{c0}$ for all cases and legends show the strength of interband scattering with power laws for each curve. The order parameters are $\Delta_1=-1.1 T_{c0}$ and $\Delta_2=1.3 T_{c0}(1+0.8\cos 2\phi)$.

deep minimum energy scale. More interesting features come with interband impurity scattering. With an interband scattering which is 90% of the intraband scattering, we see a reduction in the exponent. The temperature exponent goes to 2.14 from 2.59 of the pure intraband scattering limit. This happens due to the formation of impurity mid gap state away from the Fermi level and this makes the gap in DOS very small. In the isotropic scattering limit, when both the interband and intraband scatterings are equal, then this power is 2.46, which is smaller than the clean case and slightly larger than the
weak interband scattering case. The problem with interband scattering is that it causes a strong suppression of critical temperature as shown in Fig. 4-7, and in contradiction to experiments. In this isotropic scattering limit, the impurity band is formed on the Fermi level which causes a smaller power than the clean case. Next we consider the 122 systems.

5.3 Model for 122 Systems

Pnictides based on BaFe$_2$As$_2$ have been studied extensively by many groups. Both the electron and hole doped systems show power laws for in plane penetration depth in the low temperature regime with power $n \simeq 2$ [41, 44, 86, 87, 159]. Another experiment by Kim et al. [160] on electron doped systems with irradiation with heavy ions shows power laws in the range 2.2 to 2.8 for the in-plane penetration depth, with a decrease in exponent with increasing $T_c$ suppression [160]. The Kim et al. [160] experiment was explained with an isotropic s$_\pm$ wave model assuming interband scattering. On the other hand, recent transport measurement along the c axis have contradicted this isotropic s$_\pm$ wave model, which will give same normalized behavior in both a and c directions in contradiction to experiments. Penetration depth measurements along the c axis for Ni doped systems found linear behavior and quadratic behavior along the planes [44]. This would be impossible if these power laws extended to arbitrarily low $T_c$, and therefore suggests a more complicated interplay of gap structure and multiband physics. A recent study of thermal conductivity for Co doped systems by Reid et al. has also provided strong evidence for three dimensional nodal structure [42]. Motivated by these experiments, we consider a three dimensional model for 122 systems, which was introduced in Sec. 4.4. We consider all five cases considered in Sec. 4.4 and look at both in plane and c axis penetration depths. The parameters of the models are listed in Table 4-1.

First we consider cases 1 and 2, which have Fermi surfaces with weak c axis dispersion. Case 1 has V shaped nodes, while case 2 has horizontal line nodes. We
Figure 5-3. Residual density of states $N(\omega=0)$ normalized to the total normal state density of state at the Fermi energy $N_0$ vs. total unitary intraband scattering rate parameter $\Gamma$ in meV for cases 1 to 5, respectively.
consider two limiting cases, the clean limit and the dirty limit. In the dirty limit the total normal state scattering rate is $0.9\Gamma_{NL}$, where $\Gamma_{NL}$ is the critical disorder which removes the nodes (See Fig. 5-3). Fig. 5-4 shows the penetration depth change $\Delta \lambda$ for cases 1 and 2. In the clean limit, both the cases give power law variation with power 2.08 for the in-plane penetration depth, but the c axis is very linear. With the addition of pure intraband impurity scattering, the exponent increases for the ab-plane and the c axis $\Delta \lambda$ also deviates from linear behavior to $n > 1$ power law for V shaped nodes. For the
horizontal nodes, the c axis $\Delta \lambda$ remains linear except at very low temperatures. Cases 3 and 4 are shown in Fig. 5-5 and case 5 is shown in Fig. 5-6. Other cases also show qualitatively similar behavior to cases 1 and 2. For all cases, the electron pockets have same order parameter and two electron pockets start making significant contribution at very low temperatures. All cases give qualitatively different behavior for in plane and c axis penetration depths, similar to the experimental data on Ni doped BaFe$_2$As$_2$. Such behavior can not be obtained for an isotropic $\pm s$ wave state. At low temperatures the
Figure 5-6. Relative change in penetration depth $\Delta \lambda$ in nm as a function of temperature $T$ in Kelvin for case 5 panel a and b. Solid lines shows $\Delta \lambda$ for in plane direction and dashed line show the c axis. Blue lines denotes the clean system and red lines shows dirty system with $\Gamma = 0.9\Gamma_{NL}$, where $\Gamma_{NL}$ is the critical value of disorder to lift the nodes. The power laws are indicated for in plane direction.

The leading order temperature dependence is given by,

$$\Delta \lambda_\alpha \propto \int_0^\infty d\omega \ \text{sech}^2\left(\frac{\omega}{2T}\right) \left\langle (\mathbf{v}_F \cdot \hat{\mathbf{a}})^2 \text{Im} \left[ \frac{\bar{\Delta}^2}{(\bar{\omega}^2 - \bar{\Delta}^2)^{3/2}} \right] \right\rangle_{FS}.$$  \hspace{1cm} (5–7)

Here $< >_{FS}$ is the average over the Fermi surface. $\bar{\Delta}$ and $\bar{\omega}$ are the gap and energy renormalized by the disorder respectively. The renormalization due to the disorder does not depend on the momentum, hence we can rewrite Eq. 5–7

$$\Delta \lambda_\alpha \propto F(T) \left\langle (\mathbf{v}_F \cdot \hat{\mathbf{a}})^2 \right\rangle_{FS},$$  \hspace{1cm} (5–8)

$$F(T) = \int_0^\infty d\omega \ \text{sech}^2\left(\frac{\omega}{2T}\right) \text{Im} \left[ \frac{\bar{\Delta}^2}{(\bar{\omega}^2 - \bar{\Delta}^2)^{3/2}} \right].$$  \hspace{1cm} (5–9)

So for isotropic $s_\pm$ order parameters, the temperature dependence is the same in all directions. For another compound of 122 family, P doped BaFe$_2$As$_2$, linear $T$ behavior has been reported in the plane [123]. Microscopic calculations have found an extremely isotropic state in this material and V shaped nodes on the hole sheet [48], similar to the nodal structure found by Graser et al. for hole doped BaFe$_2$As$_2$ [40]. In such a system, electron pocket will not affect the low $T$ penetration depth and it will be purely
Figure 5-7. Penetration depth anisotropy $\gamma_\lambda$ for all cases in clean and dirty limit as a function of temperature in Kelvin.

determined by nodal hole sheet with linear behavior. Qualitatively this system will be equivalent to nodal model considered in Sec. 5.2 for 1111 family. We now investigate another important quantity, which is penetration depth anisotropy $\gamma_\lambda$ defined as,

$$\gamma_\lambda = \frac{\lambda_c}{\lambda_{ab}}.$$  \hspace{1cm} (5–10)

Here $\gamma_\lambda$ involves knowledge of absolute values of penetration depth, which require full information of the band structure. Fig. 5-7 shows the penetration depth anisotropy for all cases in clean and dirty limit. The $T = 0$ values of penetration depth calculated for our model are listed in Table 5-1. The penetration depth anisotropy is roughly constant.
Table 5-1. Zero temperature penetration depth $\lambda_0$ for all cases.

<table>
<thead>
<tr>
<th>Case</th>
<th>$\lambda_{ab}$ (nm)</th>
<th>$\lambda_c$ (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,2</td>
<td>218</td>
<td>836</td>
</tr>
<tr>
<td>3,4</td>
<td>218</td>
<td>726</td>
</tr>
<tr>
<td>5</td>
<td>218</td>
<td>825</td>
</tr>
</tbody>
</table>

over the entire low temperature range is close to 4. It is roughly close to the root mean square ratio of the in-plane and the c axis Fermi velocities.

