Ultrasonic Attenuation in Layered Superconductors

by

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Abstract

We study the ultrasonic attenuation in layered superconductors using the Green’s function formalism. General expressions are derived analytically and then calculated numerically by taking the nearest and next-nearest interactions in a disordered layered superconductor with random hoppings. Our results show huge anisotropies of ultrasonic attenuation in the superconductors and the strong dependence of ultrasonic attenuation on the temperature and the direction of polarization of the sound wave.
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Chapter 1

Introduction

Superconductivity was discovered first by H.K. Onnes in 1911 when a sharp drop of resistance of several orders of magnitude was found in mercury on lowering the temperature below 4K. After that many superconductors have been found and the critical temperature raised higher and higher. But the first theory for superconductivity appeared only 46 years after H.K. Onnes’ remarkable discovery. It is known as the BCS theory published by J. Bardeen, L. Cooper and J.R. Schrieffer, who were the first to explain the properties of superconductors from the first principles [1].

However, it took another 25 years before the high-$T_c$ era began when Bednorz and Müller found a new class of superconductors, known as high-$T_c$ cuprates. Now the critical temperature is far above the liquid nitrogen temperature and moving towards room temperature. Many novel superconductors have been found in recent years, including heavy-fermion superconductors, organic superconductors, ferromagnetic superconductors, and others.

The study of the $c$-axis transport properties in layered superconductors is one of the interesting topics which has fundamental consequences for theories of the normal state and superconducting state. In order to identify the superconducting mechanism, a variety of experiments have been done to measure the conductivity [2, 3, 4] and the penetration depth [5, 6, 7] along the $c$-axis of different high-$T_c$ superconductors. Many interesting results has been found from these works and inspired theoretical work on this topic. Now it is well accepted that high-$T_c$ superconductors have a $d_{x^2-y^2}$ wave pairing symmetry in CuO$_2$ planes, based on the measurements of the temperature dependence of the in-plane penetration depth.
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[6, 8], ARPES (angle-resolved photoemission spectroscopy) [9] and phase-sensitive measurement [10]. Some experiments also showed that the in-plane penetration depth increases linearly with $T$ at low temperature, which is in contrast to the activated behavior of conventional superconductors [11].

These interesting results have inspired theoretical work on the $c$-axis transport in the high-$T_c$ superconductors. The first theoretical work was done by A.G. Rojo and K. Levin in 1993 using a model of an anisotropic three-dimensional disordered system with the nearest-neighbor hopping [12]. Three years later K. L.e.hoppingvin compared their work [13] with P.W. Anderson’s [14] and confirmed that the interlayer transport was a tunneling process with a strong inelastic component but it was unknown whether each CuO$_2$ plane should be a Luttinger liquid or a Fermi liquid. After that, many models appeared to calculate the conductivity along the $c$-axis, based on the assumptions of Luttinger liquid or Fermi liquid [15, 16]. In 2001 M. Turlakov and A.J. Leggett were inspired by the Coulomb blockade phenomena to argue that the anomalous $c$-axis transport properties were a consequence of the strong correlations in the cuprates [17]. However, there is no agreement on this topic which can be extracted from the currently available experiments.

In recent years, ultrasonic attenuation is a new method that has been used to explore the transport properties of $c$-axis in the superconductors [18]. This method was firstly used to locate the gap line and point nodes in superconducting UPt$_3$ in 1986 [19]. In 2001 C. Lupien et al. measured the ultrasonic attenuation both in the normal and superconducting states of Sr$_2$RuO$_4$ and found huge anisotropies in the measured attenuation, both in the normal and superconducting states [18].

There has been extensive theoretical work concerning the ultrasonic attenuation in different superconductors and normal metals, including a recent one published by M.B. Walker, M.F. Smith and K.V. Samokhin [20]. They suggested a model that properly takes into account the crystalline and electronic structure of superconductors. The strong anisotropy
of the ultrasonic attenuation in superconductors is intimately connected with its layered square-lattice structure. Assuming that the interlayer electron-phonon interaction can be neglected, they calculated the attenuation attributing the electron-phonon interaction to the stretching of bonds between ions lying in a single plane.

So the ultrasonic attenuation has been shown to be an important tool of exploring the c-axis transport properties of superconductors. Motivated by this fact, especially by the recent experimental and theoretical work [18, 20], we investigated the ultrasonic attenuation in superconductors with layered square-lattice structure. In order to compare the data from our numerical simulations with the data from future experiments, many details on the Hamiltonian have to be considered. In our model, in addition to the electron-phonon interaction associated with the stretching of bonds between ions lying in a single plane, the interactions associated with the stretching of bonds between different planes have also been taken into account. In our model, we assume that the hopping amplitudes are random. This is the first time in the literature that both the nearest and the next-nearest interlayer hoppings are taken into account in a model of a three-dimensional disordered system for the purpose of the calculation of the ultrasonic attenuation in superconductors. With these considerations more information enters into the Hamiltonian, which makes the model more universal and the data much more reliable when comparisons between the numerical results and the future experiment data are made.

The thesis is organized as follows. Chap. 2 is the theoretical part in which the model Hamiltonian is introduced, and the ultrasonic attenuation coefficient is calculated using the Green's function formalism. All the numerical results are presented and analyzed in details in Chap. 3, including the solution for the self-energy and the ultrasonic attenuation lengths for longitudinal and transverse waves along the z-axis of crystals. Chap. 4 contains a conclusion and the discussion of future work.
Chapter 2

Theory and Calculation

This Chapter presents the theoretical analysis of single-electron properties and electron-phonon interaction in a disordered layered superconductor with d-wave pairing. Firstly only the nearest-neighbor electron hoppings between the sites in a single plane as well as the interlayer hoppings are considered to derive a tight-binding electron Hamiltonian. Then both the nearest and the next-nearest hoppings are taken into account. All these details are shown from Chap. 2.1 to Chap. 2.6, where the renormalized Matsubara frequency and the solutions for the electron self-energy are also discussed. In Chap. 2.7 the expression for the electron-phonon interaction are derived for both the longitudinal wave case and the transverse wave case.

The purpose of this thesis is to calculate the ultrasonic attenuation in layered superconductors, the final form of which is shown in Chap. 2.8. The ultrasonic attenuation coefficient follows from the self-energy function of phonon after taking its imaginary part. In this thesis, all the theoretical work is based on the detailed tight-binding Hamiltonian we developed and analyzed using the Green's function formalism.

2.1 The tight-binding model and Hamiltonian

Our model is based on the crystalline structure of the cuprate high-$T_c$ superconductor YBa$_2$Cu$_3$O$_7$, which is shown in Fig. 2.1. It is well accepted that the superconductivity occurs in the CuO$_2$-plane and depends mainly on the number of carriers within the CuO$_2$-
Chapter 2

Family and Environment

The family and environment play a crucial role in the development of a child. A stable and supportive family environment can significantly influence a child's well-being and future success. On the other hand, an environment filled with stress and conflict can have detrimental effects on a child's emotional and psychological health.

Research has shown that children from supportive families are more likely to develop into healthy, well-adjusted adults. These families provide a secure base from which children can explore their surroundings and develop their social and emotional skills. Conversely, children who grow up in unstable or abusive environments are at a higher risk of developing mental health problems and behavioral issues.

In addition to family dynamics, the broader environment in which a child lives also plays a role in their development. Factors such as access to quality education, healthcare, and recreational opportunities can significantly impact a child's growth and development. Policies and programs aimed at improving these conditions can have a positive effect on children's outcomes.

In conclusion, the family and environment are key determinants of a child's development. By creating supportive family environments and addressing the broader social determinants of health, we can work towards improving the well-being of all children.
plane, which is controlled by the charge reservoirs between the planes and the correlation between these carriers. The unit cell of the system is a parallelepiped with the lattice constants $a$, $b$, $c$ ($a = b < c$) for three sides respectively.

Considering the nearest-neighbor electron hopping in a single plane as well as the interlayer ones, the tight-binding electron Hamiltonian in the normal state has the form

$$H = -\sum_{n,m} \sum_{i,j} t_{nm,ij} c_{n,i,\alpha}^\dagger c_{m,j,\alpha} - \mu \sum_{n,i} c_{n,i,\alpha}^\dagger c_{n,i,\alpha}, \quad (2.1)$$

where $n$ and $m$ label different layers, $i$ and $j$ label the sites within a single layer, $\mu$ is the chemical potential, and $\alpha = \uparrow, \downarrow$ is the spin projection. We neglect in-plane disorder, then the hopping amplitudes $t_{nm,ij}$ can be written as

$$t_{nm,ij} = \begin{cases} t_{\parallel}, & \text{if } n = m \text{ and } i \text{ and } j \text{ are the nearest neighbors,} \\ t_\perp(n, i) \delta_{ij} = \left[t_\perp + \delta t_\perp(n, i)\right] \delta_{ij}, & \text{if } n = m \pm 1 \end{cases}. \quad (2.2)$$
Figure 2.2: The hopping amplitudes $t_{nm,ij}$. Only two layers of the structure are shown. The hopping $t_{||}$ appears between $O$ and $A$, $O$ and $B$, $O$ and $C$, $O$ and $D$, $O'$ and $A'$, $O'$ and $B'$, $O'$ and $C'$, $O'$ and $D'$ respectively. $t_\perp$ and $\delta t_\perp(n, i)$ appear between $O$ and $O'$. Here $t_{||}$ is the hopping amplitude between the nearest ions in a single plane, $t_\perp$ describes the coherent tunneling between two neighboring planes, and $\delta t_\perp(n, i)$ simulates the random contribution to the interlayer tunneling. By substituting (2.2) for $t_{nm,ij}$ into (2.1), one finds the detailed form of the tight-binding Hamiltonian as

$$H = -t_{||} \sum_n \sum_{\langle ij \rangle} c_{n,i,\alpha}^\dagger c_{m,j,\alpha} - t_\perp \sum_{n,i} \left[ c_{n,i,\alpha}^\dagger c_{n+1,i,\alpha} + c_{n+1,i,\alpha}^\dagger c_{n,i,\alpha} \right] - \mu \sum_{n,i} c_{n,i,\alpha}^\dagger c_{n,i,\alpha} + \sum_{n,i} \delta t_\perp(n, i) \left[ c_{n,i,\alpha}^\dagger c_{n+1,i,\alpha} + c_{n+1,i,\alpha}^\dagger c_{n,i,\alpha} \right].$$

(2.3)

The angular brackets in the first term denote the nearest neighbors. In our model, the probability distribution of $\delta t_\perp$ is assumed to be Gaussian with the averages

$$\langle \delta t_\perp(n, i) \rangle = 0,$$

(2.4)

$$\langle \delta t_\perp(n_1, i_1) \delta t_\perp(n_2, i_2) \rangle = \gamma^2 \delta_{n_1,n_2} \delta_{i_1,i_2}.$$

(2.5)

Here $\gamma$ is the measure of the disorder strength.
Now let's introduce the Fourier transforms
\[ c_{n,i}\alpha = \frac{1}{\sqrt{N}} \sum_k c_{k,\alpha} e^{ikR_{n,i}}, \]  
(2.6)
\[ \delta t_{\perp}(n,i) = \frac{1}{\sqrt{N}} \sum_Q \delta t_{\perp}(Q) e^{iQ R_{n,i}}, \]  
(2.7)
where the wave vector \( k \) takes values in the first Brillouin zone, \( N \) is the total number of unit cells in our system, and \( R_{n,i} \) are the positions of the lattice sites. The tight-binding Hamiltonian can be written in the momentum representation as follows
\[ H = H_0 + H', \]  
(2.8)
\[ H_0 = \sum_k \xi(k) c_{k,\alpha}^\dagger c_{k,\alpha}, \]  
(2.9)
\[ \xi(k) = -2t_{\parallel}(\cos k_x a + \cos k_y a) - 2t_{\perp} \cos k_z c - \mu, \]  
(2.10)
\[ H' = -\frac{1}{\sqrt{N}} \sum_{k,Q} \delta t_{\perp}(Q)(c_{k,\alpha}^\dagger c_{k-Q,\alpha} e^{-ikz c} + c_{k+Q,\alpha}^\dagger c_{k,\alpha} e^{ikz c}). \]  
(2.11)
Here, \( \delta t_{\perp}(Q) \) is a random field whose correlator is given by
\[ \langle \delta t_{\perp}(Q_1) \delta t_{\perp}(Q_2) \rangle = \gamma^2 \delta_{Q_1+Q_2,0}. \]  
(2.12)
So the above correlator is not zero only when two electrons have the opposite wave vectors, namely
\[ \langle \delta t_{\perp}(Q) \delta t_{\perp}(-Q) \rangle = \gamma^2. \]  
(2.13)
In the equation (2.8), \( H_0 \) is the free-electron Hamiltonian, while \( H' \) represents the correction due to the random interlayer tunneling.

### 2.2 The Dyson equation and self-energy in the normal state

To get the Dyson equation (see Appendix A) for our system, the first step is to calculate the corrections to the exact Green's function of the first and second order in \( H' \) [21]. The
Matsubara Green’s function is given by

\[ G(k, k', i\omega_n) = G^{(0)}(k, i\omega_n)\delta_{k, k'} + G^{(1)}(k, k', i\omega_n) + G^{(2)}(k, k', i\omega_n) + \cdots, \quad (2.14) \]

where \( G^{(0)}(k, \omega_n) \) is the unperturbed Green’s function

\[ G^{(0)}(k, i\omega_n) = \frac{1}{i\omega_n - \xi(k)}. \quad (2.15) \]

After averaging with respect to disorder, the first-order correction \( \langle G^{(1)}(k, \omega_n) \rangle \) is zero because of (2.4), and the second-order correction is

\[ G^{(2)}(k, i\omega_n) = \int \frac{d^3k_1}{(2\pi)^3} G^{(0)}(k, i\omega_n) G^{(0)}(k_1, i\omega_n) G^{(0)}(k, i\omega_n) \langle V(k, k_1) V(k_1, k) \rangle. \quad (2.16) \]

Here the angular bracket means averaging over the disorder, \( \omega_n = (2n + 1)\pi T \) is the \( n \)th Matsubara frequency, \( \xi(k) \) is the free-electron energy dispersion given in (2.10), and the disorder potential \( V(k, k_1) \) can be expressed as

\[ V(k, k_1) = -\delta t_\perp (k - k_1) \left( e^{ik_2c} + e^{-ik_1z} \right), \quad (2.17) \]

see equation (2.11). By substituting the expression (2.15) for \( G^{(0)} \) and (2.17) for \( V(k, k_1) \) into (2.16), and using the correlator (2.12), one finds the second order correction

\[ G^{(2)}(k, i\omega_n) = 2\gamma^2 G^{(0)}(k, i\omega_n) G^{(0)}(k, i\omega_n) \int \frac{d^3k_1}{(2\pi)^3} G^{(0)}(k_1, i\omega_n) \left[ 1 + \cos(k_2c + k_1z) \right]. \quad (2.18) \]

Then the final form of the Dyson equation can be obtained by substituting the expression (2.18) for \( G^{(2)} \) into (2.14) and replacing \( G^{(0)}(k_1, i\omega_n) \) by \( G(k_1, i\omega_n) \) [22]:
Figure 2.4: The Dyson equation in the case of an impure superconductor. The single solid lines are one-electron Green's function and the double solid lines are the exact Green's functions. Dotted lines with crosses correspond to the impurity averaging.

\[
G^{-1}(k, i\omega_n) = G^{(0)^{-1}}(k, i\omega_n) + 2\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} G(k_1, i\omega_n) \left[1 + \cos(k_2c + k_1z)\right],
\]

(2.19)

where

\[
G^{-1}(k, i\omega_n) = i\omega_n - \xi(k) - \Sigma(k, i\omega_n).
\]

(2.20)

Here the self-energy is different from the usual case of random potential scattering due to the momentum dependence of the impurity lines.

We seek the self-energy \(\Sigma(k, \omega_n)\) in the form

\[
\Sigma(k, i\omega_n) = i\Gamma(k, i\omega_n).
\]

(2.21)

Then the Dyson equation (2.19) yields

\[
\Gamma(k, i\omega_n) = -2\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{1}{i\omega_n - \xi(k_1) - i\Gamma(k_1, i\omega_n)}
\]

\[
-2\gamma^2 \cos(k_2c) \int \frac{d^3k_1}{(2\pi)^3} \frac{\cos(k_1z)}{i\omega_n - \xi(k_1) - i\Gamma(k_1, i\omega_n)}
\]

\[
+2\gamma^2 \sin(k_2c) \int \frac{d^3k_1}{(2\pi)^3} \frac{\sin(k_1z)}{i\omega_n - \xi(k_1) - i\Gamma(k_1, i\omega_n)}.
\]

(2.22)

This suggests separating the Matsubara frequency dependence from the wave vector dependence as follows

\[
\Gamma(k, i\omega_n) = \Gamma_0(i\omega_n) + \Gamma_1(i\omega_n) \cos(k_2c) + \Gamma_2(i\omega_n) \sin(k_2c),
\]

(2.23)
which gives the following equations for the self-energy components

\[
\begin{align*}
\Gamma_0 (i\omega_n) &= -2\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{1}{i\omega_n - \xi (k_1) - i\Gamma (k_1, i\omega_n)}, \\
\Gamma_1 (i\omega_n) &= -2\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{\cos(k_{1z}c)}{i\omega_n - \xi (k_1) - i\Gamma (k_1, i\omega_n)}, \\
\Gamma_2 (i\omega_n) &= 2\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{\sin(k_{1z}c)}{i\omega_n - \xi (k_1) - i\Gamma (k_1, i\omega_n)}.
\end{align*}
\] (2.24)

Below we solve these equations.