5.4 Conclusion

We considered models introduced in chapter 4 for the 1111 and the 122 families for calculating the low temperature penetration depth. We found that the order parameter with accidental nodes can give linear penetration depth as observed in LaFePO and BaFe$_2$(As$_{1-x}$P$_x$)$_2$. Disorder in this system, together with the mixture of different densities of quasiparticles on different bands, can lead to effective power laws observed for different materials in the 1111 family. We also investigated a model of an anisotropic $s_\pm$ state, which can give power law close to quadratic. Addition of pure intraband disorder increases the exponent, while addition of finite interband disorder reduces the exponent. Similar results were obtained by Kim et al. using isotropic $s_\pm$ wave state in the context of electron doped BaFe$_2$As$_2$ [160], but this explanation appears to be ruled out by the c axis penetration depth. For 122 family, we study gaps with three dimensional structure and find qualitatively different behavior for in plane and out of plane penetration depth.
6.1 Introduction and Review

ARPES measurements on underdoped Bi2212 cuprates have revealed disconnected arc like Fermi surfaces centered around the nodal directions instead of closed Fermi surface sheets, which are expected for normal metals [16–18]. Similar features were also found in YBCO samples by in-situ ARPES measurements [161]. On the other hand, quantum oscillation experiments on YBCO have suggested small pocket-like Fermi surfaces in high fields [162–166]. Recently, Meng et. al. have reported the existence of Fermi surface pockets in Bi2201, but whether its origin is the structural supermodulation or not, is a issue of debate [167–169]. Among many other theoretical proposals, Pereg-Barnea et. al. have shown that the quantum oscillation experiments can be explained with a phenomenological model of Fermi arcs within a semiclassical treatment of magnetic field [170]. The formation of Fermi arc is associated with a linear in temperature quasiparticle lifetime above the true phase coherence temperature [171]. Within this model, the normal state is assumed to be a mean field d wave superconductor, but inelastic scattering due to lack of phase coherence leads to formation of arcs.

In this chapter, we treat this problem from a different point of view. We start with a normal state without any superconducting order parameter and look at how the order parameter fluctuation affects the electronic structure. We consider an phenomenological model to get a d wave superconducting ground state and study the effect of fluctuation above mean field transition temperature in the long wavelength limit. Formation of Cooper pairs above $T_c$ leads to a reduction of the normal state DOS. This result was first obtained by Abrahams et. al. [172] in the context of tunneling experiments on granular Al, where DOS similar to a gapless superconductor is observed much above
the critical temperature \[173\]. Here we focus on the fluctuation effect on the Fermi surface in a similar framework, but for the d-wave case.

### 6.2 Formalism

A simple model Hamiltonian to get d-wave superconductivity is,

$$
\mathcal{H} = \sum_{k, \sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma} - g \sum_{k, k', q} \Phi(k) \Phi(k') c_{k+q_1}^\dagger c_{-k-\mathbf{q}}^\dagger c_{-k'-\mathbf{q}}^\dagger c_{k'+\mathbf{q}}.
$$

Here \(g\) is an effective coupling constant and \(\Phi(k)\) is a factor to get the d-wave symmetry, which in a gas model is \(\cos(2\phi)\) and on a lattice is \((\cos(k_x) - \cos(k_y))/2\). Such a Hamiltonian can be derived from the mean field theory of the \(t - J\) model. \(\xi_k\) is the fermion energy with respect to the Fermi energy. In the mean field theory, one restricts oneself to the \(q \to 0\) limit, i.e. pairs only time-reversed states, and gets the following result for the superconducting transition temperature for a d-wave superconductor,

$$
k_B T_c = 1.13 \omega_c e^{-\frac{2}{N_0}},
$$

where \(N_0\) is the density of states (DOS) at the Fermi surface and \(\omega_c\) is the cut off energy, which depends on the microscopic details of the pairing mechanism. Most of the physical quantities measured in experiments are measured in units of \(T_c\), hence knowledge of \(\omega_c\) is not necessary. The order parameter in the superconducting state is defined as,

$$
\Delta(k) = -g \Phi(k) \sum_{k'} \Phi(k') \langle c_{k1}^\dagger c_{-k'1}^\dagger \rangle = \Delta_0 \Phi(k).
$$

In the normal state, this anomalous expectation value is zero, which after the symmetry breaking below \(T_c\) becomes finite. But in the normal state fluctuations do exist. To get some qualitative understanding, we do the mean field decomposition of interaction term in the Hamiltonian 6–1, which gives,

$$
\mathcal{H}_{int} = \sum_{k, \mathbf{q}} \Phi(k) c_{k+q_1}^\dagger c_{-k-\mathbf{q}}^\dagger \Delta_0(\mathbf{q} \to 0) + h.c.
$$
Now to study the fluctuations, we substitute $\Delta_0(q) \rightarrow \Delta_0^{MF} + b_q$ and use the fact that in the normal state $\Delta_0^{MF} = 0$, we get an effective interaction for the electrons and the bosonic superconducting fluctuation field $b_q$.

$$H_{\text{eff}} = \sum_{k,q} \Phi(k+q) \Phi(k) c_{k+q\uparrow} c_{k\downarrow}^\dagger b_q + h.c. \quad (6–5)$$

$$H_{\text{eff}} = \sum_{k,q} \Phi(k) c_{k+q\uparrow} c_{k\downarrow}^\dagger b_q + h.c. \quad (6–6)$$

The fluctuation field is defined as,

$$b_q = \sum_k -g \Phi(k) c_{-k\downarrow} c_{k+q\uparrow}. \quad (6–7)$$

From the effective fluctuation fermion Hamiltonian we can see two things. First, the fluctuation fermion vertex is momentum dependent and comes with a factor of $\Phi(k)$, where $k$ is the fermion momentum. This tells us, that the self energy is going to have a momentum dependence corresponding to the square of the order parameter symmetry. This is illustrated in Figure 6-1. This is consistent with the angle dependence of scattering rate angular magnetoresistance oscillation (AMRO) experiments done on the cuprates [174, 175], where the scattering rate is a minimum along the nodal direction and maximum along the antinodal directions and this anisotropic scattering rate has a strong correlation with $T_c$, which suggests that it is related to superconductivity [176].

The second thing that we get from Eq. 6–6 is that the fluctuation propagator is related
to the $k$ dependent part of the full vertex function. This is also consistent with the earlier theory by Larkin [177] and Narozhny [178]. To evaluate the fluctuation propagator, if we include only the ladder diagrams in the Bethe-Salpeter equation for the vertex function, it can be written as a series of bubbles as shown in figure 6-1. The sum of the bubbles can be written as,

$$\Gamma(k, k', q) = \frac{\Phi(k)\Phi(k')}{-\Delta^{-1} + \mathcal{P}(q, i\Omega)} = \Phi(k)\Phi(k')\mathcal{L}(q, i\Omega). \quad (6–8)$$

This equation 6–8 is similar to the vertex function obtained by Narozhny [178]. The d-wave fluctuation propagator is $\mathcal{L}$ and $\mathcal{P}$ is

$$\mathcal{P}(q, i\Omega) = T \sum_{k, \omega_n} \Phi(k)\Phi(k')G(k + q, i\omega_n + i\Omega)G(-k, -i\omega_n), \quad (6–9)$$

where $\omega_n$ is the fermionic Matsubara frequency and $\Omega$ is the bosonic Matsubara frequency. $G$ is the normal state Green’s function defined as

$$G(k, i\omega_n) = \frac{1}{i\omega_n - \xi_k}. \quad (6–10)$$

The fluctuation propagator can be written as

$$\mathcal{L}^{-1}(q, i\Omega) = -\Delta^{-1} + \frac{N_0}{2} \left[ \psi \left( \frac{1}{2} + \frac{\omega_c}{2\pi T} + \frac{\Omega}{4\pi T} \right) \right]$$

$$- \psi \left( \frac{1}{2} + \frac{\Omega}{4\pi T} \right) + \frac{(v_F q)^2}{2D(4\pi T)^2} \psi'' \left( \frac{1}{2} + \frac{\Omega}{4\pi T} \right), \quad (6–11)$$

where $D$ is the dimension, $v_F$ is the Fermi velocity, $\psi$ is the Digamma function and $\psi''$ is the second derivative of the Digamma function. In deriving this expression, we assumed that $q v_F << 2\pi T$. The pole of the fluctuation propagator in the limit $q \to 0$ gives the mean field transition temperature $T_c$. The retarded propagator for small $\Omega$ can be obtained by doing an analytic continuation ($i\Omega \to \Omega + i\Omega^+$) and a Taylor’s series expansion of the Digamma functions $\psi$ and using Eq. 6–2 to eliminate $g$. We obtain

$$\mathcal{L}(q, \Omega) = \frac{2/N_0}{i\Omega \frac{\pi}{8T} - \log(T/T_c) - \lambda^2 q^2 v_F^2}. \quad (6–12)$$
Table 6-1. Value of $\delta$ in different superconductors.