First \(\Gamma_1, \Gamma_2\) are neglected and \(\Gamma_0\) is calculated. With the assumption that the density of states at the Fermi surface is constant and equal to \(N_F\), the three dimensional momentum integrals become

\[
\int \frac{d^3k}{(2\pi)^3} = N_F \int_{-\infty}^{+\infty} d\xi \int \frac{dS}{|v_F(k)|^2},
\] (2.25)

where \(v_F(k)\) is the quasiparticle velocity at the Fermi surface. Then (2.24) is simplified and \(\Gamma_0\) is reduced to the from

\[
\Gamma_0 (\omega_n) = \frac{N_F \gamma^2}{2\pi^2} \text{sign}(\omega_n) = \frac{1}{2\tau} \text{sign}(\omega_n),
\] (2.26)

where \(\tau\) is the relaxation time in the normal state. Then by introducing an expansion of \([i\omega_n - \xi (k_1) - i\Gamma (k_1, \omega_n)]^{-1}\) as follows and doing the substitution in (2.24)

\[
\frac{1}{i\omega_n - \xi (k_1) - i\Gamma (k_1, i\omega_n)} = \frac{1}{i\omega_n - \xi (k_1) - i\Gamma_0 (i\omega_n)} = \frac{i\Gamma_1 (i\omega_n) \cos(k_{1z}c) + i\Gamma_2 (i\omega_n) \sin(k_{1z}c)}{[i\omega_n - \xi (k_1) - i\Gamma_0 (i\omega_n)]^2} + \frac{[i\Gamma_1 (i\omega_n) \cos(k_{1z}c) + i\Gamma_2 (i\omega_n) \sin(k_{1z}c)]^2}{[i\omega_n - \xi (k_1) - i\Gamma_0 (i\omega_n)]^3},
\] (2.27)

we calculate the first and the second-order corrections to the integral in (2.24) and therefore to the values of \(\Gamma_0, \Gamma_1, \) and \(\Gamma_2\). After some algebra, one finds the first and the second order correction of the integral turn out to be zero. So that the only solution for the self energy is the trivial one, which can be written as

\[
\Gamma_0 (\omega_n) = \frac{1}{2\tau} \text{sign}(\omega_n), \quad \Gamma_1 (\omega_n) = 0, \quad \Gamma_2 (\omega_n) = 0.
\] (2.28)
Therefore
\[ \Gamma (k, \omega_n) = \Gamma_0 (\omega_n) = -2\gamma^2 \int d^3k_1 \frac{1}{(2\pi)^3 i\omega_n - \xi (k_1) - i\Gamma_0 (\omega_n)} \] (2.29)

Now let's make a further step to see if we can find some non-trivial solutions for the self-energy numerically. Since each \( \Gamma_i, i = 1, 2, 3 \) has a real and imaginary part, the solution of (2.24) can be written as
\[ i\Gamma_0 = A_0 + iB_0, \quad i\Gamma_1 = A_1 + iB_1, \quad i\Gamma_2 = A_2 + iB_2. \] (2.30)

After some manipulation, see Appendix B, one can write the final form for the self-energy as
\[ A_0 = 0, \quad A_1 = 0, \quad A_2 = 0, \] (2.31)

and
\[ B_0 (\omega_n) = \omega_n b_0 (\omega_n), \quad B_1 (\omega_n) = \omega_n b_1 (\omega_n), \quad B_2 (\omega_n) = \omega_n b_2 (\omega_n), \] (2.32)

\[ -\delta_n b_0 = \arccos \left( \frac{b_1}{\sqrt{b_1^2 + b_2^2}} \right) + \arccos \left( \frac{1 - b_0}{\sqrt{b_1^2 + b_2^2}} \right), \]

\[ -\delta_n b_1 = \sin \left[ \arccos \left( \frac{b_1}{\sqrt{b_1^2 + b_2^2}} \right) + \arccos \left( \frac{1 - b_0}{\sqrt{b_1^2 + b_2^2}} \right) \right], \]

\[ -\delta_n b_2 = \cos \left[ \arccos \left( \frac{b_1}{\sqrt{b_1^2 + b_2^2}} \right) + \arccos \left( \frac{1 - b_0}{\sqrt{b_1^2 + b_2^2}} \right) \right] + 1, \] (2.33)

where the following relations must be satisfied from the definition of the trigonometric function
\[ |\delta_n b_0| \leq 2\pi, \quad |\delta_n b_1| \leq 1, \quad -2 \leq \delta_n b_2 \leq 0, \quad 1 - b_0 \leq \sqrt{b_1^2 + b_2^2}. \] (2.34)

The above equations (2.33) and (2.34) are the final expressions used for numerical calculation. However, we can not find any non-trivial solutions for \( b \)'s from our numerical work, which is shown in Chap. 3. Although we can not exclude that the general nonlinear Dyson equations (2.24) have non-trivial solutions, we will make an assumption below in Chap. 2.3, that the only solution for the self energy is the trivial one, i.e. the one without \( k_z \)-dependence.
2.3 Solution of self-energy in the superconducting state

Now let us include the superconducting interactions in our model. The Hamiltonian has the form

\[ H = H_0 + H' + H_{\text{int}}, \tag{2.35} \]

\[ H_{\text{int}} = \frac{1}{2} \sum_{k,k_1} U(k, k_1) c_{-k,1}^\dagger c_{k,1} c_{k_1,1}^\dagger c_{-k_1,1}, \]

\[ U(k, k_1) = \frac{1}{2} U(k, k_1) \sum_{\Gamma} d_{\text{r}}^{\Gamma} (k) \phi_i^{\Gamma^*} (k_1), \tag{2.36} \]

where \( H_0 \) and \( H' \) are defined in (2.9) and (2.11), \( H_{\text{int}} \) is the interaction Hamiltonian including the pair attraction between the particles with opposite momenta, \( U(k, k_1) \) is the BCS interaction applying to the singlet pairing, \( \phi_i^{\Gamma} \) is the basis function of irreducible representations \( \Gamma \) of the point symmetry group of the solid with dimensionality \( d_{\text{r}} \), and \( U(k, k_1) \) is assumed to be non-zero and attractive only within a narrow layer near the Fermi surface [21].

The Green's function of a superconductor at an arbitrary temperature \( T \leq T_c \) in the presence of impurities are determined by the Gor'kov equations. In the momentum-frequency presentation, we have [21]

\[ [i\omega_n - \xi_k - \Sigma(k, i\omega_n)] G(k, \omega_n) + \Delta_k F^\dagger (k, i\omega_n) = 1, \tag{2.37} \]

\[ [i\omega_n + \xi_k - \Sigma(k, i\omega_n)] F^\dagger (k, \omega_n) + \Delta_k G(k, i\omega_n) = 0, \tag{2.38} \]

\[ [i\omega_n - \xi_k - \Sigma(k, i\omega_n)] F(k, \omega_n) - \Delta_k G(-k, -i\omega_n) = 0, \tag{2.39} \]

\[ G(k, i\omega_n) = -\frac{i\omega_n + \xi_k}{\omega_n^2 + \xi_k^2 + \Delta_k^2}, \tag{2.40} \]

\[ F(k, i\omega_n) = \frac{\Delta_k}{\omega_n^2 + \xi_k^2 + \Delta_k^2}, \tag{2.41} \]
\[ i\tilde{\omega}_n(k) = i\omega_n - \Sigma(k, i\omega_n), \]  
\[ \Delta_k = \Delta_0(T)\phi_k, \]  
\[ \phi_k = \cos(kx a) - \cos(ky a). \]  

Here \( \tilde{\omega}_n \) and \( \omega_n \) are the \( n \)th Matsubara frequencies with and without impurities respectively, \( \xi_k \) is the energy dispersion given in (2.10). \( \Delta_k \) is the energy gap, and \( \phi_k \) is the symmetry factor.

The self-energy \( \Sigma \) in (2.42) can be calculated self-consistently as follows. Substituting (2.40)–(2.44) into (2.37)–(2.39), one obtains

\[ \Sigma(k, i\omega_n) \equiv i\Gamma(k, i\omega_n) = -2\gamma^2 \left[ \frac{d^3k_1}{(2\pi)^3} \frac{i\omega_n + \xi_{k_1}}{\tilde{\omega}_n^2 + \xi_{k_1} + \Delta_k^2} \right. \]
\[ -2\gamma^2 \cos(k_z c) \int \frac{d^3k_1}{(2\pi)^3} \frac{i\omega_n + \xi_{k_1}}{\tilde{\omega}_n^2 + \xi_{k_1} + \Delta_k^2} \cos(k_{1z} c) \]
\[ +2\gamma^2 \sin(k_z c) \int \frac{d^3k_1}{(2\pi)^3} \frac{i\omega_n + \xi_{k_1}}{\tilde{\omega}_n^2 + \xi_{k_1} + \Delta_k^2} \sin(k_{1z} c). \]  

In order to separate the frequency dependence from the wave vector dependence in the self-energy, we again represent the self-energy in the following form

\[ \Gamma(k, i\omega_n) = \Gamma_0(i\omega_n) + \Gamma_1(i\omega_n) \cos(k_z c) + \Gamma_2(i\omega_n) \sin(k_z c). \]  

Then instead of (2.24) in the normal state, the equations for self-energy are now given by

\[ \Gamma_0(i\omega_n) = -2\gamma^2 \left[ \frac{d^3k_1}{(2\pi)^3} \frac{i\omega_n + \xi_{k_1}}{\tilde{\omega}_n^2 + \xi_{k_1} + \Delta_k^2} \right. \]
\[ -2\gamma^2 \cos(k_z c) \int \frac{d^3k_1}{(2\pi)^3} \frac{i\omega_n + \xi_{k_1}}{\tilde{\omega}_n^2 + \xi_{k_1} + \Delta_k^2} \cos(k_{1z} c), \]
\[ \Gamma_1(i\omega_n) = -2\gamma^2 \left. \int \frac{d^3k_1}{(2\pi)^3} \frac{i\omega_n + \xi_{k_1}}{\tilde{\omega}_n^2 + \xi_{k_1} + \Delta_k^2} \cos(k_{1z} c) \right], \]
\[ \Gamma_2(i\omega_n) = 2\gamma^2 \left[ \frac{d^3k_1}{(2\pi)^3} \frac{i\omega_n + \xi_{k_1}}{\tilde{\omega}_n^2 + \xi_{k_1} + \Delta_k^2} \sin(k_{1z} c) \right]. \]  

To find the solutions of the coupled non-linear equations (2.47), we first consider the lowest order contribution to self-energy and make an approximation as follows

\[ \tilde{\omega}_n \rightarrow \omega_n, \]  

(2.48)
then (2.47) becomes

\[
\begin{align*}
\Gamma_0 (i\omega_n) &= -2\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{i\omega_n}{\omega_n^2 + \xi_{k_1}^2 + \Delta_{k_1}^2} - 2\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{\xi_{k_1}}{\omega_n^2 + \xi_{k_1}^2 + \Delta_{k_1}^2}, \\
\Gamma_1 (i\omega_n) &= -2\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{i\omega_n \cos (k_{1z}c)}{\omega_n^2 + \xi_{k_1}^2 + \Delta_{k_1}^2} - 2\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{\xi_{k_1} \cos (k_{1z}c)}{\omega_n^2 + \xi_{k_1}^2 + \Delta_{k_1}^2}, \\
\Gamma_2 (i\omega_n) &= 2\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{i\omega_n \sin (k_{1z}c)}{\omega_n^2 + \xi_{k_1}^2 + \Delta_{k_1}^2} + 2\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{\xi_{k_1} \sin (k_{1z}c)}{\omega_n^2 + \xi_{k_1}^2 + \Delta_{k_1}^2}.
\end{align*}
\]  

(2.49)

The Monte-Carlo method was used to calculate the momentum integrals in the above equations. We looked for the non-trivial solutions of the coupled non-linear equations for the self-energy. However, we can not find any non-trivial solutions. Naturally, we come up with an assumption that the trivial solution is the only physical solution for our problem whether in the normal state case or superconducting state case.

2.4 The extended tight-binding model and Hamiltonian

The former model Hamiltonian (2.3) leads to the assumption that the trivial solution is the only solution of the self-energy in our system. Now we keep the assumption and extend the model to include more information into the Hamiltonian. The unit cell of the system is still a parallelepiped with the lattice constants \(a, b, c\) for three sides respectively. But now we consider both the nearest and the next-nearest hoppings between the ions in a single plane as well as the interlayer ones. This is the first time in the literature that the interlayer hoppings are taken into account in the topic of the ultrasonic attenuation in the superconductors. The extended tight-binding Hamiltonian of superconductors has the form

\[
H = -\sum_{n,m} \sum_{i,j} t_{nm,ij} c_{n,i,a}^\dagger c_{m,j,a} - \mu \sum_{n,i} c_{n,i,a}^\dagger c_{n,i,a},
\]  

(2.50)

where \(n\) and \(m\) label different layers, \(i\) and \(j\) label the sites within a single layer, \(\mu\) is the chemical potential, and \(\alpha = \uparrow, \downarrow\) is the spin projection. Instead of (2.2), the hopping
amplitudes \( t_{nm,ij} \) become

\[
t_{nm,ij} = \begin{cases} 
  t_{\parallel}, & \text{if } n = m \text{ and } i, j \text{ are the nearest neighbors}, \\
  \tilde{t}_{\parallel}, & \text{if } n = m \text{ and } i, j \text{ are the next-nearest neighbors}, \\
  t_{\perp} + \delta t_{\perp}(n, i), & \text{if } n = m \pm 1 \text{ and } i, j \text{ are the nearest neighbors}, \\
  \tilde{t}_{\perp} + \delta \tilde{t}_{\perp}(n, i), & \text{if } n = m \pm 1 \text{ and } i, j \text{ are the next-nearest neighbors},
\end{cases}
\]

(2.51)

Here \( t_{\parallel} \) and \( \tilde{t}_{\parallel} \) are the hopping amplitudes between the nearest and next-nearest neighbors in a single layer respectively, \( t_{\perp}, \delta t_{\perp} \) and \( \tilde{t}_{\perp}, \delta \tilde{t}_{\perp} \) describe tunneling between the two neighboring layers. The coherent hopping amplitudes \( t_{\perp} \) and \( \tilde{t}_{\perp} \) are between the nearest and next-nearest neighbors respectively, while \( \delta t_{\perp} \) and \( \delta \tilde{t}_{\perp} \) are two uncorrelated random functions. Since for each site in a layer, there are four next-nearest sites in the next layer, \( \delta \tilde{t}_{\perp} \) can be further written as

\[
\delta \tilde{t}_{\perp}(n, i) = \begin{cases} 
  \delta \tilde{t}_{\perp}^{\parallel}(n, i), & i \to i + \hat{x} \\
  \delta \tilde{t}_{\perp}^{\parallel}(n, i), & i \to i - \hat{x} \\
  \delta \tilde{t}_{\perp}^{\perp}(n, i), & i \to i + \hat{y} \\
  \delta \tilde{t}_{\perp}^{\perp}(n, i), & i \to i - \hat{y}
\end{cases}
\]

(2.52)

The details of \( \delta \tilde{t}_{\perp}^{\perp} \) and other hopping have been shown in Fig. 2.5. So the extended tight-binding Hamiltonian is given as

\[
H = -t_{\parallel} \sum_n \sum_{\langle ij \rangle} c_{n,i,\alpha}^\dagger c_{n,j,\alpha} - t_{\perp} \sum_n \sum_{\langle ij \rangle} \left[ c_{n,i,\alpha}^\dagger c_{n+1,j,\alpha} + c_{n+1,j,\alpha}^\dagger c_{n,i,\alpha} \right] \\
- \tilde{t}_{\parallel} \sum_n \sum_{\langle ij \rangle} c_{n,i,\alpha}^\dagger c_{n,j,\alpha} - \tilde{t}_{\perp} \sum_n \sum_{\langle ij \rangle} \left[ c_{n,i,\alpha}^\dagger c_{n+1,j,\alpha} + c_{n+1,j,\alpha}^\dagger c_{n,i,\alpha} \right] \\
- \sum_{n,i} \delta t_{\perp}(n, i) \left[ c_{n,i,\alpha}^\dagger c_{n+1,i,j,\alpha} + c_{n+1,i,j,\alpha}^\dagger c_{n,i,\alpha} \right] - \mu \sum_{n,i} c_{n,i,\alpha}^\dagger c_{n,i,\alpha} \\
- \sum_{n,i} \left\{ \begin{aligned} 
  & \delta \tilde{t}_{\perp}^{\parallel}(n, i) \left[ c_{n,i,\alpha}^\dagger c_{n+1,i,j+\hat{z},\alpha} + h.c. \right] \\
  + & \delta \tilde{t}_{\perp}^{\parallel}(n, i) \left[ c_{n,i,\alpha}^\dagger c_{n+1,i,j-\hat{z},\alpha} + h.c. \right] \\
  + & \delta \tilde{t}_{\perp}^{\perp}(n, i) \left[ c_{n,i,\alpha}^\dagger c_{n+1,i,j+\hat{y},\alpha} + h.c. \right] \\
  + & \delta \tilde{t}_{\perp}^{\parallel}(n, i) \left[ c_{n,i,\alpha}^\dagger c_{n+1,i,j-\hat{y},\alpha} + h.c. \right]
\end{aligned} \right. 
\]

(2.53)
Figure 2.5: The hopping amplitudes $t_{nm,ij}$ in a superconductor. Only two layers of the structure are shown. The hopping $t_{\parallel}$ appears between two sites such as $O$ and $A$, $O'$ and $A'$. $\tilde{t}_{\parallel}$ is the hopping between two sites such as $O$ and $H$, $O'$ and $H'$. $t_{\perp}$ and $\delta t_{\perp}(n, i)$ appears between $O$ and $O'$. $\tilde{t}_{\perp}$ and $\tilde{\delta t}_{\perp}(n, i)$ appears between $O'$ and $A$, $O'$ and $B$, $O'$ and $C$, $O'$ and $D$. For example, $\delta \tilde{t}_{\perp}^{1}(n, i)$ is the random hopping between $O'$ and $A$. 
where h.c. refers to the Hermitian conjugate, and \( \langle (i, j) \rangle \) means the sites i and j are the next-nearest neighbors.