<table>
<thead>
<tr>
<th>Material</th>
<th>$\delta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pb</td>
<td>$\sim 10^{-6}$</td>
</tr>
<tr>
<td>Nb$_3$Sn</td>
<td>$\sim 10^{-4}$</td>
</tr>
<tr>
<td>Tl$_2$Ba$<em>2$CuO$</em>{6+x}$</td>
<td>$\sim 0.3 - 0.5$</td>
</tr>
<tr>
<td>Bi2212</td>
<td>$\sim 0.7 - 1.0$</td>
</tr>
<tr>
<td>YBCO</td>
<td>$\sim 0.7 - 1.4$</td>
</tr>
</tbody>
</table>

Here $\Lambda^2$ is $\frac{7 \zeta(3)}{16 \pi^2 D}$, where $\zeta(3)$ is the zeta function. We are interested in the self energy near the Fermi surface;

$$\Sigma(k_F, \omega, T) = \Phi^2(k_F) \Sigma(\omega, T)$$  \hspace{1cm} (6–13)

$$\Sigma(\omega, T) = -T \sum_\Omega \int \frac{dq}{(2\pi)^D} L(q, i\Omega) G(-k + q, -i\omega + i\Omega).$$  \hspace{1cm} (6–14)

This can be rewritten after performing the Matsubara summation as

$$\Sigma(\omega, T) = -\int_0^\infty \frac{dx}{\pi} \int \frac{dq}{(2\pi)^D} L''(q, x) \frac{-x \tanh(\xi_{k+q}/2T) + (\omega + \xi_{k+q}) \coth(x/2T)}{x^2 - (\omega + \xi_{k+q})^2}. \hspace{1cm} (6–15)$$

To understand the effect of long wavelength fluctuations on the Fermi surface, which are most important, we can drop the $q$ dependence of the electron Green’s function and self energy reduces to

$$\Sigma(\omega, T) = -\int_0^\infty \frac{dx}{\pi} \int \frac{dq}{(2\pi)^D} L''(q, x) \frac{(\omega) \coth(x/2T)}{x^2 - (\omega)^2}. \hspace{1cm} (6–16)$$

where the imaginary part of the fluctuation propagator $L''$

$$L''(q, x) = \frac{-2 N_0^{-1}x\pi/8T}{(\pi/8T)^2x^2 + (\varepsilon + \Lambda_0^2 v_F^2 / T^2 q^2)^2}, \hspace{1cm} (6–17)$$

where $\varepsilon$ is $\log(T/T_c)$. We can rewrite Eq. 6–16 after integrating out the momentum as,

$$\Sigma(\omega, T) = \frac{T^2}{2\pi^2 N_0 v_F^2 \Lambda^2} \int_0^\infty dy \left[ \frac{\pi}{2} - \tan^{-1} \left( \frac{\varepsilon 8T}{\omega \pi} \right) \right] \frac{(\omega / T) \coth(y/2)}{y^2 - (\omega / T)^2}. \hspace{1cm} (6–18)$$

The denominator in Eq. 6–18 has dimensions of temperature, hence we introduce a
temperature scale $T_\theta$,  

$$T_\theta = \pi^2\Lambda^2 N_0 \nu_F^2 = \frac{7 \zeta(3)}{16D} N_0 \nu_F^2. \quad (6–19)$$

For a layered two dimensional system $N_0 \nu_F^2$ is $\rho_s d/m$, where $d$ is the interlayer distance. Using this we rewrite $T_\theta$ as,  

$$T_\theta = \frac{7 \zeta(3) \rho_s d}{16D} = A \frac{\rho_s d}{4m}, \quad (6–20)$$

where $A$ is $1.1058$. A similar analysis for three dimensions gives,  

$$T_\theta = A \frac{\rho_s \ell}{4m}, \quad (6–21)$$

with $A = 1.6391$ and $\ell = \sqrt{\pi \nu_F/\pi \Delta_0}$. Emery and Kivelson proposed a similar temperature scale known as the phase ordering temperature with $A = 0.9$ for 2D and $A = 2.2$ for an isotropic 3D system. This we can rewrite the self energy as  

$$\Sigma/T_c = \delta \frac{T^2}{2T_c^2} \int_0^\infty dy \left[ \frac{\pi}{2} - \tan^{-1} \left( \frac{\nu}{\pi} \right) \right] \frac{(\omega/T) \coth(y/2)}{y^2 - (\omega/T)^2}, \quad (6–22)$$

where $\delta$ is $T_c/T_\theta$. The dimensionless parameter $\delta$ for some superconductors is listed in Table 6-1. The imaginary part of the self energy can be calculated analytically and is given as,  

$$\frac{\Sigma''(\omega/T, T)}{T_c} = -\delta \frac{T^2}{T_c^2} \left[ \frac{\pi}{2} - \tan^{-1} \left( \frac{\nu}{\omega} \right) \right] \coth(\omega/2T) \frac{\pi}{4}. \quad (6–23)$$

The real part comes from the principal value of the integral in Eq. 6–22. In next section, I discuss the effect of fluctuations on the one-electron spectral function.

### 6.3 Spectral Function

The spectral function is related to the imaginary part of the retarded Green’s function and reads as,  

$$A(k, \omega) = -\frac{1}{\pi} \text{Im} G(k, \omega). \quad (6–24)$$

In normal metals, the spectral function is peaked at the Fermi energy and in the superconducting state the peak shifts to the gap energy scale. To track the Fermi arc,
we look at the peak position of spectral function using the ARPES criterion, where half of peak value is measured from a reference Fermi level. Fig. 6-2 shows, the spectral gap determined using the ARPES criterion for different temperatures above $T_c$. The value of $\delta$ is taken to be 1.5, which is comparable for slightly underdoped Bi2212 samples. The Fermi arc is the angular region around the node where the spectral gap is zero.

Next we look at the temperature dependence of the arc length, which is shown in Fig. 6-3, with experimental data from Kanigel et. al. [17]. The experiments claim a universal temperature dependence with point like Fermi surface for samples with $T_c$ of zero Kelvin, and the arc closing temperature is much higher than most of the pseudo gap temperature scales coming from other scales. Pure d-wave fluctuations seem to give a qualitatively good fit for the weakly underdoped case, but can not account for the behavior of strongly underdoped samples. We calculate the value of $\delta$ for different dopings using the data from Storey et. al. [179], and construct a phase diagram for the
Figure 6-3. Arc length as a function of temperature normalized to arc closing temperature $T_F$. The experimental data is taken from Kangiel et. al. [17]. The end point of the green curve is $1.05 T_c$, the arc length goes to zero at $T_c$ and within our model, we do not consider the superconducting state. The curve is for $\delta = 1.5$.

The arc closing temperature ($T_F$) from pure d-wave fluctuations. Fig. 6-4 shows the doping dependence of arc length closing temperature within the model considered here. There is also some evidence for the existence of higher harmonic terms in the gap function, which could affect the temperature dependence of arc, because the fluctuation self energy carries the full information of the gap structure. To model this, we consider a simple model gap function with d-wave symmetry, written as,

$$\Delta(\phi) = \Delta_0 (\cos 2\phi + B_6 \cos 6\phi).$$  \hfill (6–25)

Here $B_6$ is a parameter to control the strength of the higher harmonic term. In Fig. 6-5, we plot the Fermi arc length as a function of temperature normalized to the arc closing
Figure 6-4. Doping dependence of arc length closing temperature $T^F$ with temperature scale $T_c$ (from [179]), pseudogap temperature $T^*$ (from [180]) and Nernst effect’s onset temperature $T^\nu$ (from [22]).

temperature. This clearly shows that the arc length closing strongly depends on the gap function symmetry. In the next section, I discuss the effect of magnetic fluctuations.