After introducing the Fourier transforms

\[
\begin{align*}
\hat{c}_{n,i,\alpha} &= \frac{1}{\sqrt{N}} \sum_k c_{k,\alpha} e^{i k R_{n,i}}, \\
\delta t_{\perp}(n, i) &= \frac{1}{\sqrt{N}} \sum_Q \delta t_{\perp}(Q) e^{i Q R_{n,i}}, \\
\delta \tilde{t}_{\perp}^m(n, i) &= \frac{1}{\sqrt{N}} \sum_Q \delta \tilde{t}_{\perp}^m(Q) e^{i Q R_{n,i}}, m = 1, 2, 3, 4,
\end{align*}
\]

the Hamiltonian in the momentum space can be written in the following form

\[
H = H_0 + H',
\]

\[
H_0 = \sum_k \xi(k) c_{k,\alpha}^+ c_{k,\alpha},
\]

\[
H' = -\frac{1}{\sqrt{N}} \sum_{k, Q} \left\{ \begin{array}{l}
\delta t_{\perp}(Q) \left[ c_{k,\alpha}^+ c_{k-Q,\alpha} e^{-i k z_e} + c_{k+Q,\alpha}^+ c_{k,\alpha} e^{i k z_e} \right] \\
\delta \tilde{t}_{\perp}^1(Q) \left[ c_{k,\alpha}^+ c_{k-Q,\alpha} e^{-i (k_x a + k_z e)} + c_{k+Q,\alpha}^+ c_{k,\alpha} e^{i (k_x a + k_z e)} \right] \\
+ \delta \tilde{t}_{\perp}^2(Q) \left[ c_{k,\alpha}^+ c_{k-Q,\alpha} e^{-i (k_y a + k_e)} + c_{k+Q,\alpha}^+ c_{k,\alpha} e^{i (k_y a + k_e)} \right] \\
+ \delta \tilde{t}_{\perp}^3(Q) \left[ c_{k,\alpha}^+ c_{k-Q,\alpha} e^{-i (k_z e - k_y a)} + c_{k+Q,\alpha}^+ c_{k,\alpha} e^{i (k_z e - k_y a)} \right]
\end{array} \right\}.
\]

Here

\[
\xi(k) = -2 t_{\|} (\cos k_x a + \cos k_y a) - 2 t_{\perp} \cos k_z c \\
- 4 \tilde{t}_{\|} \cos (k_x a) \cos (k_y a) - 4 t_{\perp} [\cos (k_x a) + \cos (k_y a)] \cos (k_z c) - \mu
\]

is the extended single-electron dispersion, \( \delta t_{\perp}(Q) \) and \( \delta \tilde{t}_{\perp}^m(Q) \) are the random fields, whose correlators are given by

\[
\langle \delta t_{\perp}(Q_1) \delta t_{\perp}(Q_2) \rangle = \gamma^2 \delta_{Q_1+Q_2,0},
\]

\[
\langle \delta \tilde{t}_{\perp}^m(Q_1) \delta \tilde{t}_{\perp}^m(Q_2) \rangle = \gamma^2 \delta_{mn} \delta_{Q_1+Q_2,0},
\]
\[ \langle \delta t_{\perp}(Q_1)\delta t_{\perp}^n(Q_2) \rangle = 0, \tag{2.63} \]

where \( \gamma \) and \( \tilde{\gamma} \) are the measures of disorder strength in the nearest and next-nearest hoppings respectively.

### 2.5 The Dyson Equation and self-energy in the normal State

To get the Dyson equation (see Appendix A) for the self-energy, one can perform the same manipulation as in Chap. 2.2. Instead of (2.17) we now have

\[
V(k, k') = -\delta t_{\perp}(k - k') \left[ e^{ik_xc} + e^{-ik_xc} \right]
- \delta t_{\perp}^2(k - k') \left[ e^{i(k_xa + k_zc)} + e^{-i(k_xa + k_zc)} \right]
- \delta t_{\perp}^2(k - k') \left[ e^{i(k_xc - k_xa)} + e^{-i(k_xc - k_xa)} \right]
- \delta t_{\perp}^3(k - k') \left[ e^{i(k_ya + k_zc)} + e^{-i(k_ya + k_zc)} \right]
- \delta t_{\perp}^4(k - k') \left[ e^{i(k_xc - k_ya)} + e^{-i(k_xc - k_ya)} \right]. \tag{2.64}
\]

Then the second order correction has the form

\[
G^{(2)}(k, i\omega_n) = \int \frac{d^3k_1}{(2\pi)^3} G^{(0)}(k, i\omega_n) G^{(0)}(k_1, i\omega_n) G^{(0)}(k, i\omega_n) G^{(0)}(k_1, i\omega_n) \times \begin{cases} 2\gamma^2 (1 + \cos [(k_x + k_{1x})c]) \\ +2\tilde{\gamma}^2 (1 + \cos [(k_x + k_{1x})c + (k_z + k_{1z})a]) \\ +2\tilde{\gamma}^2 (1 + \cos [(k_x + k_{1x})c - (k_z + k_{1z})a]) \\ +2\tilde{\gamma}^2 (1 + \cos [(k_y + k_{1y})c + (k_z + k_{1z})a]) \\ +2\tilde{\gamma}^2 (1 + \cos [(k_y + k_{1y})c - (k_z + k_{1z})a]) \end{cases}. \tag{2.65}
\]

So the Dyson equation can be written as

\[
G^{-1}(k, i\omega_n) = G^{(0)-1}(k, i\omega_n) + \int \frac{d^3k_1}{(2\pi)^3} G(k_1, i\omega_n)
\]
Here the exact Green’s function is

\[
G^{-1} (k, i\omega_n) = i\omega_n - \xi_k - \Sigma (k, i\omega_n) = G^{0-1} (k, i\omega_n) - \Sigma (k, i\omega_n),
\]  

(2.67)

where \(\xi_k\) is given in (2.60). Inserting (2.67) into (2.66), one gets the following equation for the self-energy

\[
\Sigma (k, i\omega_n) = -2 \int \frac{d^3k_1}{(2\pi)^3} \frac{1}{i\omega_n - \xi_k - \Sigma (k_1, i\omega_n)}
\times \left\{ \begin{array}{l}
\gamma^2 + \gamma^2 \cos (k_z c) \cos (k_{1z} c) - \gamma^2 \sin (k_z c) \sin (k_{1z} c) \\
+4\tilde{\gamma}^2 + 2\tilde{\gamma}^2 \cos (k_z c) \cos (k_x c) \cos (k_{1z} c) \cos (k_{1x} c) \\
+2\tilde{\gamma}^2 \cos (k_z c) \cos (k_y a) \cos (k_{1z} c) \cos (k_{1y} a) \\
+2\tilde{\gamma}^2 \sin (k_z c) \sin (k_x c) \sin (k_{1z} c) \sin (k_{1x} a) \\
+2\tilde{\gamma}^2 \sin (k_z c) \sin (k_y a) \sin (k_{1z} c) \sin (k_{1y} a) \\
-2\tilde{\gamma}^2 \cos (k_z c) \sin (k_x a) \cos (k_{1z} c) \sin (k_{1x} a) \\
-2\tilde{\gamma}^2 \cos (k_z c) \sin (k_y a) \cos (k_{1z} c) \sin (k_{1y} a) \\
-2\tilde{\gamma}^2 \sin (k_z c) \cos (k_x a) \sin (k_{1z} c) \cos (k_{1x} a) \\
-2\tilde{\gamma}^2 \sin (k_z c) \cos (k_y a) \sin (k_{1z} c) \cos (k_{1y} a)
\end{array} \right\}.
\]  

(2.68)

As before, separating the wave vector dependence from the frequency dependence, we seek the self-energy in the form

\[
\Sigma (k, i\omega_n) = \Sigma_0 (i\omega_n) + \Sigma_1 (i\omega_n) \cos (k_z c) + \Sigma_2 (i\omega_n) \sin (k_z c)
\]

\[
+ \Sigma_3 (i\omega_n) \cos (k_x c) \cos (k_y a) + \Sigma_4 (i\omega_n) \cos (k_z c) \cos (k_y a)
\]
Chapter 2. Theory and Calculation

\[ + \Sigma_5 (i\omega_n) \sin (k_z c) \sin (k_x a) + \Sigma_6 (i\omega_n) \sin (k_z c) \sin (k_y a) \]
\[ + \Sigma_7 (i\omega_n) \cos (k_z c) \sin (k_x a) + \Sigma_8 (i\omega_n) \cos (k_z c) \sin (k_y a) \]
\[ + \Sigma_9 (i\omega_n) \sin (k_z c) \cos (k_x a) + \Sigma_{10} (i\omega_n) \sin (k_z c) \cos (k_y a), \]  
(2.69)

where

\[
\Sigma_0 (i\omega_n) = -2 \left( \gamma^2 + 4\gamma^2 \right) \int \frac{d^3 k_1}{(2\pi)^3} \frac{1}{i\omega_n - \xi_{k_1} - \Sigma(k_1, i\omega_n)} 
\]
(2.70)

\[
\Sigma_1 (i\omega_n) = -2\gamma^2 \int \frac{d^3 k_1}{(2\pi)^3} \frac{\cos (k_{1z} c)}{i\omega_n - \xi_{k_1} - \Sigma(k_1, i\omega_n)} 
\]
(2.71)

\[
\Sigma_2 (i\omega_n) = 2\gamma^2 \int \frac{d^3 k_1}{(2\pi)^3} \frac{\sin (k_{1z} c)}{i\omega_n - \xi_{k_1} - \Sigma(k_1, i\omega_n)} 
\]
(2.72)

\[
\Sigma_3 (i\omega_n) = -4\gamma^2 \int \frac{d^3 k_1}{(2\pi)^3} \frac{\cos (k_{1z} c) \cos (k_{1x} a)}{i\omega_n - \xi_{k_1} - \Sigma(k_1, i\omega_n)} 
\]
(2.73)

\[
\Sigma_4 (i\omega_n) = -4\gamma^2 \int \frac{d^3 k_1}{(2\pi)^3} \frac{\cos (k_{1z} c) \cos (k_{1y} a)}{i\omega_n - \xi_{k_1} - \Sigma(k_1, i\omega_n)} 
\]
(2.74)

\[
\Sigma_5 (i\omega_n) = -4\gamma^2 \int \frac{d^3 k_1}{(2\pi)^3} \frac{\sin (k_{1z} c) \sin (k_{1x} a)}{i\omega_n - \xi_{k_1} - \Sigma(k_1, i\omega_n)} 
\]
(2.75)

\[
\Sigma_6 (i\omega_n) = -4\gamma^2 \int \frac{d^3 k_1}{(2\pi)^3} \frac{\sin (k_{1z} c) \sin (k_{1y} a)}{i\omega_n - \xi_{k_1} - \Sigma(k_1, i\omega_n)} 
\]
(2.76)

\[
\Sigma_7 (i\omega_n) = 4\gamma^2 \int \frac{d^3 k_1}{(2\pi)^3} \frac{\cos (k_{1z} c) \sin (k_{1x} a)}{i\omega_n - \xi_{k_1} - \Sigma(k_1, i\omega_n)} 
\]
(2.77)

\[
\Sigma_8 (i\omega_n) = 4\gamma^2 \int \frac{d^3 k_1}{(2\pi)^3} \frac{\cos (k_{1z} c) \sin (k_{1y} a)}{i\omega_n - \xi_{k_1} - \Sigma(k_1, i\omega_n)} 
\]
(2.78)

\[
\Sigma_9 (i\omega_n) = 4\gamma^2 \int \frac{d^3 k_1}{(2\pi)^3} \frac{\sin (k_{1z} c) \cos (k_{1x} a)}{i\omega_n - \xi_{k_1} - \Sigma(k_1, i\omega_n)} 
\]
(2.79)

\[
\Sigma_{10} (i\omega_n) = 4\gamma^2 \int \frac{d^3 k_1}{(2\pi)^3} \frac{\sin (k_{1z} c) \cos (k_{1y} a)}{i\omega_n - \xi_{k_1} - \Sigma(k_1, i\omega_n)} 
\]
(2.80)

One can easily check the following assumption is self-consistent for the above equation

\[
\Sigma_j (i\omega_n) = 0, j = 1, 2...10. 
\]
(2.81)

So the self-energy is momentum-independent and satisfies the following equation

\[
\Sigma (k, i\omega_n) = \Sigma_0 (\omega_n) = -2 \left( \gamma^2 + 4\gamma^2 \right) \int \frac{d^3 k_1}{(2\pi)^3} \frac{1}{i\omega_n - \xi_{k_1} - \Sigma_0 (\omega_n)} 
\]
(2.82)
By comparing this result of the self-energy with (2.29) in Chap. 2.2, one can find the self-energy for the extended model is different from the former one only by the coefficient which is a measure of the disorder in a superconductor. Thus the assumption that the momentum-independent solution is the only solution still holds.