6.4 Fluctuation in Dirty Limit

In the presence of impurities, the impurity lifetime enters the single particle Green’s function and fermion fluctuation vertex get renormalized. The normal state electron Green’s function becomes,

$$G(k, i\omega) = \frac{1}{i\omega + i\frac{1}{2\tau} \text{sgn}\omega - \xi_k}, \quad (6-26)$$

where $\tau$ is the single particle lifetime. The renormalized vertex within the ladder approximation is written as,

$$\lambda(q, \tilde{\omega}_1, \tilde{\omega}_2) = \frac{|\tilde{\omega}_1 - \tilde{\omega}_2|}{|\omega_1 - \omega_2| + \Theta(-\tilde{\omega}_1\tilde{\omega}_2)D/|\tilde{\omega}_1 - \tilde{\omega}_2|^3}. \quad (6-27)$$
Here $D$ is the diffusion constant ($v_F^2\tau/2$) and $\Theta(x)$ is the Heavyside theta function within the approximation $|(\tilde{\omega}_1 - \tilde{\omega}_2)| \ll \max(T, \tau^{-1})$ and $\tilde{\omega} = \omega + 1/2\tau \text{sgn}\omega$. The fluctuation propagator takes the form,

$$L(q, \Omega) = \frac{2/N_0}{i\Omega \frac{\pi}{8F} - \log(T/T_c) - \Lambda^2 q^2 v_F^2 \tau}$$  \hspace{1cm} (6–28)$$

where $T_c$ is the critical temperature for the dirty system. The self energy is calculated to lowest order including the vertex correction, and for the dirty limit this can be calculated in closed form by taking only the leading contributions in the Matsubara sum. It comes out to be exactly the same as originally calculated by Abraham et. al. [172]. The only difference due to d-wave symmetry comes in the momentum dependence of self energy. In the clean limit quantum fluctuations dominate, but in the dirty case classical
Figure 6-6. Fermi arc length as a function of disorder, $\tau^{-1}$ is the single particle scattering time and $T_c$ is the critical temperature for the corresponding system.

fluctuations play dominant role. The fluctuation self energy can be written as,

$$\Sigma(i\omega) = -i\frac{\tilde{\omega}^2}{T N_0 v_F^2 \tau} \int_0^\infty dq \frac{1}{2\pi} \frac{1}{\varepsilon + \lambda^2 q^2 v_F^2} \left[ \left( \frac{8\varepsilon + \lambda^2 q^2 v_F^2}{\pi} + 2\omega + \frac{q^2 v_F^2}{2} \right)^2 \right].$$  

(6–29)

Here $\omega$ is the fermionic Matsubara frequency. We can integrate out $q$, and on the Fermi surface the self energy becomes,

$$\Sigma(\omega) = -i\frac{\tilde{\omega}}{\pi T N_0 v_F^2 \tau} \left[ \log \left( \frac{\lambda^2(16\varepsilon T + 4\pi \omega)}{\pi(16\lambda^2 T + \pi \tau)} \right) + \frac{16\lambda^2 T + \pi \varepsilon T}{(4\lambda^2 \omega - \varepsilon T)^2 (16\varepsilon T + 4\pi \omega)} \right].$$  

(6–30)

To compare with clean limit behavior, I replace $N v_F^2$ in Eq. 6–30 with $4 T_\alpha/1.1$. Fig. 6-6 shows the effect of disorder on the Fermi arcs for $\delta = 1.5$. We can clearly see that the arc closing temperature $T_F$ still can be much higher than $T_c$ for dirtier systems, although the temperature dependence is qualitatively different from the experimental
observations. Another point to note here is $T_c$ going to zero limit of the curve, which appears to be finite. In the context of cuprates, disorder doesn’t seem to be very important because the coherence length $\xi_0$ is much shorter than mean free path $\ell$, which is equivalent to the condition $\tau^{-1} \ll T_c$.

6.5 Effect of Magnetic Fluctuations

The proximity to antiferromagnetism makes the role of antiferromagnetic fluctuations important in normal and superconducting states of cuprates, although there is no clear evidence of coexisting magnetic and superconducting ground states in hole doped cuprates. Magnetic fluctuations will scatter fermions and cannot be ignored. We treat the magnetic fluctuations in a similar way as the superconducting fluctuations. The SDW fluctuation propagator or the effective antiferromagnetic spin fluctuation potential is written as [181, 182],

$$\mathcal{L}_{SDW}(q, \Omega) = \frac{2/N_0}{i\Omega \frac{\pi}{8T} - \log(T/T_{SDW}) - \Lambda^2 \frac{q^2 \tilde{\nu}^2}{T^2} - 1}.$$  \hfill (6–31)

where $q$ is near the order vector $Q$, $\tilde{\nu}$ is the velocity at $k = k_F + Q$ and the mean SDW transition temperature $T_{SDW}$ is given as,

$$T_{SDW} = 1.13 E_F e^{-1/N_0 \tilde{U}}.$$  \hfill (6–32)

Here $\tilde{U}$ is the effective electron electron interaction. The lowest order self energy is calculated in a similar way as in last section but in this section we consider a tight binding dispersion,$$
\xi_k = -2t (\cos k_x + \cos k_y) + 1.6t \cos k_x \cos k_y + 1.1t.  \hfill (6–33)
$$

We focus the qualitative aspect of co-existing magnetic fluctuation, hence use the same propagator as in the electron gas model. The ordering vector that we consider is $(\pi, \pi)$. A tight binding dispersion will give slightly different prefactor for $q$ in the fluctuation propagator, but the qualitative form will remain same for small $q$ fluctuations. In the self
energy calculation, we assume that $q \ll k_F + Q$ and set $t = 1$. The superconducting transition temperature $T_c$ is taken as $0.1t$ and SDW transition temperature is taken to be smaller than $T_c$ ($T_{SDW} = 0.9T_c$). It is assumed that superconductivity is the leading instability and system first goes through a superconducting transition. We do not address the question of whether there will be a co-existing phase of magnetic and superconducting order below $T_c$, because we are primarily interested in the temperature range above $T_c$. The self energy is written as,

$$\Sigma(k, \omega, T)_{SDW} = -\int_0^\infty \frac{dx}{\pi} \int \frac{d\mathbf{q}}{(2\pi)^D} \Delta_{SDW}''(\mathbf{q}, x) \times \frac{-x \tanh(\xi_{k+Q+q}/2T)}{x^2 - (\omega + \xi_{k+Q+q})^2}$$

(6–34)

We also calculate the self energy for the superconducting state with tight-binding dispersion and the full Green’s function is,

$$G(k, \omega) = [\omega - \xi_k - \Sigma_{SC} - \Sigma_{SDW}]^{-1}.$$  

(6–35)

Fig. 6-7 shows the spectral function on k space for $\omega = 0$, with the normal state Fermi surface. Panel (a) shows the effect of pure SDW fluctuations, we can clearly see that the Fermi Surface moves away from its original position, and a transition to SDW state leads to a reconstruction of the Fermi surface with small pockets. In case of SC fluctuations, we have an arc like Fermi surface along the original Fermi surface as shown in the panel (b). In presence of both fluctuations, we get again arc like Fermi surface, which is shifted from the original Fermi surface and its larger than the arc from pure SC fluctuations.

### 6.6 Conclusion

We considered the effect of superconducting order parameter fluctuations on spectral function above transition, and we found that the d-wave superconducting fluctuations in the normal state can lead to arc-like Fermi surface segments as observed in Bi2212 cuprates. Our studies show that clean limit results are in better qualitative agreement with experiments. We also considered effect of magnetic fluctuations along...
Figure 6-7. Spectral function $A(k, \omega = 0)$ for (a) SDW fluctuations (b) d wave SC fluctuation and (c) in presence of both kinds of fluctuations. The temperature for all three plots is $1.1 T_c$ and $T_{SDW}$ is $0.9 T_c$. The red dashed line shows the Fermi surface without any fluctuation effect.

with superconducting fluctuations give very small qualitative difference between the two cases. Our work is in good agreement with weakly underdoped Bi2212 systems, but not for extremely underdoped regimes.
APPENDIX A
T-MATRIX FOR TWO BAND SYSTEM

A.1 Basic Formalism

For low impurity concentrations, one can ignore the processes which involve scattering from multiple impurity sites. Within this single site approximation, we sum all possible scattering events from a single site to calculate the T-matrix, which is related to the self energy as

\[ \Sigma = n_{\text{imp}} T, \]  
\[ (A-1) \]

where \( n_{\text{imp}} \) is the impurity concentration. \( T \) denotes a quantity in the two band Nambu basis \( \tilde{c}_k = (c_{k\alpha}, c_{k\alpha}^\dagger, c_{k\beta}, c_{k\beta}^\dagger) \). Here \( \alpha, \beta \) denote the bands, \( c \) and \( c^\dagger \) are annihilation and creation operators respectively. In a multiband superconductor, an impurity can scatter within the same band or in between two different bands. Fig. A-1 shows the impurity averaged diagrams up to third order. Any process which involves odd number of interband scatterings does not contribute to the self energy, because at the end the final state belong to the other band. The sum of all the diagrams from a single impurity site can be expressed as

\[ T_1 = \frac{1}{1 - U_{11}^{\text{eff}} G_1}(U_{11}^{\text{eff}}). \]  
\[ (A-2) \]

In the Nambu basis,

\[ U_{ij} = U_{ij} \hat{\tau}_3, \]  
\[ (A-3) \]

\[ \langle G_i \rangle_k = g_{i,0} \hat{\tau}_0 + g_{i,1} \hat{\tau}_1 \]  
\[ (A-4) \]

The effective impurity scattering potential is given as,

\[ U_{11}^{\text{eff}} = U_{11} + U_{12} \left[ G_2 \frac{1}{1 - U_{22} G_2} \right] U_{12} \]  
\[ (A-5) \]

The second term in the Eq. A–5 is due to scattering in the second band before coming back to the initial band, and contains terms like \( U_{12} G_2 U_{22} G_2 U_{12} \). This is going to modify
Figure A-1. These are the impurity averaged diagrams, which contribute to the self energy of the first band Green’s function. Here the interband contribution comes through processes, which involve even number of interband scatterings. The diagrams also takes into account the order of inter and intraband scatterings. $U_{ij}$ is the impurity potential strength, where $i,j$ are the band indexes. $i=j$ denotes the intraband and $i\neq j$ denotes the interband potential strength. $G_i$ is the bare Green’s function and $T_i$ is T-matrix for $i^{th}$ band.

The effective interband vertex, which is illustrated in fig. A-2. In Eq. A–5, $U_{11}, U_{22}$ are the “Intra-band” impurity potential strengths in band 1 and 2 respectively. $U_{12}$ is the “Inter-band” impurity potential strength, which scatters between the bands. After doing the Pauli matrices ($\tau$) algebra, we can write the expression for the self energy in terms of $g_{i,\alpha}$, the Green’s function, where the momentum has been integrated out. Self energies
Figure A-2. Diagrams contributing to second term of Eq. A–5, which can be regarded as a modified effective vertex $\Gamma_1$ for the interband scattering, which takes into account for the intraband scattering process in the second band after getting scattered by the first band and before coming back to the first band again.

$\Sigma$’s can be written as,

$$
\Sigma_{1,0} = n_{\text{imp}} \frac{U_{12}^2 g_{1,0} + U_{12}^2 g_{2,0} - g_{1,0} (U_{12} - U_{11} U_{22})^2 (g_{2,0} - g_{2,1})}{D},
$$

(A–7)

$$
\Sigma_{1,1} = -n_{\text{imp}} \frac{U_{11}^2 g_{1,1} + U_{12}^2 g_{2,2} - g_{1,1} (U_{12} - U_{11} U_{22})^2 (g_{2,0} - g_{2,1})}{D}.
$$

(A–8)

The first subscript in $\Sigma_{i,\alpha}$ represents the band index and the second subscript $\alpha$ denotes the Nambu components.
A.2 Special Cases

A.2.1 One Band

For a one band superconductor, there is no interband scattering, so $U_{12} = 0$ and we can simplify the expressions for the self-energies as,

$$
\Sigma_{1,0} = n_{imp} \frac{U^2 g_{1,0}}{1 - U^2 (g_{1,0}^2 - g_{1,1}^2)},
$$  \hspace{1cm} (A–9)

$$
\Sigma_{1,1} = -n_{imp} \frac{U^2 g_{1,1}}{1 - U^2 (g_{1,0}^2 - g_{1,1}^2)}.
$$  \hspace{1cm} (A–10)

Here intraband scattering strength $U_{11}$ has been replaced by "$U$" [82].

A.2.2 Born Limit of Two Band Case

In the Born limit, we will keep the terms up to second order in "$U_{ij}$", so the denominator becomes 1 and we get,

$$
\Sigma_{1,0} = n_{imp} (U_{11}^2 g_{1,0} + U_{12}^2 g_{2,0}),
$$  \hspace{1cm} (A–11)

$$
\Sigma_{1,1} = -n_{imp} (U_{11}^2 g_{1,1} + U_{12}^2 g_{2,2}),
$$  \hspace{1cm} (A–12)

$$
\Sigma_{2,0} = n_{imp} (U_{22}^2 g_{2,0} + U_{12}^2 g_{1,0}),
$$  \hspace{1cm} (A–13)

$$
\Sigma_{2,1} = -n_{imp} (U_{22}^2 g_{2,2} + U_{12}^2 g_{1,2}).
$$  \hspace{1cm} (A–14)

A.2.3 Unitary Limit

Due to the presence of an additional band, a new parameter comes into play in the unitary limit. This parameter is the ratio of the interband scattering to the intraband scattering. If one assumes that the interband scattering is weaker than intraband scattering, then in the unitary limit, there is no role for the interband scattering, but if interband scattering is not small and grows with the intraband scattering, then their relative strength could be important. In this first scenario, we define the unitary limit as,

$$
U_{11} N_1 \gg 1, \; U_{22} N_2 \gg 1, \; (U_{12}^2 N_1 N_2) \ll U_{11} N_1 \; \text{and} \; (U_{12}^2 N_1 N_2) \ll U_{22} N_2.
$$

$N_1$ is the density of states (DOS) at the Fermi surface of the first band and $N_2$ is the DOS at the Fermi
surface for the second band. This means in the unitary limit, $1/U_{11}^2 \to 0, 1/U_{22}^2 \to 0$ and $U_{12}^2/U_{11}^2 \to 0$. So the self energies become

$$\Sigma_{1,0} = -n_{\text{imp}} \frac{g_{1,0}}{(g_{1,0}^2 - g_{1,1}^2)}, \quad (A\text{-}15)$$

$$\Sigma_{1,1} = n_{\text{imp}} \frac{g_{1,1}}{(g_{1,0}^2 - g_{1,1}^2)}, \quad (A\text{-}16)$$

$$\Sigma_{2,0} = -n_{\text{imp}} \frac{g_{2,0}}{(g_{2,0}^2 - g_{2,1}^2)}, \quad (A\text{-}17)$$

$$\Sigma_{2,1} = n_{\text{imp}} \frac{g_{2,1}}{(g_{2,0}^2 - g_{2,1}^2)}. \quad (A\text{-}18)$$

We obtain exactly same results as above for the case when interband scattering is stronger than the intraband scattering. This happens due the fact that only an even number of interband scattering processes contribute to the self energy and in the unitary limit two successive interband scattering events between two bands are equivalent to one intraband scattering event.

Now we consider the special limiting case of isotropic unitary scattering, when interband and intraband scatterings have equal potential strength. For this $U_{11} = U_{22} = U_{12}$ limit we get,

$$\Sigma_{1,0} = -n_{\text{imp}} \frac{g_{1,0} + g_{2,0}}{(g_{1,0} + g_{2,0})^2 - (g_{1,1} + g_{2,1})^2}, \quad (A\text{-}19)$$

$$\Sigma_{1,1} = n_{\text{imp}} \frac{g_{1,1} + g_{2,1}}{(g_{1,0} + g_{2,0})^2 - (g_{1,1} + g_{2,1})^2}, \quad (A\text{-}20)$$

$$\Sigma_{2,0} = \Sigma_{1,0}, \quad (A\text{-}21)$$

$$\Sigma_{2,1} = \Sigma_{1,1}. \quad (A\text{-}22)$$

In this limit, the self energies are the same for all the bands, because the isotropic scattering mixes all momentum states, not just the states within the same band.
APPENDIX B
GENERAL EXPRESSION FOR PENETRATION DEPTH