2.6 The self-energy and Matsubara frequency in the superconducting state

Now let us include the superconducting interactions in our extended Hamiltonian which has the form

\[ H = H_0 + H' + H_{int}, \tag{2.83} \]

where \( H_0, H' \) and \( H_{int} \) are defined in (2.58), (2.59) and (2.36) respectively. The Dyson equation is given in Appendix A as (A.21)

\[
\hat{G}^{-1}(k, i\omega_n) = \begin{pmatrix}
i(\omega_n - \text{Im}\Sigma_a) - (\xi_k + \text{Re}\Sigma_a) & -\left(\Delta_k + \text{Re}\Sigma_2\right) - i\text{Im}\Sigma_2 \\
-\left(\Delta_k + \text{Re}\Sigma_2\right) + i\text{Im}\Sigma_2 & i(\omega_n - \text{Im}\Sigma_a) + (\xi_k - \text{Re}\Sigma_a)
\end{pmatrix}, \tag{2.84}
\]

where \( \Sigma_a \) and \( \Sigma_2 \) are the matrix elements of the self-energy in the momentum-frequency representation (see Appendix A). After some algebra, one can get the terms of the Green's function matrix as

\[
G_{11}(k, i\omega_n) = \frac{i\omega_n + \xi_k - \Sigma_a}{\det(\hat{G}^{-1}(k, i\omega_n))}, \tag{2.85}
\]

\[
G_{12}(k, i\omega_n) = \frac{\Delta_k + \Sigma_2}{\det(\hat{G}^{-1}(k, i\omega_n))}, \tag{2.86}
\]

where

\[
\det(\hat{G}^{-1}(k, i\omega_n)) = -\left\{ (\omega_n - \text{Im}\Sigma_a)^2 + \xi_k^2 - (\text{Re}\Sigma_a)^2 + (\text{Im}\Sigma_2)^2 \right. \\
+ \left. (\Delta_k + \text{Re}\Sigma_2)^2 + 2i(\text{Re}\Sigma_2)(\omega_n - \text{Im}\Sigma_a) \right\}. \tag{2.87}
\]
A possible solution of the self-energy (see Appendix C) in the superconducting state is

$$\Sigma(i\omega_n) = -2 \left( \gamma^2 + 4\gamma^2 \right) \frac{d^3k_1}{(2\pi)^3} \frac{i\omega_n + \xi_k - \Sigma_a}{\det (\hat{G}^{-1}(k, i\omega_n))}. \quad (2.88)$$

So that the imaginary part of the self-energy is given by

$$\text{Im}\Sigma(i\omega_n) = -2 \left( \gamma^2 + 4\gamma^2 \right) \int \frac{d^3k_1}{(2\pi)^3} \frac{\omega_n - \text{Im}\Sigma_a(i\omega_n)}{[\omega_n - \text{Im}\Sigma_a(i\omega_n)]^2 + \xi_k^2 - [\text{Re}\Sigma_a(i\omega_n)]^2 + \Delta_k^2}. \quad (2.89)$$

The $n$th Matsubara frequencies with impurities can be written as

$$i\tilde{\omega}_n = i\omega_n - i\text{Im}\Sigma_a(i\omega_n). \quad (2.90)$$

Let us consider alongside the Matsubara function $G$ the function $G^R(k, \epsilon)$, which is analytic in the upper half-plane of $\omega_n$. Here $G^R(k, \epsilon)$ is known as the retarded Green's function [22] and can be obtained from the Matsubara Green's function $G$ by changing $i\omega_n$ to $\epsilon + i\delta$, where $\delta$ is a positive infinitesimal:

$$G^R(k, \epsilon) = \frac{t(\epsilon) + \xi_k}{t^2(\epsilon) - \xi_k^2 - \Delta_k^2}. \quad (2.91)$$

Here

$$t(\epsilon) \equiv i\tilde{\omega}_n|_{i\omega_n \rightarrow \epsilon + i\delta}. \quad (2.92)$$

Another retarded Green's function $F^R(k, \epsilon)$ can be obtained similarly [22]:

$$F^R(k, \epsilon) = \frac{\Delta_k}{t^2(\epsilon) - \xi_k^2 - \Delta_k^2}. \quad (2.93)$$

Putting (2.89)-(2.91) into (2.92), one finds that the equation for the function $t(\epsilon)$ in the superconducting state can be written as

$$t(\epsilon) = \epsilon + i\Gamma \frac{\int \frac{d^3k}{(2\pi)^3} \frac{t(\epsilon)}{\sqrt{t^2(\epsilon) - \Delta_k^2}} \delta (\xi_k)}{\int \frac{d^3k}{(2\pi)^3} \delta (\xi_k)}. \quad (2.94)$$

$$\Gamma = 2\pi N_F \left( \gamma^2 + 4\gamma^2 \right) = \frac{1}{2\tau_n}, \quad (2.95)$$
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where $\Gamma$ is a measure of the disorder, $\tau_n$ defines the mean free time in the normal state. In this thesis, only the weak disorder is considered, which means $\Gamma$ is very small. So we made an approximation in equation (2.94), i.e. neglected the difference between $t(\epsilon)$ and $\epsilon$ on the right side. Then we have

$$t(\epsilon) \cong \epsilon + i\Gamma \frac{\int \frac{d^3k}{(2\pi)^3} \frac{\epsilon}{\sqrt{\epsilon^2 - \Delta_k^2}} \delta(\xi_k)}{\int \frac{d^3k}{(2\pi)^3} \delta(\xi_k)}.$$  \hspace{1cm} (2.96)

Replacing the delta function with a Gaussian function in the above equation, we calculated the three dimensional integral and obtained the value of the imaginary part of $t(\epsilon)$ when $\Gamma$ is very small in Chap. 3.

2.7 The electron-phonon interaction

In order to get the ultrasonic attenuation theoretically, we calculate the self-energy for the phonon Green's function and take its imaginary part, which is proportional to the rate of ultrasonic attenuation. In what follows, the form of the electron-phonon interaction will be discussed in details for both the longitudinal wave case and the transverse wave case. After that the expression of ultrasonic attenuation will be derived, which will be used for the numerical calculations in Chap. 3.

The tight-binding Hamiltonian is given by (2.83). In order to get the expressions for the electron-phonon interaction from the Hamiltonian, all the hoppings between different sites have to be calculated.

For the hopping between any two sites in a superconductor, see Fig. 2.6, the positions of the ions are changed by $u(r_1^{(0)})$ and $u(r_2^{(0)})$ because of the sound waves. So the electron hopping can be written as

$$t(r_1, r_2) = t(R) + \frac{\partial t}{\partial R} [u(r_2^{(0)}) - u(r_1^{(0)})],$$  \hspace{1cm} (2.97)
Figure 2.6: Diagram of the hopping between two sites in the unit cell. \( r_1^{(0)} \) and \( r_2^{(0)} \) are the locations of two ions with a displacement \( R \). \( u(r_1^{(0)}) \) and \( u(r_2^{(0)}) \) are small deviations of the lattice ions from their equilibrium positions because of the sound waves.

Figure 2.7: The layered square-lattice structure of YBa$_2$Cu$_3$O$_7$. The wave vector \( q \), polarization \( u \) are the indices for (a) longitudinal sound propagation and (b) transverse sound propagation.
where \( \mathbf{R} = \mathbf{r}_2^{(0)} - \mathbf{r}_1^{(0)}, \mathbf{r}_1 = \mathbf{r}_1^{(0)} + \mathbf{u} (\mathbf{r}_1^{(0)}), \mathbf{r}_2 = \mathbf{r}_2^{(0)} + \mathbf{u} (\mathbf{r}_2^{(0)}) \). Then (2.97) becomes

\[
 t (\mathbf{r}_1, \mathbf{r}_2) = t (\mathbf{R}) + \frac{\partial t}{\partial R_i} R_j \frac{\partial u_i}{\partial r_j} = t (\mathbf{R}) + R \frac{\partial \mathbf{u}}{\partial \mathbf{r}} \frac{\partial u_i}{\partial r_j} = t (\mathbf{R}) + t' \hat{R}_i \hat{R}_j \frac{\partial u_i}{\partial r_j}. \tag{2.98}
\]

Here \( i \) labels the vector components. This is the general expression which will now be analyzed separately both for the longitudinal and transverse waves along the \( z \)-axis with different directions of the polarization.

a). \( t = t_{||} \) is the hopping between the nearest neighbors in a single plane. Here \( R \) is a \( (|a| = |b| = a) \). Then the expression (2.98) takes the form

\[
 t_{||} (r + u (r'), r' + u (r')) = t_{||} + at_{||} \frac{\partial u_x}{\partial x}, \tag{2.99}
\]

if the hopping is along the \( x \)-axis or

\[
 t_{||} (r + u (r'), r' + u (r')) = t_{||} + at_{||} \frac{\partial u_y}{\partial y}. \tag{2.100}
\]

if the hopping is along the \( y \)-axis.

b). \( t = \tilde{t}_{||} \) is the hopping between the next-nearest neighbors in a single plane. Then the expression is

\[
 \tilde{t}_{||} (r + u (r'), r' + u (r')) = \tilde{t}_{||} + \tilde{R}_i \hat{R}_j \frac{\partial u_i (r)}{\partial r_j}. \tag{2.101}
\]

For a longitudinal wave along the \( z \)-axis, for which \( \mathbf{q} = q (0, 0, 1), \mathbf{u} = u (0, 0, 1) \), and \( \mathbf{R} = (\pm a, \pm a, 0) \), we have

\[
 \tilde{t}_{||} (r + u (r), r' + u (r')) = \tilde{t}_{||}. \tag{2.102}
\]

For a transverse wave along the \( z \)-axis, for which \( \mathbf{q} = q (0, 0, 1), \mathbf{u} = u (\cos \theta, \sin \theta, 0) \), where \( \theta \) shows the direction of polarization, and \( \mathbf{R} = (\pm a, \pm a, 0) \), we have

\[
 \tilde{t}_{||} (r + u (r), r' + u (r')) = \tilde{t}_{||} + \frac{\sqrt{2}}{2} \tilde{a} \frac{\partial u_x}{\partial r_z} \tag{2.103}
\]

if the hopping is along the \( x \)-axis or

\[
 \tilde{t}_{||} (r + u (r), r' + u (r')) = \tilde{t}_{||} + \frac{\sqrt{2}}{2} \tilde{a} \frac{\partial u_y}{\partial r_y} \tag{2.104}
\]
if the hopping is along the y-axis.

c). \( t = t_\perp \) is the hopping between the nearest neighbors in the neighboring two planes. We have

\[
t_\perp (r + u(r), r' + u(r')) = t_\perp + ct_\perp \frac{\partial x}{\partial z}. \tag{2.105}
\]

d). \( t = \tilde{t}_\perp \) is the hopping between the next-nearest neighbors in the neighboring two planes. We have

\[
\tilde{t}_\perp (r + u(r), r' + u(r')) = \tilde{t}_\perp + R\tilde{t}_\perp \frac{\partial u_i(r)}{\partial r_j}. \tag{2.106}
\]

For a longitudinal wave along the z-axis, for which \( q = q(0, 0, 1), u = u(0, 0, 1) \), and \( R = (\pm a, 0, c) \) or \( R = (0, \pm a, c) \), we have

\[
\tilde{t}_\perp (r + u(r), r' + u(r')) = \tilde{t}_\perp + \frac{c^2}{\sqrt{a^2 + c^2}} \frac{\partial u_i(r)}{\partial r_j}. \tag{2.107}
\]

For a transverse wave along the z-axis, for which \( q = q(0, 0, 1), u = u(\cos \theta, \sin \theta, 0) \), and \( R = (\pm a, 0, c) \) or \( R = (0, \pm a, c) \), we have

\[
\tilde{t}_\perp (r + u(r), r' + u(r')) = \tilde{t}_\perp + \sqrt{a^2 + c^2} \frac{\partial u_i(r)}{\partial r_j}. \tag{2.108}
\]

This can be further written as

\[
\tilde{t}_\perp (r + c \pm a, r) = \tilde{t}_\perp + \frac{ac}{\sqrt{a^2 + c^2}} \frac{\partial u_x}{\partial z}, \tag{2.109}
\]

\[
\tilde{t}_\perp (r + c \pm b, r) = \tilde{t}_\perp + \frac{ac}{\sqrt{a^2 + c^2}} \frac{\partial u_y}{\partial z}, \tag{2.110}
\]

\[
\tilde{t}_\perp (r - c \pm a, r) = \tilde{t}_\perp + \frac{ac}{\sqrt{a^2 + c^2}} \frac{\partial u_x}{\partial z}, \tag{2.111}
\]

\[
\tilde{t}_\perp (r - c \pm b, r) = \tilde{t}_\perp + \frac{ac}{\sqrt{a^2 + c^2}} \frac{\partial u_y}{\partial z}. \tag{2.112}
\]

Substituting all above hoppings into the tight-binding Hamiltonian in (2.83), one obtains the electron-phonon interaction for the longitudinal wave and the transverse wave as follows.
For a longitudinal wave along the z-axis, for which \( u = u(0,0,1) \) and \( q = q(0,0,1) \), the electron-phonon interaction has the form

\[
H_{e-p,L} = -t_1' \int \frac{d^3r}{(2\pi)^3} \left[ c_\alpha^\dagger (r) c_\alpha (r + c) + c_\alpha^\dagger (r) c_\alpha (r - c) \right] \frac{\partial u_z}{\partial z} \\
- t_1'' \int \frac{d^3r}{(2\pi)^3} \left[ c_\alpha^\dagger (r) c_\alpha (r + c + a) + c_\alpha^\dagger (r) c_\alpha (r - c - a) + c_\alpha^\dagger (r) c_\alpha (r + c - a) + c_\alpha^\dagger (r) c_\alpha (r - c + a) + c_\alpha^\dagger (r) c_\alpha (r + c + b) + c_\alpha^\dagger (r) c_\alpha (r - c - b) + c_\alpha^\dagger (r) c_\alpha (r + c - b) + c_\alpha^\dagger (r) c_\alpha (r - c + b) \right] \frac{\partial u_z}{\partial z},
\]

After introducing the Fourier transform

\[
u(r) = \int \frac{d^3q}{(2\pi)^3} \left[ u_q e^{iqr} + u_q^* e^{-iqr} \right],
\]

\[c(r) = \int \frac{d^3k}{(2\pi)^3} c_k e^{ikr},\]

the electron-phonon interaction turns out to be

\[
H_{e-p,L} = -2i \int \frac{d^3q}{(2\pi)^3} \int \frac{d^3k}{(2\pi)^3} u_q f_L(k,q) c_{k+q,\alpha}^\dagger c_{k,\alpha} \\
-2i \int \frac{d^3q}{(2\pi)^3} \int \frac{d^3k}{(2\pi)^3} u_q^* f_L(k,q) c_{k-q,\alpha}^\dagger c_{k,\alpha},
\]

where \( f_L(k,q) \) is the electron-phonon interaction matrix for the longitudinal wave

\[
f_L(k,q) = q \left\{ t_{1\perp} \cos(k_z c) + 2t_{1\perp} \cos(k_z c) [\cos(k_x a) + \cos(k_y a)] \right\}.
\]

For a transverse wave along the z-axis that yields \( u = u(\cos \theta, \sin \theta, 0) \) and \( q = q(0,0,1) \), we have the following form for the electron-phonon interaction

\[
H_{e-p,T} = -t_2' \int \frac{d^3r}{(2\pi)^3} \left[ c_\alpha^\dagger (r) c_\alpha (r + a) + c_\alpha^\dagger (r) c_\alpha (r - a) \right] \frac{\partial u_x}{\partial z} \\
- t_2'' \int \frac{d^3r}{(2\pi)^3} \left[ c_\alpha^\dagger (r) c_\alpha (r + a + c) + c_\alpha^\dagger (r) c_\alpha (r - a - c) + c_\alpha^\dagger (r) c_\alpha (r - a + c) + c_\alpha^\dagger (r) c_\alpha (r + a - c) \right] \frac{\partial u_x}{\partial z},
\]
After introducing the Fourier transform for the electron-phonon interaction, it can be expressed as

\[
H_{e-p,T} = -2i \int \frac{d^3q}{(2\pi)^3} \int \frac{d^3k}{(2\pi)^3} u_q f_T (k, q) c_{k+q,\alpha}^{\dagger} c_{k,\alpha} \\
+2i \int \frac{d^3q}{(2\pi)^3} \int \frac{d^3k}{(2\pi)^3} u_q f_T (k, q) c_{k-q,\alpha}^{\dagger} c_{k,\alpha},
\]

(2.119)

where \( f_T (k, q) \) is the electron-phonon interaction matrix for the transverse wave

\[
f_T (k, q) = 2q_{\perp} \cos (k_z c) \left[ \cos \theta \cos (k_x a) + \sin \theta \cos (k_y a) \right].
\]

(2.120)

So the general form for the electron-phonon interaction is

\[
H_{e-p} = -2i \int \frac{d^3q}{(2\pi)^3} \int \frac{d^3k}{(2\pi)^3} u_q f (k, q) c_{k+q,\alpha}^{\dagger} c_{k,\alpha} \\
+2i \int \frac{d^3q}{(2\pi)^3} \int \frac{d^3k}{(2\pi)^3} u_q f (k, q) c_{k-q,\alpha}^{\dagger} c_{k,\alpha},
\]

(2.121)

where \( f (k, q) \) is given by the expressions (2.117) and (2.120) for the longitudinal and transverse waves respectively. For both the longitudinal and the transverse waves, the phonon creation operator can be written as

\[
u (q) = \frac{1}{\sqrt{2\rho \omega_0 (q)}} b_q,
\]

(2.122)

\[
\omega_0 (q) = v (\hat{q}) |q|.
\]

(2.123)
Figure 2.8: The phonon self-energy in the case of an impure superconductor. Solid lines are the one-electron Green's functions. Zigzag lines are the bare phonon propagators.

Here $\omega_0(q)$ is the frequency of a phonon and $v(q)$ is the sound velocity, which in general depends on the direction of propagation. Then the electron-phonon interaction in (2.121) can be expressed as

$$H_{e-p} = -2i \int \frac{d^3q}{(2\pi)^3} \int \frac{d^3k}{(2\pi)^3} \frac{1}{\sqrt{2q\rho v(q)}} f(k, q) b_q c_{k+q, \alpha} c_{k, \alpha}$$

$$+ 2i \int \frac{d^3q}{(2\pi)^3} \int \frac{d^3k}{(2\pi)^3} \frac{1}{\sqrt{2q\rho v(q)}} f(k, q) b_q^\dagger c_{k-q, \alpha} c_{k, \alpha}. \quad (2.124)$$

### 2.8 The ultrasonic attenuation

The phonon Green’s function is given as

$$D(q, \omega_m) = \frac{1}{i\omega_m - \omega_0(q) - \Pi(q, \omega_m)}, \quad (2.125)$$

where $\Pi(q, \omega_m)$ is the phonon self-energy. In the second-order approximation

$$\Pi(q, \omega_m) = \frac{4}{q\rho v(q)} T \sum_n \int \frac{d^3k}{(2\pi)^3} f^2(k, q)$$

$$\times \left\{ G(k + q, \epsilon_n + \omega_m) G(k, \epsilon_n) - F(k + q, \epsilon_n + \omega_m) F^\dagger(k, \epsilon_n) \right\}, \quad (2.126)$$

where $F$ and $F^\dagger$ are anomalous Green’s functions [22]. The rate of ultrasonic attenuation is proportional to the imaginary part of the self energy.