B.1 Introduction

In this Appendix, I discuss some details involved in the derivation of the current response for an anisotropic singlet superconductor in the case of a lattice Hamiltonian, in a way general enough to include all kinds of scattering processes excluding the vertex corrections. The kinetic energy term in a tight binding Hamiltonian is given as,

\[ H_0 = \sum_{i,j} \left( t_{ij} c_i^\dagger c_j + h.c. \right), \]  

(B-1)

where \( i, j \) denotes the sites and \( t_{ij} \) is the hoping matrix element between the \( i^{th} \) and \( j^{th} \) sites. \( c_i^\dagger, c_i \) are the creation and annihilation operators respectively on the \( i^{th} \) site. In the presence of a vector potential \( t_{ij} \rightarrow t_{ij} \exp (ieA \cdot r_{ij} \cdot \hat{x}) \) where \( \hbar = c = 1 \) and \( r_{ij} = r_j - r_i \) [80, 183]. We make a Taylor series expansion for the phase factor due to vector potential and only keep the term which has \( A \cdot \hat{x} \).

\[ H(A \cdot \hat{x}) = H_0 + \sum_{i,j} \left( t_{ij} c_i^\dagger c_j \left( ieA \cdot \hat{x} r_{ij} \cdot \hat{x} - (eA \cdot \hat{x} r_{ij} \cdot \hat{x})^2 / 2 \right) + h.c. \right), \]  

(B-2)

where \( H_0 \) is the part of the Hamiltonian which is independent of \( A \cdot \hat{x} \). Note we have chosen the \( \hat{x} \) direction arbitrarily as being the direction of the current, thus the only terms in the Hamiltonian which will contribute are those which give projections onto the \( x \)-direction. To obtain the total current, we operate with \( -\frac{\hat{x}}{\partial A \cdot \hat{x}} \). This gives

\[ j^{\hat{x}}_{\text{total}} = \sum_{i,j \in \mathbb{R}} \left( t_{ij} c_i^\dagger c_j \left( -ier_{ij} \cdot \hat{x} + (er_{ij} \cdot \hat{x})^2 A \cdot \hat{x} \right) + h.c. \right), \]  

(B-3)

where we define

\[ j^{\hat{x}}_{\text{dia}} = \sum_{i,j \in \mathbb{R}} (r_{ij} \cdot \hat{x})^2 \left( t_{ij} c_i^\dagger c_j + h.c. \right), \]  

(B-4)

and

\[ j^p = \sum_{i,j \in \mathbb{R}} i r_{ij} \cdot \hat{x} \left( t_{ij} c_i^\dagger c_j - h.c. \right). \]  

(B-5)
Now we have to calculate the expectation value of the total current. The second term is the Eq. (B–3) is already linear in external field. So we can directly calculate the expectation value with the unperturbed ground state, because any correction to the ground state wave function due to the external potential will not contribute in first order. For the paramagnetic current which is independent of $\mathbf{A} \cdot \hat{\mathbf{x}}$, we need to consider the effect of an external field on wave function up to first order in the field. So in the interaction representation the wave function acquires a factor $T \exp \left[ -i \int_{-\infty}^{t} H'(t') dt' \right] |0\rangle$ (see any many-body text, e.g. [75]). In this case, the zeroth order contribution is zero, because there is no current in the absence of a field, and we keep terms which are first order in $\mathbf{A} \cdot \hat{\mathbf{x}}$. We write down the response function $K_{ij}$, which is defined as:

$$\langle j_{\text{total}} \rangle = J_i(q, \omega) = -e^2 K_{ij}(q, \omega) A_j(q, \omega), \quad (B–6)$$

where $K_{ij}$ is,

$$K_{ij}(q, \omega) = \langle -j_{\text{dia}} \rangle \delta_{ij} - \int_0^\beta d\tau \langle T_{\tau} [j^p_i(q, \tau) j^p_j(-q, 0)] \rangle$$

$$= K^\text{dia}_{ij}(q, \omega) + K^\text{para}_{ij}(q, \omega). \quad (B–7)$$

Eq. B–7 has two terms, the diamagnetic term

$$K^\text{dia}_{ij}(q, \omega) = \langle -j_{\text{dia}} \rangle \delta_{ij}, \quad (B–8)$$

and the paramagnetic term,

$$K^\text{para}_{ij}(q, \omega) = -\int_0^\beta d\tau \langle T_{\tau} [j^p_i(q, \tau) j^p_j(-q, 0)] \rangle, \quad (B–9)$$

with this definition of response function superfluid weight $D_s/e^2/\pi = n_s/m$ is given by [2, 80, 184],

$$\frac{D_s}{\pi e^2} = \frac{n_s}{m} = K_{ij}(q \rightarrow 0, \omega = 0). \quad (B–10)$$
Now the terms of first order in external field in Eq. (B–3) will give the diamagnetic response (B–8). For the diamagnetic term we can easily take the expectation value, 

\[ j^x_{\text{dia}} = \sum_{i,j} \left( t_{ij} c_i^\dagger c_j + \text{h.c.} \right) \left( -(r^x_{ij})^2 \right). \]  

(B–11)

Taking \( t_{ij} = -t \), \( r^x_{ij} = a \) for nearest neighbor and \( t_{ij} = -t', r^x_{ij} = a \) and we will sum only along the direction where \( r^x_{ij} \neq 0 \). So the expression in Fourier space becomes,

\[ j^x_{\text{dia}} = \sum_k \left( c_k^\dagger c_k \right) \left( -(a^2) \right) \left( -2t \cos(k_x) - 4t' \cos(k_x) \cos(k_y) \right). \]  

(B–12)

Here we notice that,

\[ (-2t \cos(k_x) - 4t' \cos(k_x) \cos(k_y)) = -a^2 \frac{d^2 \epsilon_k}{dk_x^2}. \]  

(B–13)

This term has dimensions of inverse mass, and this is in general true for any tight binding Hamiltonian. For a general hoping matrix element \( t_{ij} \), we can write

\[ t_{ij(=i+a)} = t_x \delta(x + a) + t_y \delta(y \pm b) + t' \delta(x + a) \delta(y \pm b) + \ldots \]  

(B–14)

Only terms which have projection along \( \hat{x} \) will contribute to the response. In the presence of an external field, \( t_{ij} \rightarrow t_{ij} \exp(iA_x \cdot r_{ij}) \). So for the term linear in external field, along \(+\hat{x}\) it becomes

\[ \sum_k t_{ij} c_k^\dagger c_k \exp(i k \cdot r_{ij} + i k' \cdot r_{ij}) = \sum_k c_k^\dagger c_k \left[ \sum_n a_n t^n_x \exp(i k_x a_n) \right. \]  

(B–15)

\[ + \sum_{n,n'} a_{n'} t^n_{xy} \exp(i k_x a_{n'}) \left( 2 \cos(k_y b) \right) \left] \right. \right. \]

Here the superscript \( n \) denotes the neighbor distance along the \( a \) and \( b \) axis and \( n' \) along the diagonals in the lattice, e.g. \( n = 1 \) is nearest neighbor, \( n' = 1 \) is next nearest neighbor and so on. For the diamagnetic current term, we need \( t_{ij} + t'_{ij} \), which follows
from Eq. (B–16),

\[
\sum_k t_{ij} c_k^\dagger c_{k'} \exp(i k \cdot r_i + i k' \cdot r_j) + h. c. = \sum_{k,n,n'} c_k^\dagger c_k \left[ (na)^2 t_{x}^n (2 \cos(k_xa)) + (n'a)^2 t_{xy}^n (2 \cos(k_xa')/(2 \cos(k_yb))) \right],
\]

and for the corresponding tight binding dispersion,

\[
\epsilon_k = t_x(2 \cos(k_xa)) + t_y(2 \cos(k_ya) + t'(2 \cos(k_xa)(2 \cos(k_yb))) + \sum_n t_{x}^n (2 \cos(k_xan)) + \sum_n t_{xy}^n (2 \cos(k_xan))(2 \cos(k_ybn)),
\]

Using Eq. (B–17), we can write the diamagnetic term as

\[
\sum_k t_{ij} c_k^\dagger c_{k'} \exp(i k \cdot r_i + i k' \cdot r_j) = \sum_k c_k^\dagger c_k \left( -\frac{d^2 \epsilon_k}{dk_x^2} \right)
\]