We introduce the retarded Green’s function and use the spectral representation of the Green’s function

$$G(k, \epsilon_n) = \int_{-\infty}^{\infty} \frac{dz}{\pi} \frac{\text{Im} G^R(k, \epsilon_n)}{z - i\epsilon_n}. \quad (2.127)$$
The integration over $k$ and the sum over $\epsilon_n$ in (2.126) are exchanged and the sum can be expressed as

$$
T \sum_n \left\{ \begin{array}{l}
G(k + q, \epsilon_n + \omega_m) G(k, \epsilon_n) \\
- F(k + q, \epsilon_n + \omega_m) F^\dagger(k, \epsilon_n)
\end{array} \right. 

= \frac{1}{2} \int_{-\infty}^{\infty} \frac{dz_1 dz_2}{\pi} \frac{1}{\pi} \left\{ \begin{array}{l}
\text{Im} G^R(k + q, z_1) \text{Im} G^R(k, z_2) \\
- \text{Im} F^R(k + q, z_1) \text{Im} F^R(k, z_2)
\end{array} \right. 

\times \left\{ \tanh \left( \frac{z_1}{2T} \right) - \tanh \left( \frac{z_2}{2T} \right) \right\} \frac{1}{z_1 - z_2 - i\omega_n}.

(2.128)

Setting $i\omega_m \rightarrow \omega + i\delta$ in the above equation, we have

$$
\text{Im} T \sum_n \left\{ \begin{array}{l}
G(k + q, \epsilon_n + \omega_m) G(k, \epsilon_n) \\
- F(k + q, \epsilon_n + \omega_m) F^\dagger(k, \epsilon_n)
\end{array} \right. |_{i\omega_m \rightarrow \omega + i\delta} 

= \int_{-\infty}^{\infty} \frac{dz}{2\pi} \left\{ \begin{array}{l}
\text{Im} G^R(k + q, z + \omega) \text{Im} G^R(k, z) \\
- \text{Im} F^R(k + q, z + \omega) \text{Im} F^R(k, z)
\end{array} \right. 

\times \left\{ \tanh \left( \frac{z + \omega}{2T} \right) - \tanh \left( \frac{z}{2T} \right) \right\}.

(2.129)

So the imaginary part of the phonon self-energy can be written as

$$
\text{Im} \Pi(q, \omega) = \frac{4\omega(q)}{q^2 \rho v^2(q)} \int \frac{d^3k}{(2\pi)^3} \frac{d\epsilon}{2\pi} f^2(k, q) \left\{ \tanh \left( \frac{\epsilon + \omega}{2T} \right) - \tanh \left( \frac{\epsilon}{2T} \right) \right\} 

\times \left\{ \begin{array}{l}
\text{Im} G^R(k + q, \epsilon + \omega) \text{Im} G^R(k, \epsilon) \\
- \text{Im} F^R(k + q, \epsilon + \omega) \text{Im} F^R(k, \epsilon)
\end{array} \right. .

(2.130)

In the hydrodynamic approximation the electron quasiparticle mean free path is much shorter than the phonon wave length. So the equation (2.130) becomes

$$
\text{Im} \Pi^R(q, \omega) = \frac{2\omega^2}{q^2 \rho v^2(q)} \frac{1}{T} \int \frac{d^3k}{(2\pi)^3} \frac{d\epsilon}{2\pi} f^2(k, q) \frac{1}{\cosh^2(\epsilon/2T)} 

\times \left\{ \text{Im} G^R(k, \epsilon) \text{Im} G^R(k, \epsilon) - \text{Im} F^R(k, \epsilon) \text{Im} F^R(k, \epsilon) \right\}.

(2.131)
We use the following relations in the above equation [22]

\[
\text{Im} \left\{ \begin{array}{c}
G^R \\
F^R
\end{array} \right\} = \frac{1}{2i} \left\{ \begin{array}{c}
G^R - G^A \\
F^R - F^A
\end{array} \right\},
\]

\[
(\text{Im}G^R)^2 - (\text{Im}F^R)^2 = \left\{ \begin{array}{c}
-\frac{1}{4} \left( G^R G^R - F^R F^R \right) \\
-\frac{1}{4} \left( G^A G^A - F^A F^A \right) + \frac{1}{2} \left( G^R G^A - F^R F^A \right)
\end{array} \right\},
\]

\[
\int d\xi \left( G^R G^R - F^R F^R \right) = \int d\xi \left( G^A G^A - F^A F^A \right) = 0.
\]

Thus (2.131) can be written as

\[
\text{Im}\Pi^R (q, \omega) = \frac{N_F \omega^2}{2q^2 \rho v^2 (\hat{q})} \frac{1}{T} \int_0^\infty \frac{d\epsilon}{\cosh^2 (\epsilon/2T)} \times \left\langle f^2 (k, q) \int d\xi \left( G^R (k, \epsilon) G^A (k, \epsilon) - F^R (k, \epsilon) F^A (k, \epsilon) \right) \right\rangle_{FS}, \quad (2.132)
\]

where \( \langle \cdots \rangle_{FS} \) means Fermi surface averaging. Substituting the retarded Green’s functions (2.91) and (2.93) into above equation, one obtains the expression for the imaginary part of the phonon self-energy as

\[
\text{Im}\Pi^R (q, \omega) = \frac{N_F \omega^2}{2q^2 \rho v^2 (\hat{q})} \frac{1}{T} \int_0^\infty \frac{d\epsilon}{\cosh^2 (\epsilon/2T)} \times \left\langle f^2 (k, q) \frac{1}{|\text{Ret}(\epsilon)|} \frac{1}{|\text{Im}(\epsilon)|} \frac{\text{Re} |t(\epsilon)|^2 + t^2(\epsilon) - 2\Delta_k^2}{\sqrt{t^2(\epsilon) - \Delta_k^2}} \right\rangle_{FS}. \quad (2.133)
\]

In the normal state, \( t(\epsilon) = \epsilon + i\Gamma \) and \( \Delta_k = 0 \), the imaginary part of phonon self-energy is

\[
\text{Im}\Pi^R (q, \omega) = \frac{4N_F T_n \omega^2}{q^2 \rho v^2 (\hat{q})} \left\langle f^2 (k, q) \right\rangle_{FS}. \quad (2.134)
\]

Since the ratio of ultrasonic attenuation in the normal state and superconducting state is proportional to the ratio of imaginary parts of the self-energy in the normal state and superconducting state, which are given by (2.133) and (2.134), the ratio of ultrasonic attenuation coefficients can be finally obtained as follows

\[
\frac{\alpha^s (q, \omega)}{\alpha^n (q, \omega)} = \frac{1}{8 T_n} \frac{1}{|f^2 (k, q)|_{FS}} \int_0^\infty \frac{d\epsilon}{\cosh^2 (\epsilon/2T)} \frac{1}{|\text{Ret}(\epsilon)|} \frac{1}{|\text{Im}(\epsilon)|} \left\langle f^2 (k, q) \frac{|t(\epsilon)|^2 + t^2(\epsilon) - 2\Delta_k^2}{\sqrt{t^2(\epsilon) - \Delta_k^2}} \right\rangle_{FS}. \quad (2.135)
\]
In our numerical calculation, we only consider the weak disorder and have the following relations for the energy gap

\[
\frac{\Delta_0 (0)}{T_c} = 1.30, \quad (2.136)
\]

\[
\Delta_0 (T) = \Delta_0 (0) \left[ 1 - \left( \frac{T}{T_c} \right)^3 \right]^\frac{1}{2}, \quad (2.137)
\]

\[
\Delta_k (T) = \Delta_0 (T) \left( \cos (k_x a) - \cos (k_y a) \right), \quad (2.138)
\]

see equations (2.43) and (2.44). Here the expression (2.137) is only a convenience approximation for the energy gap [23]. The exact form of \( \Delta_0 (T) \) can be obtained from the self-consistent equation, which is shown in Chap. 3.5. The real and imaginary part of \( t (\epsilon) \) can be obtained from (2.94) and (2.96), which is presented in details in Chap. 3.3. Then the final form of the ratio of ultrasonic attenuation between superconducting state and normal state for the numerical work can be written as

\[
\frac{\alpha^s (\mathbf{q}, \omega)}{\alpha^n (\mathbf{q}, \omega)} = \frac{1}{2T} \frac{1}{\langle f^2 (\mathbf{k}, \mathbf{q}) \rangle_{FS}} \times \int_0^\infty \frac{d\epsilon}{\cosh^2 (\epsilon/2T)} \frac{1}{\epsilon} \left\langle \frac{f^2 (\mathbf{k}, \mathbf{q}) \sqrt{\epsilon^2 - \Delta_k^2 (T)}}{\epsilon / \sqrt{\epsilon^2 - \Delta_k^2 (T)}} \right\rangle_{FS}. \quad (2.139)
\]

When \( \Delta_k \) is zero in the above equation one can find that the ratio of \( \alpha^s (\mathbf{q}, \omega) / \alpha^n (\mathbf{q}, \omega) \) is 1, which means the metal reduces to the normal state.
Chapter 3

Numerical Results and Analysis

In the previous Chapter we introduced the general theoretical framework for the calculation of the ultrasonic attenuation in layered superconductors. The model Hamiltonian includes the nearest and next-nearest interactions in superconductors. The electron self-energies are calculated in the normal state as well as in the superconducting state. Then the ultrasonic attenuation is calculated by taking the imaginary part of the self-energy of the phonon Green's function. In this Chapter, the computational procedures are presented and all the numerical results of above research are shown and discussed in detail. We will present and explain the ultrasonic attenuation length, the gap equation, and the solution for the self-energy.

3.1 The numerical methods for 3D integrals

We use two methods to calculate the 3D momentum integrals in our work. One is the Monte-Carlo method and the other is the Gaussian smearing method. The procedures for these two methods are outlined below.

Let us first discuss the Monte-Carlo method [24]. A multidimensional integral can be expressed as

\[ s = \int_{a_1}^{b_1} \int_{a_2}^{b_2} \cdots \int_{a_n}^{b_n} f(x_1, x_2 \cdots x_n) \, dx_1 \, dx_2 \cdots dx_n, \]  

(3.1)

where \( f(x_1, x_2 \cdots x_n) \) is the integration function and \( a \)'s and \( b \)'s define the boundaries of integration region. First we generate some random numbers in the range from 0 to 1 as
Chapter 3

Chapter 3: Data Preparation and Analysis

This chapter focuses on the preparation and analysis of data. It covers the basics of data cleaning, handling missing values, and exploring data distributions. We will also learn about statistical methods for summarizing data and identifying patterns. By the end of this chapter, you should be able to prepare your data for further analysis and effectively analyze data using various statistical techniques.
Chapter 3. Numerical Results and Analysis

$t_1^i, t_2^i...t_n^i, i = 1, 2...m$ and set

\[ x_j^i = a_j + (b_j - a_j)t_j^i, \quad j = 1, 2...n. \] (3.2)

Then the value of the integral can be estimated from the following expression

\[ s = \frac{1}{m} \left[ \sum_{i=1}^{m} f\left(x_1^i, x_2^i \cdots x_n^i\right) \right] \prod_{j=0}^{n} (b_j - a_j), \] (3.3)

where \( m \) is the number of the sets of random numbers. It is very important to have a large enough \( m \), which means there are enough samples to ensure that a satisfactory degree of accuracy be yielded in our research. Generally \( m \) is \( 10^6 \). We set \( m \) as \( 10^7 \) in our calculation.

As to the Gaussian smearing method, it is used to do a 3D integral over the Fermi surface with a technique of the Gaussian broadening of the band energies [25]. As we know, the average of any function \( F(k) \) over the Fermi surface can be written as

\[ \langle F(k) \rangle_{FS} = \frac{\int_{k \in FBZ} d^3k F(k) \delta(\xi_k)}{\int_{k \in FBZ} d^3k \delta(\xi_k)}, \] (3.4)

where \( \xi_k \) is the energy dispersion and we perform our integration in the momentum space where \( k = (k_x, k_y, k_z) \) spans the first Brillouin zone (FBZ) with the boundaries \( k_x = \pm \pi/a, k_y = \pm \pi/b, k_z = \pm \pi/c \). Then the \( \delta \)-function in the above equation is replaced by a Gaussian distribution as follows

\[ \delta(\xi_k) = \lim_{\varepsilon \rightarrow 0} \frac{1}{\sqrt{2\pi \varepsilon^2}} \exp\left(-\frac{\xi_k^2}{2\varepsilon^2}\right), \] (3.5)

where \( \varepsilon \) is the width of the Gaussian distribution. After the substitution, equation (3.5) changes into

\[ \langle F(k) \rangle_{FS} \cong \lim_{\varepsilon \rightarrow 0} \frac{\sum N \sum_{k \in FBZ} F(k) \exp\left(-\frac{\xi_k^2}{2\varepsilon^2}\right)}{\sum N \sum_{k \in FBZ} \exp\left(-\frac{\xi_k^2}{2\varepsilon^2}\right)}. \] (3.6)

Here the FBZ is divided into \( N \times N \times N \) lattice cells when the calculation is done numerically in our Fortran program. The lattice size has to be large enough, so that there are enough \( k \) points over which the momentum dependent quantities are summed to yield reliable results. Generally, the larger \( N \) leads to higher degree of accuracy, but longer run time of the program.
Figure 3.1: Diagram of the 3D Fermi surface when \( t_\parallel = 1 \), \( t_\perp/t_\parallel = 0.1 \), \( \Delta_0/t_\parallel = 0.04 \), \( t_\parallel/t_\parallel = -0.3 \), \( t_\perp/t_\parallel = -0.03 \), \( \mu/t_\parallel = -1.0 \). This Fermi surface is corresponding to the curve A in Fig. 3.7 and \( t_\parallel, t_\perp \) are \( \tilde{t}_\parallel, \tilde{t}_\perp \) in the body text respectively.

### 3.2 Fermi surfaces

In this thesis we consider several different kinds of Fermi Surfaces to calculate \( t(\epsilon) \) in \((2.96)\) at \( \epsilon = 0 \). The energy dispersion is given in \((2.60)\) and the shapes of the Fermi surfaces are shown from Fig. 3.1 to Fig. 3.6. The values of the corresponding coefficients in \((2.60)\) are given as the following six sets by setting \( t_\parallel \) as the unit of all coefficients:

<table>
<thead>
<tr>
<th></th>
<th>( t_\parallel )</th>
<th>( t_\perp/t_\parallel )</th>
<th>( \Delta_0/t_\parallel )</th>
<th>( \tilde{t}<em>\parallel/t</em>\parallel )</th>
<th>( \tilde{t}<em>\perp/t</em>\parallel )</th>
<th>( \mu/t_\parallel )</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>1.0</td>
<td>0.1</td>
<td>0.04</td>
<td>-0.3</td>
<td>-0.03</td>
<td>-1.0</td>
</tr>
<tr>
<td>B</td>
<td>1.0</td>
<td>0.1</td>
<td>0.04</td>
<td>-0.3</td>
<td>-0.03</td>
<td>-0.5</td>
</tr>
<tr>
<td>C</td>
<td>1.0</td>
<td>0.01</td>
<td>0.04</td>
<td>-0.3</td>
<td>-0.003</td>
<td>-1.0</td>
</tr>
<tr>
<td>D</td>
<td>1.0</td>
<td>0.01</td>
<td>0.04</td>
<td>-0.03</td>
<td>-0.003</td>
<td>-0.5</td>
</tr>
<tr>
<td>E</td>
<td>1.0</td>
<td>0.3</td>
<td>0.04</td>
<td>0</td>
<td>0</td>
<td>-1.9</td>
</tr>
<tr>
<td>F</td>
<td>1.0</td>
<td>0.0</td>
<td>0.04</td>
<td>0</td>
<td>0</td>
<td>-1.9</td>
</tr>
</tbody>
</table>

The three dimensional Fermi surfaces are different with each other. By comparison
Figure 3.2: Diagram of the 3D Fermi surface when $t_{\parallel} = 1$, $t_{\perp}/t_{\parallel} = 0.1$, $\Delta_0/t_{\parallel} = 0.04$, $t_{\parallel}/t_{\parallel} = -0.3$, $t_{\perp}/t_{\parallel} = -0.03$, $\mu/t_{\parallel} = -0.5$. This Fermi surface is corresponding to the curve B in Fig. 3.7 and $t_{\parallel}, t_{\perp}$ are $\tilde{t}_{\parallel}, \tilde{t}_{\perp}$ in the body text respectively.