This expression is true in general for any lattice dispersion. Now for the diamagnetic term, the expectation value of \( < c_k^\dagger c_k > = < \hat{n}_k > \) is equal to \( 1/\beta \sum \frac{i \omega}{\omega_m} G(i \omega, \xi_k) \exp(i \omega_m \beta^+). \)

So the diamagnetic current operator becomes

\[
j_{\text{dia}}^x = -\sum_k \left( c_k^\dagger c_k \right) \left( -\frac{d^2 \epsilon_k}{dk_x^2} \right),
\]

and the final expression for the diamagnetic response is

\[
<j_{\text{dia}}^x> = 2 T \sum_{i\omega_m} \sum_k \left( \frac{d^2 \epsilon_k}{dk_x^2} \right) G(i \omega_m, k),
\]

where \( G \) is the diagonal Matsubara Green's function in the superconducting state,

\[
G(i \omega_n, k) = \frac{i \omega_n + \xi_k}{(i \omega_n)^2 - \xi_k^2 - \Delta_k^2}.
\]

Next we calculate the paramagnetic response. The paramagnetic current comes from the first term in Eq. (B–3). This term is independent of \( A_x \). So we will use the Kubo formula, which requires the calculation of the current-current correlation function. In
In general, the paramagnetic current on a lattice is

$$j^p = \sum_{ij} \left( t_{ij} c^\dagger_i c_j - h.c. \right) (i \mathbf{r}^*_{ij}),$$  \hspace{1cm} (B–22) 

which for nearest neighbor hoping is given as,

$$j^p_{nn} = \sum_k \left( -2t \sin(k_x) c^\dagger_k c_k \right) (-a),$$  \hspace{1cm} (B–23) 

and for next nearest neighbor hoping is,

$$j^p_{nnn} = \sum_k \left( -4t' \sin(k_x) \cos(k_y) c^\dagger_k c_k \right) (-a).$$  \hspace{1cm} (B–24) 

So in general it is the velocity and is expressed as,

$$j^p = \sum_{k,\sigma} \left( \frac{d\epsilon_k}{dk_x} c^\dagger_{k\sigma} c_{k\sigma} \right),$$  \hspace{1cm} (B–25) 

In the Nambu basis, we define \( c^\dagger_k = \{ c^\dagger_{k,\uparrow} \ c_{-k,\downarrow} \} \) and the paramagnetic current operator may be written as,

$$j^p = \sum_{k,\sigma} \left( \frac{d\epsilon_k}{dk_x} c^\dagger_{0\sigma} c_{0\sigma} \right)$$  \hspace{1cm} (B–26) 

Now we need to calculate the current current correlation function defined as

$$\Lambda(q, i\nu) = \int_0^\beta \exp(i\nu\tau) \langle j^p(\tau)j^p(0) \rangle$$  \hspace{1cm} (B–27) 

so we need \( \langle c^\dagger_{k}(\tau)\tau_0 c_{k+q}(\tau) c^\dagger_{k'}(0)\tau_0 c_{k'-q}(0) \rangle \). Within the Hartree-Fock approximation, we keep only terms corresponding to BCS pairing, such that the product may be written \( Tr[G(k + q, \tau)G(k, -\tau)] \). In Fourier space the current current correlation function becomes,

$$\Lambda(q, i\nu) = \int_0^\beta d\tau \exp(i\nu\tau) T^2 \sum_{\omega_m,\omega_n} \exp(-i\omega_m\tau) \exp(i\omega_n\tau) \ Tr[G(k + q, \omega_m)G(k, \omega_n)],$$ \hspace{1cm} (B–28)
and after integrating out $\tau$, we get,

$$\Lambda(q, i\nu) = T^2 \sum_{\omega_m, \omega_n} (\beta \delta_{\nu+\omega_m = \omega_n}) \text{Tr}[G(k+q, \omega_m)G(k, \omega_n)],$$

which can be simplified as

$$\Lambda(q, i\nu) = T \sum_{\omega_m} \text{Tr}[G(k+q, \omega_m)G(k, \omega_m - \nu)].$$

Where we have introduced the Nambu (matrix) Green’s function

$$G = \begin{pmatrix} G(k, i\omega_n) & F(k, i\omega_n) \\ F^\dagger(k, i\omega_n) & G(-k, i\omega_n) \end{pmatrix},$$

and $G$ and $F$ are defined as

$$G(k, i\omega_n) = \frac{i\omega_n + \xi_k}{(i\omega_n)^2 - \xi_k^2 - \Delta_k^2},$$

$$F(k, i\omega_n) = \frac{\Delta_k}{(i\omega_n)^2 - \xi_k^2 - \Delta_k^2}.$$  

So finally the expression for the current current correlation function becomes,

$$\Lambda(q, i\nu) = T \sum_{\omega_m, k} \text{Tr}[G(k+q, \omega_m)G(k, \omega_m - \nu)] \left[ \frac{d\epsilon_k}{dk_x} \right]^2.$$  

In the last expression the finite 'q' terms in velocity have been ignored because the main contribution to this integral comes from the region near the Fermi surface, and in the small q limit $k + q \approx k$. In the next section, I show that the superfluid density is zero in the normal state.

**B.2 Normal State Cancellation**

In the normal state the Green's function reduces to a simple normal state Green’s function. So for the diamagnetic component we can write,

$$< \hat{J}_{dia}^x > = 2T \sum_{\omega_m} \sum_k \left( \frac{d^2 \epsilon_k}{dk_x^2} \right) \frac{1}{i\omega - \epsilon_k}.$$
Summation over Matsubara frequencies gives,

$$< j_{\text{dia}}^x > = 2 \sum_k \left( \frac{d^2 \epsilon_k}{dk_x^2} \right) f(\epsilon_k), \quad (B-36)$$

and now we perform integration by parts on the diamagnetic term,

$$< j_{\text{dia}}^x > = \frac{1}{4\pi^2} \int_{k_y} \int_{k_x} \left( \frac{d\epsilon_k}{dk_x} \right)^2 \frac{df(\epsilon_k)}{d\epsilon_k}. \quad (B-37)$$

The first term is zero in Eq. (B-38) and in the second term \( \frac{df(\epsilon_k)}{d\epsilon_k} \to \frac{df(\epsilon_k)}{d\epsilon_k} \frac{d\epsilon_k}{dk_x} \). So finally we have,

$$< j_{\text{dia}}^x > = -\frac{1}{4\pi^2} \int_{k_y} \int_{k_x} \left( \frac{d\epsilon_k}{dk_x} \right)^2 \frac{df(\epsilon_k)}{d\epsilon_k}. \quad (B-38)$$

Now in the paramagnetic term, it’s very important to first set \( i\nu = 0 \) and then taking the limit \( q \to 0 \), for the cancellation in the normal state [80]. This gives,

$$\Lambda(q \to 0, i\nu = 0) = 2 \frac{1}{4\pi^2} \int_k T \sum_{\omega_m} \left[ \frac{1}{i\omega_m - \epsilon_k + q} \frac{1}{i\omega_m - \epsilon_k} \right] \left( \frac{d\epsilon_k}{dk_x} \right)^2, \quad (B-39)$$

which can be written after doing summation over the Matsubara frequencies

$$\Lambda(q \to 0, i\nu = 0) = 2 \frac{1}{4\pi^2} \int_k \left[ \frac{f(\epsilon_k + q) - f(\epsilon_k)}{\epsilon_k + q - \epsilon_k} \right] \left( \frac{d\epsilon_k}{dk_x} \right)^2, \quad (B-40)$$

which in limit \( q \to 0 \) becomes,

$$\Lambda(q \to 0, i\nu = 0) = 2 \frac{1}{4\pi^2} \int_k \left[ \frac{df(\epsilon_k)}{d\epsilon_k} \right] \left( \frac{d\epsilon_k}{dk_x} \right)^2, \quad (B-41)$$

which exactly cancels the diamagnetic response given by Eq. B–38. In the next section, I express the superfluid density in terms of spectral functions, which is easier to handle in the presence of complicated scattering processes.
B.3 Total Current Response

The diamagnetic term can be written as,

\[
\langle j_{\text{dia}}^x \rangle = -2 T \sum_{i \omega_n} \int \sum_k \left( \frac{d^2 \epsilon_k}{dk_x^2} \right) \frac{A(k, \epsilon)}{i \omega_n - \epsilon} = -2 \sum_k \left( \frac{d^2 \epsilon_k}{dk_x^2} \right) A(k, \epsilon) f(\epsilon),
\]