Figure 3.3: Diagram of the 3D Fermi surface when $t_{\parallel} = 1$, $t_{\perp}/t_{\parallel} = 0.1$, $\Delta_0/t_{\parallel} = 0.04$, $t_{\parallel}/t_{\parallel} = -0.03$, $t_{\perp}/t_{\parallel} = -0.003$, $\mu/t_{\parallel} = -1.0$. This Fermi surface is corresponding to the curve C in Fig. 3.8 and $t_{\parallel}, t_{\perp}$ are $\tilde{t}_{\parallel}, \tilde{t}_{\perp}$ in the body text respectively.
Figure 3.4: Diagram of the 3D Fermi surface when \( t_\parallel = 1 \), \( t_\perp/t_\parallel = 0.1 \), \( \Delta_0/t_\parallel = 0.04 \), \( t_\parallel/t_\parallel = -0.03 \), \( t_\perp/t_\parallel = -0.003 \), \( \mu/t_\parallel = -0.5 \). This Fermi surface is corresponding to the curve D in Fig. 3.8 and \( t_\parallel, t_\perp \) are \( \tilde{t}_\parallel, \tilde{t}_\perp \) in the body text respectively.

Figure 3.5: Diagram of the 3D Fermi surface when \( t_\parallel = 1 \), \( t_\perp/t_\parallel = 0.3 \), \( \Delta_0/t_\parallel = 0.04 \), \( t_\parallel/t_\parallel = 0 \), \( t_\perp/t_\parallel = 0 \), \( \mu/t_\parallel = -1.9 \). This Fermi surface is corresponding to the curve E in Fig. 3.9 and \( \tilde{t}_\parallel, \tilde{t}_\perp \) are \( \tilde{t}_\parallel, \tilde{t}_\perp \) in the body text respectively.
Figure 3.6: Diagram of the 3D Fermi surface when \( t_{\parallel} = 1, \ t_{\perp}/t_{\parallel} = 0, \ \Delta_0/t_{\parallel} = 0.04, \ t_{\parallel}/t_{\parallel} = 0, \ t_{\perp}/t_{\parallel} = 0, \ \mu/t_{\parallel} = -1.9 \). This Fermi surface is corresponding to the curve F in Fig. 3.9 and \( t_{\parallel}, t_{\perp} \) are \( \tilde{t}_{\parallel}, \tilde{t}_{\perp} \) in the body text respectively.

between Fig. 3.1 and Fig. 3.2, or between Fig. 3.3 and Fig. 3.4, we see that the effect of the chemical potential variation on the shape of the Fermi surface is that the \( xy \) cross-section of the Fermi surface becomes more like a square as \( \mu \) increases. By comparison between Fig. 3.1 and Fig. 3.3, or between Fig. 3.2 with Fig. 3.4, we see that the Fermi surface becomes more corrugated along the \( z \) axis when the nearest hopping \( t_{\perp} \) and next nearest hopping \( \tilde{t}_{\perp} \) and \( \tilde{t}_{\parallel} \) increase.

### 3.3 Calculation of \( t(\epsilon) \)

When we calculate the ultrasonic attenuation, the values of imaginary part of \( t(\epsilon) \) as a function of energy are required for the deduction from (2.135) to (2.139). The details are shown as follows. The final form of \( t(\epsilon) \) for numerical calculation in the superconducting state is given by (2.94) in Chap. 2:

\[
t(\epsilon) = \epsilon + i\Gamma \frac{\int \frac{d^3k}{(2\pi)^3} \frac{\tilde{t}(\epsilon)}{\sqrt{i^2(\epsilon) - \Delta_k^2}} \delta(\xi_k)}{\int \frac{d^3k}{(2\pi)^3} \delta(\xi_k)} .
\]  

(3.7)
By using the Gaussian smearing method, we calculated the three dimensional momentum integrals and obtained the value of \( t(\epsilon) \) at \( \epsilon = 0 \) as well as when \( \Gamma \) is very small.

When \( \epsilon = 0 \), \( t(\epsilon) \) is imaginary and can be written as

\[
 t(\epsilon) = it_0. \tag{3.8}
\]

Then (3.7) changes into

\[
 1 = \Gamma \frac{\sum N \sum_{k \in FBZ} \frac{1}{\sqrt{t_0^2 + \Delta_k^2}} \exp \left(-\frac{\xi_k}{2\epsilon^2}\right)}{\sum N \sum_{k \in FBZ} \exp \left(-\frac{\xi_k}{2\epsilon^2}\right)}, \tag{3.9}
\]

where \( \Delta_k(T) \) and \( \Delta_0(T) \) have been defined in (2.136)-(2.138), which have been used by Jian-Xin Zhu et al. in their model [23]. The relation between \( t_0/\Delta_0 \) and \( \Gamma/\Delta_0 \) is shown in Fig. 3.7, Fig. 3.8, and Fig. 3.9 for different kinds of energy dispersion, which are corresponding to different Fermi surfaces from Fig. 3.1 to Fig. 3.6. From the comparison between Fig. 3.7-Fig. 3.9 and Fig. 3.10, one can find that the Fermi surfaces will have significant effect on the imaginary part of \( t(\epsilon = 0) \) only if the disorder is as weak as \( \Gamma/\Delta_0 < 1.0 \). In Fig 3.10 the values of \( t_0/\Delta_0 \) for different Fermi surfaces vary several orders of magnitude for a same value of \( \Gamma/\Delta_0 \). By comparison between the curves A and B, and A and C, we also find that the smaller the interlayer hopping disorder and the chemical potential, the larger the values of \( t_0/\Delta_0 \).

So we just consider the case when \( \Gamma \) is very small. Then the self-consistency between \( t(\epsilon) \) and \( \epsilon \) on the right side of (3.7) can be neglected, i.e. \( t(\epsilon) \) is replaced with \( \epsilon \) there and the following expression is obtained

\[
 t(\epsilon) = \epsilon + i\Gamma \frac{\int \frac{d^2k}{(2\pi)^2} \frac{\epsilon}{\sqrt{\epsilon^2 - \Delta_k^2}} \delta(\xi_k)}{\int \frac{d^2k}{(2\pi)^2} \delta(\xi_k)}. \tag{3.10}
\]

Now we do the calculation of \( \text{Im} t(\epsilon) / \Gamma \) vs \( \epsilon/\Delta_0 \) with the coefficients used for curve A in Fig. 3.7 with the above equation. The result is shown in Fig. 3.11, where the curve is almost linear when energy is smaller than \( \Delta_0 \). This linear relation between \( \text{Im} t(\epsilon) / \Gamma \) and \( \epsilon/\Delta_0 \) is
put into (2.135) and the final form (2.139) for ultrasonic attenuation is obtained after some algebra in Chap. 2.8.

### 3.4 The ultrasonic attenuation

The final form for the ratio of ultrasonic attenuation between superconducting state and normal state is given by (2.139) in Chap. 2

\[
\frac{\alpha_s(q, \omega)}{\alpha_n(q, \omega)} = \frac{1}{2T} \left\langle f^2(k, q) \right\rangle_{FS} \frac{1}{\int_0^\infty d\epsilon \frac{1}{\cosh^2(\epsilon/2T)} \frac{1}{\epsilon} \frac{\left\langle f^2(k, q) \sqrt{\epsilon^2 - \Delta_k^2(T)} \right\rangle_{FS}}{\epsilon} \right. \left. \epsilon \right\rangle_{FS}.
\]

Introducing the function \( A(\epsilon, q) \) and \( B(\epsilon) \) as follows

\[
A(\epsilon, q) = \left\langle f^2(k, q) \sqrt{\epsilon^2 - \Delta_k^2(T)} \right\rangle_{FS},
\]

\[
B(\epsilon) = \left\langle \epsilon/\sqrt{\epsilon^2 - \Delta_k^2(T)} \right\rangle_{FS},
\]

then (3.11) changes into

\[
\frac{\alpha_s(q, \omega)}{\alpha_n(q, \omega)} = \frac{1}{2T} \left\langle f^2(k, q) \right\rangle_{FS} \frac{1}{\int_0^\infty d\epsilon \frac{1}{\cosh^2(\epsilon/2T)} \frac{1}{\epsilon} A(\epsilon, q)} B(\epsilon).
\]

So we need to calculate the values of \( \left\langle f^2(k, q) \right\rangle_{FS} \), \( A(\epsilon, q) \) and \( B(\epsilon) \) for longitudinal waves and transverse waves. In this thesis we calculated \( \alpha_s/\alpha_n \) only in the range of low temperature \((0 < T < 0.2T_c)\) since the calculation in the whole range will take quite a long time.

For a longitudinal wave along the z axis, \( q = q(0, 0, 1) \) and \( u = u(0, 0, 1) \), the result of \( \left\langle f^2(k) \right\rangle_{FS} \) in our numerical calculation is \( 4.245 \times 10^{-3} \) and the ultrasonic attenuation is shown in Fig. 3.13. For a transverse wave along the z axis, \( q = q(0, 0, 1) \) and \( u = u(\cos \theta, \sin \theta, 0) \), the value of \( \left\langle f^2(k) \right\rangle_{FS} \) is a periodic function of \( \theta \) in Fig. 3.12. The ultrasonic attenuation of a transverse wave with the polarization \( u = u(1, 0, 0) \) is shown in Fig. 3.14, and that with the polarization \( u = u(\sqrt{2}/2, \sqrt{2}/2, 0) \) is shown in Fig. 3.15.
From the comparison of Fig. 3.13 and Fig. 3.14, one finds that the ultrasonic attenuation of a longitudinal wave along the z-axis with the polarization \( \mathbf{u} = u(1, 0, 0) \) is about one orders of magnitude larger than that of a transverse wave along the z-axis with the polarization \( \mathbf{u} = u(1, 0, 0) \), which means it is easier for a longitudinal wave to transport in the superconductors than a transverse wave. As to the ultrasonic attenuation of a transverse wave along the z-axis with the polarization \( \mathbf{u} = u(1, 0, 0) \), the result in Fig. 3.15 is much more interesting. The ultrasonic attenuation is about three orders of magnitude smaller than those in Fig. 3.13 and Fig. 3.14. For example, at \( T = 0.1T_c \), the ultrasonic attenuation in Fig. 3.15 is \( 4.98 \times 10^{-4} \), which is much smaller than 0.27 in Fig. 3.13 and 0.04 in Fig. 3.14. But it increases much more rapidly as the temperature goes up, which means a much stronger temperature dependence on the polarization.

So our data show the huge anisotropy of the ultrasonic attenuation in the superconductors. We also conclude that the ultrasonic attenuation depends strongly on the polarization \( \mathbf{u} \) and the temperature. However, our data only show a part of the story because the range of the temperature is limited. Further more, the data at \( 0 < T < 0.1T_c \) in Fig. 3.13 and Fig. 3.14 don’t show a rapid decrease to zero as the temperature goes down. The reason is that higher precision should be required during these computation since the accumulated round off error is much larger when we do the integrals in the range \( 0 < T < 0.1T_c \).

### 3.5 Gap equation in the superconducting state

To calculate the ultrasonic attenuation, one needs not only the \( \tilde{\omega}_n \) but also the temperature-dependent energy gap. Although we use an approximation for the gap equation as (2.136)-(2.138) in our numerical calculation, we will show the theoretical approach to the exact values of the energy gap with a simple example as follows.
Figure 3.7: Diagram of $t_0/\Delta_0$ vs $\Gamma/\Delta_0$ at $\epsilon = 0$. The coefficients of the two curves are corresponding to different Fermi surfaces shown in Fig. 3.1 and Fig. 3.2.

Figure 3.8: Diagram of $t_0/\Delta_0$ vs $\Gamma/\Delta_0$ at $\epsilon = 0$. The coefficients of the two curves are corresponding to different Fermi surfaces shown in Fig. 3.3 and Fig. 3.4.
Chapter 3. Numerical Results and Analysis

Figure 3.9: Diagram of $t_0/\Delta_0$ vs $\Gamma/\Delta_0$ at $\epsilon = 0$. The coefficients of the two curves are corresponding to different Fermi surfaces shown in Fig. 3.5 and Fig. 3.6.

Figure 3.10: Diagram of $t_0/\Delta_0$ vs $\Gamma/\Delta_0$ at $\epsilon = 0$ for all six kinds of Fermi surfaces when the disorder $\Gamma$ is weak. The coefficients of the six curves are shown in Chap. 3.2.
Chapter 3. Numerical Results and Analysis

Figure 3.11: Diagram of $\text{Im}t(\epsilon)/\Gamma$ vs $\epsilon/\Delta_0$ with the coefficients used for curve A in Fig. 3.7 when the disorder $\Gamma$ is weak. Here $\Gamma = 0.1\Delta_0$ are used in our calculation.

Figure 3.12: Diagram of the $\langle f^2(k, q) \rangle_{FS}$ vs $\theta$ for a transverse wave along the $z$-axis. Here the angle $\theta$ expresses the direction of polarization as $\mathbf{u} = u(\cos \theta, \sin \theta, 0)$. 
Figure 3.13: Diagram of the ultrasonic attenuation in the superconducting state as a function of temperature in the lower temperature range for a longitudinal wave along the z-axis with the polarization as \( \mathbf{u} = (0, 0, 1) \). The black dots are the numerical results and the fitted line is shown as a guide to the eye only.

Figure 3.14: Diagram of the ultrasonic attenuation in the superconducting state as a function of temperature in the lower temperature range for a transverse wave along the z-axis with the polarization as \( \mathbf{u} = (1, 0, 0) \). The black dots are the numerical results and the fitted line is shown as a guide to the eye only.
Figure 3.15: Diagram of the ultrasonic attenuation in the superconducting state as a function of temperature in the lower temperature range for a transverse wave along the z-axis with the polarization as \( u = u(\sqrt{2}/2, \sqrt{2}/2, 0) \). The black dots are the numerical results and the fitted line is shown as a guide to the eye only.

We set \( t_\perp = 0 \) in (2.10), which makes the system 2-dimensional, that is

\[
H = H_0 + H' + H_{int},
\]

(3.15)

\[
H_0 = \sum_k \xi(k)c_{k,\alpha}^\dagger c_{k,\alpha},
\]

(3.16)

\[
\xi(k) = -2t_{||}(\cos k_x a + \cos k_y a) - \mu,
\]

(3.17)

where \( H' \) and \( H_{int} \) are defined in (2.11) and (2.36) respectively. For this 2-dimensional system, the Fermi surface is cylindrical and the symmetry factor can be written as

\[
\phi_k = \sqrt{2}\cos(2\varphi),
\]

(3.18)

where \( \sqrt{2} \) is the normalization factor. After performing manipulations similar to those in Chap. 2.2, one finds the self-energy has the form

\[
\Sigma(\omega_n) = -2i\gamma^2\omega_n N_F \int_0^{2\pi} \frac{d\varphi}{2\pi} \frac{\pi}{\sqrt{\bar{\omega}_n^2 + \Delta_k^2}},
\]

(3.19)
where \( N_F \) is the density of the states at the Fermi surface. So the renormalized Matsubara frequencies (2.42) become

\[
i \tilde{\omega}_n = i \omega_n + 2i \gamma^2 \pi N_F \int_0^{2\pi} \frac{d\varphi}{2\pi} \frac{\tilde{\omega}_n}{\sqrt{\tilde{\omega}_n^2 + \Delta_k^2}}.
\]  

(3.20)

For the normal state, \( \Delta_k = 0 \), it yields

\[
\tilde{\omega}_n = \omega_n + \frac{1}{2\tau} \text{sign}(\tilde{\omega}_n),
\]

(3.21)

\[
\frac{1}{2\tau} = 2\gamma^2 \pi N_F,
\]

(3.22)

where \( \tau \) is the relaxation time in the normal state. For the superconducting state, it yields

\[
\tilde{\omega}_n = \omega_n + \frac{1}{2\tau} \int_0^{2\pi} \frac{d\varphi}{2\pi} \frac{\tilde{\omega}_n}{\sqrt{\tilde{\omega}_n^2 + \Delta_k^2}}.
\]

(3.23)

The general form of the gap equation for a superconductor is [21]

\[
1 = VT \sum_n \int \frac{d^3k}{(2\pi)^3} \frac{\phi_k^2}{\bar{\omega}_n^2 + \xi_k^2 + \Delta_k^2} = VT \sum_n \pi N_F \left\langle \frac{\phi_k^2}{\sqrt{\bar{\omega}_n^2 + \Delta_k^2}} \right\rangle_{FS},
\]

(3.24)

where \( \phi_k \) is defined by (3.18), \( \langle \phi_k^2 \rangle_{FS} = 1 \), and \( V \) is the coupling constant. The value of \( \langle \phi_k^2/\sqrt{\bar{\omega}_n^2 + \Delta_k^2} \rangle_{FS} \) at \( \tau^{-1} = 0 \) and \( \Delta_k = 0 \), i.e. in a clean sample in the normal state is \( 1/|\omega_n| \). To guarantee convergence of the Matsubara sum, the term \( 1/|\omega_n| \) is added and subtracted in (3.24). Then

\[
\frac{1}{VN_F} = \pi T \sum_n \left[ \left\langle \frac{\phi_k^2}{\sqrt{\bar{\omega}_n^2 + \Delta_k^2}} \right\rangle_{FS} - \frac{1}{|\omega_n|} \right] + \pi T \sum_n \frac{1}{|\omega_n|},
\]