(B–42)

where \( f(\epsilon) \) is the Fermi function and \( A(k, \epsilon) \) is the spectral function defined as,

\[
A(k, \omega) = -\frac{1}{\pi} \text{Im} \frac{\omega + \epsilon_k}{\omega^2 - E_k^2}.
\]

(B–43)

Where \( E_k = \sqrt{\epsilon_k^2 + \Delta_k^2} \), \( \omega_\pm = \omega + i \Gamma \) and \( \Gamma \) is the single particle scattering rate, assumed here to modify only the \( \omega \) term in the Green’s function. The paramagnetic term can be expressed using

\[
\Lambda(q, i \nu) = T \sum_{\omega_n} \text{Tr} \left[ G(k + q, \omega_n) G(k, \omega_n - \nu) \right] \left( \frac{d \epsilon_k}{dk_x} \right)^2,
\]

\[
= T \sum_{\omega_n} \int_{\epsilon_1, \epsilon_2} \frac{\text{Tr} \left[ \text{Im}(G(k + q, \epsilon_1)) \text{Im}(G(k, \epsilon_2)) \right]}{(i \omega_n - \epsilon_1)(i \omega_n - \nu - \epsilon_2)} \left( \frac{d \epsilon_k}{dk_x} \right)^2,
\]

\[
= \int_{\epsilon_1, \epsilon_2, k} \frac{\text{Tr} \left[ \text{Im}(G(k + q, \epsilon_1)) \text{Im}(G(k, \epsilon_2)) \right]}{(\epsilon_1 - \epsilon_2 - i \nu)} \left[ f(\epsilon_1) - f(\epsilon_2) \right] \left( \frac{d \epsilon_k}{dk_x} \right)^2,(B–44)
\]

and specifically for the limit \( i \nu \to 0 \), we have

\[
\Lambda(q, 0) = \int \frac{d \epsilon_1}{2\pi} \frac{d \epsilon_2}{2\pi} \text{Tr} \left[ \text{Im}(G(k + q, \epsilon_1)) \text{Im}(G(k, \epsilon_2)) \right] \left( \frac{f(\epsilon_1) - f(\epsilon_2)}{\epsilon_1 - \epsilon_2} \right) \left( \frac{d \epsilon_k}{dk_x} \right)^2(\text{B–45})
\]

\[
= 2 \int \frac{d \epsilon_1}{2\pi} \frac{d \epsilon_2}{2\pi} [A(k + q, \epsilon_1) A(k, \epsilon_2)] \left( \frac{f(\epsilon_1) - f(\epsilon_2)}{\epsilon_1 - \epsilon_2} \right) \left( \frac{d \epsilon_k}{dk_x} \right)^2,(\text{B–46})
\]

\[
+ B(k + q, \epsilon_1) B(k, \epsilon_2) \left( \frac{f(\epsilon_1) - f(\epsilon_2)}{\epsilon_1 - \epsilon_2} \right) \left( \frac{d \epsilon_k}{dk_x} \right)^2,
\]

where \( B(k, \omega) \) is,

\[
B(k, \omega) = -\frac{1}{\pi} \text{Im} \frac{\Delta_k}{\omega^2 - E_k^2}.
\]

(B–47)

This is usually sufficient in a \( d \)-wave superconductor, but not completely general. For superconductors other than \( d \) wave, \( \Delta \) is replaced by a renormalized \( \Delta \) and particle-hole asymmetric systems the single particle energy \( \xi_k \) must be renormalized as well. We can
further simplify the diamagnetic term,

\[ K_{\text{dia}} = 2 T \sum_\omega \sum_k \frac{d^2 \epsilon_k}{dk_x^2} \frac{i \omega + \xi_k}{(i \omega)^2 - \xi_k^2 - \Delta_k^2}. \]  

(B–48)

Now we perform an integration by parts over the variable \( k_x \), The diamagnetic term is

\[ K_{\text{dia}} = 2 T \sum_\omega \left[ \left( \int_{k_y} d \epsilon_k \frac{i \omega + \xi_k}{(i \omega)^2 - \xi_k^2 - \Delta_k^2} \right)_{\pi}^{-\pi} - \sum_k \frac{d \epsilon_k}{dk_x} \frac{1}{(i \omega)^2 - \xi_k^2 - \Delta_k^2} \frac{d \epsilon_k}{dk_x} + \frac{i \omega + \xi_k}{[(i \omega)^2 - \xi_k^2 - \Delta_k^2]^2} \frac{d E_k^2}{dk_x} \right]. \]  

(B–49)

The first term in the above expression is zero, and the second term can be written as:

\[ K_{\text{dia}} = 2 T \sum_\omega \sum_k \left[ -V_x^2 \frac{1}{(i \omega)^2 - \xi_k^2 - \Delta_k^2} - 2 \frac{i \omega + \xi_k}{((i \omega)^2 - \xi_k^2 - \Delta_k^2)^2} \left( \xi_k V_x + \Delta_k V_x^\Delta \right) \right]. \]  

(B–50)

Here \( V_x = \frac{d \epsilon_k}{dk_x} \) and \( V_x^\Delta = \frac{d \Delta_k}{dk_x} \). Now the paramagnetic term in total current response is

\[ K_{\text{para}} = 2 T \sum_\omega \sum_k V_x^2 \left[ \frac{(i \omega)(i \omega') + \xi_k^2 + \Delta_k^2 + \xi_k(i \omega + i \omega')}{((i \omega)^2 - E_k^2)((i \omega')^2 - E_k^2)} \right], \]  

(B–51)

\[ = 2 T \sum_\omega \sum_k V_x^2 \left[ \frac{1}{(i \omega)^2 - \xi_k^2 - \Delta_k^2} \right. 
\]  

\[ + \left. \frac{(i \omega)(i \omega') - (i \omega')^2 + 2 E_k^2 + \xi_k(i \omega + i \omega')}{((i \omega)^2 - E_k^2)((i \omega')^2 - E_k^2)} \right]. \]  

(B–52)

Now we can combine both terms, noting that the divergent contribution comes with opposite signs in both the equation, hence canceled. Now we can also set \( \Omega \rightarrow 0; \omega = \omega' \). The remaining terms can be written as,

\[ K = 2 T \sum_\omega \sum_k \left[ V_x^2 \frac{2 \Delta_k^2}{((i \omega)^2 - E_k^2)^2} - V_x^\Delta \frac{2 \Delta_k(i \omega + \xi_k)}{((i \omega)^2 - E_k^2)^2} \right]. \]  

(B–53)

In presence of self energy corrections, \( \omega \rightarrow \omega - \Sigma_0 \) and \( \Delta \rightarrow \Delta + \Sigma_1 \). Eq. B–53 is valid as long as the self energies are not momentum dependent.
B.4 Spectral Representation of Total Current Response

The total current response can be expressed in terms of spectral functions as

\[ K = 4 \sum_k \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \left[ V_x^2 B(k, x) B(k, y) \right] \]

\[ - V_x V_x^\Delta B(k, x) A(k, y) \left[ f(x) - f(y) \right] \]

\[ x - y + i\delta, \]

\[ B(k, x) = -\frac{1}{\pi} \text{Im} \left[ \frac{\Delta_k}{x^2 - E_k^2} \right], \quad \text{(B–55)} \]

\[ A(k, x) = -\frac{1}{\pi} \text{Im} \left[ \frac{x + \xi_k}{x^2 - E_k^2} \right], \quad \text{(B–56)} \]

\[ V_x = \frac{d\epsilon_k}{dk_x}, \quad \text{(B–57)} \]

\[ V_x^\Delta = \frac{d\Delta_k}{dk_x}. \quad \text{(B–58)} \]
REFERENCES


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BIOGRAPHICAL SKETCH

Vivek Mishra was born in February 1983, in Jagdalpur, India. He obtained his Higher Secondary School Certificate with mathematics, physics and chemistry in his hometown, and admitted to Indian Institute of Technology, Kanpur, India in 2001, where he graduated with Master of Science (Integrated) in physics in 2006. In 2006, he went to University of Florida, Gainesville, United States America and completed his Doctor of Philosophy in physics in 2011.