(3.25)

where the second term can be written in the following form after some algebra (see Appendix D):

\[
\pi T \sum_n \frac{1}{|\omega_n|} = \ln \left( \frac{2e^C \omega_c T_c^{(0)}}{\pi T_c^{(0)} T} \right).
\]

(3.26)

Here \( n_c = \omega_c/2\pi T >> 1 \), \( C \) is Euler's constant, and \( T_c^{(0)} \) is the critical temperature at \( \tau^{-1} = 0 \) (no disorder). Then the gap equation (3.24) takes the form

\[
\ln \left( \frac{T_c^{(0)}}{T} \right) = 2\pi T \sum_{n=0}^{\infty} \left[ \frac{1}{|\omega_n|} - \left\langle \frac{\phi_k^2}{\sqrt{\bar{\omega}_n^2 + \Delta_k^2}} \right\rangle_{FS} \right].
\]

(3.27)
Defining the dimensionless temperature $T^\delta$ as $T^\delta = T/T_c^{(0)}$, $0 < T^\delta < 1$, we obtain

$$\ln T^\delta = 2\pi T \sum_{n=0}^{\infty} \left[ \frac{1}{(2n+1)\pi T} - \left< \frac{\phi_k^2}{\sqrt{\omega_n^2 + \Delta_k^2}} \right>_{FS} \right].$$

(3.28)

Now introducing the non-self-consistent approximation

$$\tilde{\omega}_n = \omega_n + \frac{1}{2\tau} = 2\pi T \left( n + \frac{1}{2} + \frac{1}{4\pi T \tau} \right),$$

(3.29)

the final form for the gap equation can be written as

$$\ln T^\delta = \sum_{n=0}^{\infty} \left[ \frac{1}{n+\frac{1}{2}} - \int_0^{2\pi} \frac{d\varphi}{2\pi} \frac{2 \cos^2(2\varphi)}{\sqrt{(n + \frac{1}{2} + \frac{\alpha}{t})^2 + 2(\delta_0 \cos(2\varphi)/t)^2}} \right],$$

(3.30)

where $\alpha = 1/4\pi T_c^{(0)} \tau$ is the dimensionless strength of disorder and $\delta_0 = \Delta_0/2\pi T_c^{(0)}$. We did the calculation numerically and obtained Fig. 3.16, which gives the exact values of temperature-dependent energy gap for different disorder strength. The curve $\alpha = 0$ matches the data in the previous work by Takada [26]. Our data also shows that the superconductivity can be suppressed by the disorder and there is a critical disorder strength $\alpha = 0.1404$ where superconductors will change to normal metals.

### 3.6 Solutions of the self-energy in the normal state

In this section we will show that the non-trivial solutions for the self-energy in the normal state can not be found numerically. In Chap. 2.2 the equations for the $b_0$, $b_1$ and $b_2$ are given by (2.33) and (2.34) as follows

$$-\delta_n b_0 = \arccos \left( \frac{b_1}{\sqrt{b_1^2 + b_2^2}} \right) + \arccos \left( \frac{1 - b_0}{\sqrt{b_1^2 + b_2^2}} \right),$$

$$-\delta_n b_1 = \sin \left[ \arccos \left( \frac{b_1}{\sqrt{b_1^2 + b_2^2}} \right) + \arccos \left( \frac{1 - b_0}{\sqrt{b_1^2 + b_2^2}} \right) \right],$$

$$-\delta_n b_2 = \cos \left[ \arccos \left( \frac{b_1}{\sqrt{b_1^2 + b_2^2}} \right) + \arccos \left( \frac{1 - b_0}{\sqrt{b_1^2 + b_2^2}} \right) \right] + 1,$$

(3.31)
Figure 3.16: The diagram of $\delta_0$ vs $T/T_c^{(0)}$. Here $\alpha = 1/4\pi T_c^{(0)}/\tau$ is the dimensionless strength of disorder, $\delta_0 = \Delta_0/2\pi T_c^{(0)}$ is the dimensionless gap. The black point $\alpha = 0.1404$ corresponds to the critical disorder strength above which the superconductivity is suppressed.

$$|\delta_n b_0| \leq 2\pi, \quad |\delta_n b_1| \leq 1, \quad -2 \leq \delta_n b_2 \leq 0, \quad 1 - b_0 \leq \sqrt{b_1^2 + b_2^2}. \quad (3.32)$$

We solve these equations numerically and draw the curves $b_0$ vs $b_1$ of (3.31) in a same Cartesian coordinates for different values of $\delta_n$. Two typical pictures are presented in Fig. 3.17 and Fig. 3.18, and for the range of $\delta_n$ from $8.0 \times 10^{-4}$ to 0.1 no intersection of the curves $b_0$ vs $b_1$ of (3.31) was found. When the values of $\delta_n$ increase from 0.1 to 1.8, the curves behave roughly as Fig. 3.17. When the values of $\delta_n$ decrease from 0.1 to $8.0 \times 10^{-4}$, the curves behave roughly as Fig. 3.18. In both cases, whether $\delta_n$ increase or decrease, curves $a$ move away from curve $c$ and no intersection has been found. So we conclude that for $\delta_n > 1.8$ and $\delta_n < 8.0 \times 10^{-4}$, there is no non-trivial solutions. Then we come to the conclusion that there is no non-trivial solutions for the self-energy for all possible values of $\delta_n$. Thus the trivial solution (2.29) is the only solution for the self-energy in our model.
Figure 3.17: Diagram of the solutions of equations (3.31) when $\delta_n = 1.0$. The shadow $a$, $b$, $c$ in the figure are the solutions of the three equations in (3.31) respectively. Although the shadow $b$ and shadow $c$ overlap a lot, there is no intersection of shadow $a$ and shadow $c$.

Figure 3.18: Diagram of the solutions of equations (3.31) when $\delta_n = 0.002$. The shadow $a$, $b$, $c$ in the figure are the solutions of the three equations in (3.31) respectively. Although the shadow $b$ and shadow $c$ overlap a lot, there is no intersection of shadow $a$ and shadow $c$. 
Chapter 4

Conclusion and Discussion

We performed the theoretical analysis of single-electron properties and electron-phonon interaction in a disordered layered superconductor with d-wave pairing. Firstly only the nearest-neighbor electron hopping between the sites in a single plane as well as the interlayer hopping were considered to derive a simple tight-binding electron Hamiltonian. Then we calculated the electron self-energy function both analytically and numerically, and concluded that the trivial solution is the only solution for the electron self-energy function. Then we used this conclusion as an assumption in the extended model, where both the nearest and the next-nearest hoppings in the plane as well as between planes were taken into account. With the extended model the renormalized Matsubara frequency and the solutions for the electron self-energy, both in the normal state and superconducting state, were calculated. We also derived the expression for the electron-phonon interaction, for both the longitudinal wave and the transverse wave. Then the ultrasonic attenuation was calculated by taking the imaginary part of the self-energy of the phonon Green’s function, which is proportional to the rate of ultrasonic attenuation. After that the expression of ultrasonic attenuation for numerical calculations was given and numerical work was done. Three important conclusions were obtained from the theoretical work and the analysis of all numerical data:

1). The solutions for the self-energy of the single-electron Green’s function in the normal state and the superconducting state were calculated by the analytical approach as well as by the numerical method with a simple tight-binding model, which just takes the nearest hoppings into account in the Hamiltonian. The only solution for the self-energy is a
Chapter 4

Confirmation of Residence
momentum-independent one. Some symmetry may be responsible for this behaviour. This important conclusion was used as an assumption for the extended tight-binding model, which takes both the nearest and next-nearest hoppings in the plane as well between planes into account in the three-dimensional Hamiltonian. Then the ultrasonic attenuation was calculated analytically with the extended model by taking the imaginary part of the self-energy for the phonon Green’s function. We also find that in the normal state the self-energy for the extended model is different from that for the simple model only by a coefficient which is a measure of the disorder in the superconductor.

2). The effect of the interlayer hopping disorder and the chemical potential greatly depends on the shape of Fermi surface. The \( xy \) cross-section of the Fermi surface becomes more like a square than a circle as chemical potential increases and the Fermi surface becomes more corrugated along the \( z \) axis when the nearest hopping \( t_\perp \), and next-nearest hopping \( \tilde{t}_\perp \) and \( \tilde{t}_\parallel \) increase. We also see that the smaller the interlayer hopping disorder and the chemical potential, the larger the values of the renormalized Matsubara frequency. However, that effect on the renormalized Matsubara frequency is strong only when the disorder is as weak as \( \Gamma/\Delta_0 < 1.0 \), where a difference of several orders of magnitude of \( t_0/\Delta_0 \) shows up for different interlayer hopping disorder and chemical potentials. An important linear relationship between \( \text{Im} t(\epsilon)/\Gamma \) and \( \epsilon/\Delta_0 \) is also found when the disorder is weak, which makes our final form of ultrasonic attenuation much more simple and easy for simulation.

3). As for the ultrasonic attenuation, first it is about 10 to \( 10^3 \) times larger for a longitudinal wave in the superconductors than for a transverse wave. We also find a strong dependence of ultrasonic attenuation on the direction of the polarization for a transverse wave, which shows a difference of several orders of magnitude of the values for different polarization along x-axis (\( \theta = 0 \)) and x-y direction (\( \theta = \pi/4 \)). There is also a significant anisotropy in the temperature dependence of the ultrasonic attenuation. We find that the ultrasonic attenuation of the transverse wave decreases much faster than that of the longitu-
dinal wave as the temperature goes down, especially when the polarization for a transverse wave is along the x-y direction ($\theta = \pi/4$). Thus our data show different kinds of anisotropies of the ultrasonic attenuation in the layered superconductors when the sound propagation is along the c-axis of the crystal. The values of ultrasonic attenuation depend strongly on the temperature, and the direction of the polarization of the sound wave.

However, much more work can be done in the future. Firstly, we should do more numerical work on this topic with some high speed computer. We can calculate the ultrasonic attenuation in the layered superconductors for not only the lower range but also the whole range of the temperature with proper required precision. Then the future experimental data can be compared with our results. Secondly, we can enhance the accuracy of the present calculation and reduce the accumulated round-off error at $0 < T < 0.1T_c$. Besides these simulations, we can also find out the symmetry in the self-energy that makes the trivial solution the only solution in our tight-binding model, which must be important for understanding the mechanism of the anisotropy of the ultrasonic attenuation in the layered superconductors.
Appendix A

Dyson equation

In this Appendix we derive the Dyson equation for electron self-energy. The general form for the single-particle Matsubara Green’s function is given as [22]

\begin{align}
G_{\uparrow\uparrow}^{(1,2)} &= -\langle T_\tau c_{r_1\uparrow}(\tau_1)c_{r_2\uparrow}^\dagger(\tau_2) \rangle, \quad (A.1) \\
G_{\uparrow\downarrow}^{(1,2)} &= -\langle T_\tau c_{r_1\uparrow}(\tau_1)c_{r_2\downarrow}^\dagger(\tau_2) \rangle, \quad (A.2) \\
F_{\uparrow\downarrow}^{(1,2)} &= -\langle T_\tau c_{r_1\downarrow}(\tau_1)c_{r_2\uparrow}^\dagger(\tau_2) \rangle, \quad (A.3) \\
F_{\uparrow\uparrow}^{(1,2)} &= -\langle T_\tau c_{r_1\downarrow}(\tau_1)c_{r_2\uparrow}^\dagger(\tau_2) \rangle. \quad (A.4)
\end{align}

Here the arrows show the direction of the spin up and down respectively. \((1,2)\) means \((r_1\tau_1, r_2\tau_2)\), where \(r\) is the location of the site \((n, i)\). The capital \(C_r(\tau)\) and \(C_r^\dagger(\tau)\) are the creator operator and annihilator operator, which are defined as

\begin{align}
C_r(\tau) &= \begin{pmatrix} C_{r\uparrow}(\tau) \\ C_{r\downarrow}(\tau) \end{pmatrix}, \quad (A.5) \\
C_r^\dagger(\tau) &= \begin{pmatrix} C_{r\uparrow}(\tau) \\ C_{r\downarrow}(\tau) \end{pmatrix}. \quad (A.6)
\end{align}

So the Nambu matrix Green’s function has the form

\[
\hat{G}^{(1,2)} = \begin{pmatrix} G_{\uparrow\uparrow}^{(1,2)} & F_{\uparrow\downarrow}^{(1,2)} \\ F_{\uparrow\downarrow}^{(1,2)} & -G_{\uparrow\downarrow}^{(1,2)} \end{pmatrix}. \quad (A.7)
\]
With the assumption that $G$ is spin independent, the above equation in the Momentum-frequency representation can be expressed as

$$\hat{G}(k, \omega_n) = \begin{pmatrix} G(k, \omega_n) & F(k, \omega_n) \\ F^\dagger(k, \omega_n) & -G(-k, -\omega_n) \end{pmatrix}. \tag{A.8}$$

The self-energy in the Momentum-frequency representation has the form

$$\hat{\Sigma}(k, \omega_n) = \begin{pmatrix} \Sigma_1(k, \omega_n) & \Sigma_2(k, \omega_n) \\ \Sigma_2^*(k, \omega_n) & -\Sigma_1(-k, -\omega_n) \end{pmatrix}, \tag{A.9}$$

where

$$\Sigma_1(k, \omega_n) = \Sigma_s(k, \omega_n) + \Sigma_a(k, \omega_n), \tag{A.10}$$

$$-\Sigma_1(-k, -\omega_n) = -\Sigma_s(-k, \omega_n) + \Sigma_a(-k, \omega_n), \tag{A.11}$$

With the assumption that $\Sigma_1(-k) = \Sigma_1(k)$, we have

$$\Sigma_s(k, \omega_n) = \frac{1}{2} [\Sigma_1(k, \omega_n) + \Sigma_1(k, -\omega_n)] \tag{A.12}$$

$$\Sigma_a(k, \omega_n) = \frac{1}{2} [\Sigma_1(k, \omega_n) - \Sigma_1(k, -\omega_n)] \tag{A.13}$$

From the equations (A.10)~(A.13), one can check the following two equations are equivalent

$$\begin{cases} \text{Im} \Sigma_1(-\omega_n) = -\text{Im} \Sigma_1(\omega_n) \\ \text{Re} \Sigma_1(-\omega_n) = \text{Re} \Sigma_1(\omega_n) \end{cases} \iff \begin{cases} \text{Im} \Sigma_a(-\omega_n) = -\text{Im} \Sigma_a(\omega_n) \\ \text{Re} \Sigma_a(-\omega_n) = \text{Re} \Sigma_a(\omega_n) \end{cases}. \tag{A.14}$$

So the following relations hold

$$\text{Re} \Sigma_a(k, \omega_n) = 0, \tag{A.15}$$

$$\text{Im} \Sigma_s(k, \omega_n) = 0. \tag{A.16}$$

Then the Dyson equation for the superconductor can be written as the following

$$\hat{G}^{-1}(k, \omega_n) = \begin{pmatrix} i\omega_n - \xi_k - \Sigma_s(k, \omega_n) - \Sigma_a(k, \omega_n) & -(\Delta_k + \Sigma_2) \\ -(\Delta_k + \Sigma_2)^* & i\omega_n + \xi_k + \Sigma_s(-k, \omega_n) - \Sigma_a(-k, \omega_n) \end{pmatrix}. \tag{A.17}$$
Including $\Sigma_s$ in the chemical potential, the above equation changes into

$$
\hat{\mathcal{G}}^{-1}(\mathbf{k}, \omega_n) = \begin{pmatrix}
i\omega_n - \xi_k - \Sigma_a(\mathbf{k}, \omega_n) & - (\Delta_k + \Sigma_2) \\
-(\Delta_k + \Sigma_2)^* & i\omega_n + \xi_k - \Sigma_a(\mathbf{k}, \omega_n)
\end{pmatrix}.
$$  \hspace{1cm} (A.18)

Now we separate the real and imaginary part of the self-energy, namely

$$
\Sigma_a(\mathbf{k}, \omega_n) = \text{Re}\Sigma_a + i\text{Im}\Sigma_a,
$$  \hspace{1cm} (A.19)

$$
\Sigma_2(\mathbf{k}, \omega_n) = \text{Re}\Sigma_2 + i\text{Im}\Sigma_2.
$$  \hspace{1cm} (A.20)

Then the final form of Dyson equation can be written as

$$
\hat{\mathcal{G}}^{-1}(\mathbf{k}, \omega_n) = \begin{pmatrix}
i(\omega_n - \text{Im}\Sigma_a) - (\xi_k + \text{Re}\Sigma_a) & - (\Delta_k + \text{Re}\Sigma_2) - i\text{Im}\Sigma_2 \\
-(\Delta_k + \text{Re}\Sigma_2) + i\text{Im}\Sigma_2 & i(\omega_n - \text{Im}\Sigma_a) - (\xi_k - \text{Re}\Sigma_a)
\end{pmatrix}.
$$  \hspace{1cm} (A.21)
Appendix B

The self-energy in the normal state

Now let’s try to find some non-trivial solutions for the self-energy. Since each $\Gamma_i$, $i = 1, 2, 3$ has a real and imaginary part, the solution of (2.24) can be written as

$$\Gamma_0 = A_0 + iB_0, \quad \Gamma_1 = A_1 + iB_1, \quad \Gamma_2 = A_2 + iB_2. \quad (B.1)$$

The Green’s function in (2.24) can be expressed as

$$G(k_1, \omega_n) = -\frac{I_1 + iI_2}{I_0}, \quad (B.2)$$

where

$$I_1 = \xi_{k_1} + A_0 + A_1 \cos(k_{1z}c) + A_2 \sin(k_{1z}c), \quad (B.3)$$

$$I_2 = \omega_n - B_0 - B_1 \cos(k_{1z}c) - B_2 \sin(k_{1z}c), \quad (B.4)$$

$$I_0 = I_1^2 + I_2^2. \quad (B.5)$$

So (2.24) change into

$$\Gamma_0 = -2\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{I_1 + iI_2}{I_0}, \quad (B.6)$$

$$\Gamma_1 = -2\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{I_1 \cos(k_{1z}c) + iI_2 \cos(k_{1z}c)}{I_0}, \quad (B.7)$$

$$\Gamma_2 = 2\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{I_1 \sin(k_{1z}c) + iI_2 \sin(k_{1z}c)}{I_0}. \quad (B.8)$$

In order to get the values of $\Gamma_i$, $i = 1, 2, 3$ for the self-energy, one needs to calculate the values of all $A$’s and $B$’s, namely

$$A_0 = -2\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{I_1}{I_1^2 + I_2^2}. \quad (B.9)$$
Appendix B. The self-energy in the normal state

First the integrations over energies and over angles in the above equations are separated as follows

\[
\int \frac{d^3k_1}{(2\pi)^3} = N_F \int_{-\infty}^{\infty} d\xi \int_{-\pi}^{\pi} \frac{dk_{1z}}{2\pi},
\]

where \( N_F \) is the density of the state at the Fermi surface. After some algebra one finds all \( A \)'s are zero and the \( B \)'s can be written as

\[
B_0 = -\gamma^2 N_F \int_{-\pi}^{\pi} dk_{1z} \text{sign} [\omega_n - B_0 - B_1 \cos(k_{1z}) - B_2 \sin(k_{1z})],
\]

\[
B_1 = -\gamma^2 N_F \int_{-\pi}^{\pi} dk_{1z} \text{sign} [\omega_n - B_0 - B_1 \cos(k_{1z}) - B_2 \sin(k_{1z})] \cos(k_{1z}),
\]

\[
B_2 = \gamma^2 N_F \int_{-\pi}^{\pi} dk_{1z} \text{sign} [\omega_n - B_0 - B_1 \cos(k_{1z}) - B_2 \sin(k_{1z})] \sin(k_{1z}).
\]

These are the iterative equations for the \( B \)'s. Introducing the \( b \)'s as the following

\[
B_0 (\omega_n) = \omega_n b_0 (\omega_n), \quad B_1 (\omega_n) = \omega_n b_1 (\omega_n), \quad B_2 (\omega_n) = \omega_n b_2 (\omega_n).
\]

The solutions for the self-energy can be expressed as

\[
A_0 = 0, \quad A_1 = 0, \quad A_2 = 0,
\]

\[
B_0 (\omega_n) = -\frac{\gamma^2 N_F}{c} \int_{-\pi}^{\pi} dk_{1z} \text{sign} [1 - b_0 - b_1 \cos(k_{1z}) - b_2 \sin(k_{1z})],
\]

\[
B_1 (\omega_n) = -\frac{\gamma^2 N_F}{c} \int_{-\pi}^{\pi} dk_{1z} \text{sign} [1 - b_0 - b_1 \cos(k_{1z}) - b_2 \sin(k_{1z})] \cos(k_{1z}),
\]

\[
B_2 (\omega_n) = -\frac{\gamma^2 N_F}{c} \int_{-\pi}^{\pi} dk_{1z} \text{sign} [1 - b_0 - b_1 \cos(k_{1z}) - b_2 \sin(k_{1z})] \sin(k_{1z}).
\]
\[ B_2 (\omega_n) = \frac{\gamma^2 N_F}{c} \int_{-\pi}^{\pi} dk_{1z} \text{sign} \left[ 1 - b_0 - b_1 \cos(k_{1z}) - b_2 \sin(k_{1z}) \right] \sin(k_{1z}). \quad (B.23) \]

In what follows, the sign in the above equations will be considered and the equation will be simplified. If \( \text{sign} \left[ 1 - b_0 - b_1 \cos(k_{1z}) - b_2 \sin(k_{1z}) \right] = 1 \), then \( 1 - b_0 - b_1 \cos(k_{1z}) - b_2 \sin(k_{1z}) > 0 \), that is

\[ 1 - b_0 > b_1 \cos(k_{1z}) + b_2 \sin(k_{1z}). \quad (B.24) \]

By setting \( \beta = (1 - b_0) / \sqrt{b_1^2 + b_2^2} \) and \( \cos \varphi = b_1 / \sqrt{b_1^2 + b_2^2} \), one can reduce the above equation to the form

\[ \beta > \cos(k_{1z} - \varphi). \quad (B.25) \]

Then \( x_0 \) and \( \alpha \) are introduced here and defined as

\[ x_0 = \varphi + \arccos(\beta), \quad (B.26) \]

\[ \alpha = \frac{N_F \gamma^2}{C}. \quad (B.27) \]

So the final form for \( B' \)'s can be expressed as

\[ B_0 (\omega_n) = -2\alpha x_0, \quad B_1 (\omega_n) = -2\alpha \sin(x_0), \quad B_2 (\omega_n) = -2\alpha (\cos(x_0) + 1). \quad (B.28) \]

In order to do the calculation numerically, it is more convenience to deal with the \( b' \)'s than the \( B' \)'s. So introducing \( \delta_n \) as

\[ \delta_n = \frac{\omega_n}{2\alpha} = \frac{(2n + 1) \pi T c}{2N_F \gamma^2}, \quad (B.29) \]

one can write the final form for the \( b' \)'s as

\[ -\delta_n b_0 = \arccos \left( \frac{b_1}{\sqrt{b_1^2 + b_2^2}} \right) + \arccos \left( \frac{1 - b_0}{\sqrt{b_1^2 + b_2^2}} \right), \]

\[ -\delta_n b_1 = \sin \left[ \arccos \left( \frac{b_1}{\sqrt{b_1^2 + b_2^2}} \right) + \arccos \left( \frac{1 - b_0}{\sqrt{b_1^2 + b_2^2}} \right) \right], \]

\[ -\delta_n b_2 = \cos \left[ \arccos \left( \frac{b_1}{\sqrt{b_1^2 + b_2^2}} \right) + \arccos \left( \frac{1 - b_0}{\sqrt{b_1^2 + b_2^2}} \right) \right] + 1. \quad (B.30) \]
where the following relations must be satisfied from the definition of the trigonometric function

\[ 1 - b_0 \leq \sqrt{b_1^2 + b_2^2}, \quad |\delta_n b_0| \leq 2\pi, \quad |\delta_n b_1| \leq 1, \quad -2 \leq \delta_n b_2 \leq 0. \]  

(B.31)
Appendix C

The self-energy in the superconducting state

The self-energy in the superconducting state with the extended Hamiltonian can be expressed as

\[
\Sigma_1 (k_i \omega_n) = -2 \int \frac{d^3k}{(2\pi)^3} G_{11}(k, i\omega_n) \left\{ \begin{array}{c}
\gamma^2 + \gamma^2 \cos (k_x c) \cos (k_{1z} c) - \gamma^2 \sin (k_x c) \sin (k_{1z} c) \\
+4\tilde{\gamma}^2 + 2\tilde{\gamma}^2 \cos (k_x c) \cos (k_{1z} c) \cos (k_{1z} a) \\
\quad +2\tilde{\gamma}^2 \cos (k_x c) \cos (k_{1z} c) \cos (k_{1y} a) \\
\quad +2\tilde{\gamma}^2 \sin (k_x c) \sin (k_{1z} c) \sin (k_{1z} a) \\
\quad +2\tilde{\gamma}^2 \sin (k_x c) \sin (k_{1z} c) \sin (k_{1y} a) \\
\quad -2\tilde{\gamma}^2 \cos (k_x c) \sin (k_{1z} c) \cos (k_{1z} a) \\
\quad -2\tilde{\gamma}^2 \cos (k_x c) \sin (k_{1z} c) \cos (k_{1y} a) \\
\quad -2\tilde{\gamma}^2 \sin (k_x c) \sin (k_{1z} c) \cos (k_{1z} a) \\
\quad -2\tilde{\gamma}^2 \sin (k_x c) \sin (k_{1z} c) \cos (k_{1y} a)
\end{array} \right\}
\] (C.1)
The self-energy in the superconducting state

\[ \Sigma_2 (k, i\omega_n) = -2 \int \frac{d^3k}{(2\pi)^3} G_{12} (k, i\omega_n) \left\{ \begin{array}{l}
\gamma^2 + \gamma^2 \cos (k_z c) \cos (k_{1z} c) - \gamma^2 \sin (k_z c) \sin (k_{1z} c) \\
+4\gamma^2 + 2\gamma^2 \cos (k_z c) \cos (k_{1z} c) \cos (k_{1x} a) \\
+2\gamma^2 \cos (k_z c) \cos (k_{1y} a) \cos (k_{1z} c) \cos (k_{1y} a) \\
+2\gamma^2 \sin (k_z c) \sin (k_{1x} a) \sin (k_{1z} c) \sin (k_{1y} a) \\
-2\gamma^2 \cos (k_z c) \sin (k_{1x} a) \cos (k_{1z} c) \sin (k_{1z} a) \\
-2\gamma^2 \cos (k_z c) \cos (k_{1x} a) \sin (k_{1z} c) \sin (k_{1y} a) \\
-2\gamma^2 \sin (k_z c) \cos (k_{1x} a) \sin (k_{1z} c) \cos (k_{1y} a) \\
-2\gamma^2 \sin (k_z c) \cos (k_{1x} a) \sin (k_{1z} c) \cos (k_{1y} a) \\
\end{array} \right\} \]

(C.2)

To separate the frequency from the wave vector in the self-energy, the self-energy is writing as the following form

\[ \Sigma_1 (k, i\omega_n) = \left\{ \begin{array}{l}
\Sigma_1^{(0)} (i\omega_n) + \Sigma_1^{(1)} (i\omega_n) \cos (k_z c) + \Sigma_1^{(2)} (i\omega_n) \sin (k_z c) \\
+ \Sigma_1^{(3)} (i\omega_n) \cos (k_z c) \cos (k_{1x} a) + \Sigma_1^{(4)} (i\omega_n) \cos (k_z c) \cos (k_{1y} a) \\
+ \Sigma_1^{(5)} (i\omega_n) \sin (k_z c) \sin (k_{1x} a) + \Sigma_1^{(6)} (i\omega_n) \sin (k_z c) \sin (k_{1y} a) \\
+ \Sigma_1^{(7)} (i\omega_n) \cos (k_z c) \sin (k_{1x} a) \sin (k_{1z} c) \sin (k_{1y} a) \\
+ \Sigma_1^{(8)} (i\omega_n) \cos (k_z c) \cos (k_{1x} a) \sin (k_{1z} c) \sin (k_{1y} a) \\
+ \Sigma_1^{(9)} (i\omega_n) \sin (k_z c) \cos (k_{1x} a) \sin (k_{1z} c) \cos (k_{1y} a) \\
\end{array} \right\}, \quad (C.3) \]

\[ \Sigma_2 (k, i\omega_n) = \left\{ \begin{array}{l}
\Sigma_2^{(0)} (i\omega_n) + \Sigma_2^{(1)} (i\omega_n) \cos (k_z c) + \Sigma_2^{(2)} (i\omega_n) \sin (k_z c) \\
+ \Sigma_2^{(3)} (i\omega_n) \cos (k_z c) \cos (k_{1x} a) + \Sigma_2^{(4)} (i\omega_n) \cos (k_z c) \cos (k_{1y} a) \\
+ \Sigma_2^{(5)} (i\omega_n) \sin (k_z c) \sin (k_{1x} a) + \Sigma_2^{(6)} (i\omega_n) \sin (k_z c) \sin (k_{1y} a) \\
+ \Sigma_2^{(7)} (i\omega_n) \cos (k_z c) \sin (k_{1x} a) \sin (k_{1z} c) \sin (k_{1y} a) \\
+ \Sigma_2^{(8)} (i\omega_n) \cos (k_z c) \cos (k_{1x} a) \sin (k_{1z} c) \sin (k_{1y} a) \\
+ \Sigma_2^{(9)} (i\omega_n) \sin (k_z c) \cos (k_{1x} a) \sin (k_{1z} c) \cos (k_{1y} a) \\
\end{array} \right\}, \quad (C.4) \]

where

\[ \Sigma_1^{(0)} (i\omega_n) = -2 (\gamma^2 + 4\gamma^2) \int \frac{d^3k_1}{(2\pi)^3} \frac{i\omega_n + \xi_k - \Sigma_0}{\det \left( \hat{G}^{-1} (k, i\omega_n) \right)}, \quad (C.5) \]
Appendix C. The self-energy in the superconducting state

\[
\Sigma_{1}^{(1)}(i\omega_n) = -2\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{i\omega_n + \xi_k - \Sigma}{\det(\tilde{G}^{-1}(k, i\omega_n))} \cos(k_{1z}c),
\]

(C.6)

\[
\Sigma_{1}^{(2)}(i\omega_n) = 2\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{i\omega_n + \xi_k - \Sigma}{\det(\tilde{G}^{-1}(k, i\omega_n))} \sin(k_{1z}c),
\]

(C.7)

\[
\Sigma_{1}^{(3)}(i\omega_n) = -4\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{i\omega_n + \xi_k - \Sigma}{\det(\tilde{G}^{-1}(k, i\omega_n))} \cos(k_{1z}c) \cos(k_{1x}a),
\]

(C.8)

\[
\Sigma_{1}^{(4)}(i\omega_n) = -4\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{i\omega_n + \xi_k - \Sigma}{\det(\tilde{G}^{-1}(k, i\omega_n))} \cos(k_{1z}c) \cos(k_{1y}a),
\]

(C.9)

\[
\Sigma_{1}^{(5)}(i\omega_n) = -4\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{i\omega_n + \xi_k - \Sigma}{\det(\tilde{G}^{-1}(k, i\omega_n))} \sin(k_{1z}c) \sin(k_{1x}a),
\]

(C.10)

\[
\Sigma_{1}^{(6)}(i\omega_n) = -4\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{i\omega_n + \xi_k - \Sigma}{\det(\tilde{G}^{-1}(k, i\omega_n))} \sin(k_{1z}c) \sin(k_{1y}a),
\]

(C.11)

\[
\Sigma_{1}^{(7)}(i\omega_n) = 4\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{i\omega_n + \xi_k - \Sigma}{\det(\tilde{G}^{-1}(k, i\omega_n))} \cos(k_{1z}c) \sin(k_{1x}a),
\]

(C.12)

\[
\Sigma_{1}^{(8)}(i\omega_n) = 4\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{i\omega_n + \xi_k - \Sigma}{\det(\tilde{G}^{-1}(k, i\omega_n))} \cos(k_{1z}c) \sin(k_{1y}a),
\]

(C.13)

\[
\Sigma_{1}^{(9)}(i\omega_n) = 4\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{i\omega_n + \xi_k - \Sigma}{\det(\tilde{G}^{-1}(k, i\omega_n))} \sin(k_{1z}c) \cos(k_{1x}a),
\]

(C.14)

\[
\Sigma_{1}^{(10)}(i\omega_n) = 4\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{i\omega_n + \xi_k - \Sigma}{\det(\tilde{G}^{-1}(k, i\omega_n))} \sin(k_{1z}c) \cos(k_{1y}a),
\]

(C.15)

\[
\Sigma_{2}^{(0)}(i\omega_n) = -2(\gamma^2 + 4\gamma^2) \int \frac{d^3k_1}{(2\pi)^3} \frac{\Delta + \Sigma_2}{\det(\tilde{G}^{-1}(k, i\omega_n))},
\]

(C.16)

\[
\Sigma_{2}^{(1)}(i\omega_n) = -2\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{\Delta + \Sigma_2}{\det(\tilde{G}^{-1}(k, i\omega_n))} \cos(k_{1z}c),
\]

(C.17)

\[
\Sigma_{2}^{(2)}(i\omega_n) = 2\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{\Delta + \Sigma_2}{\det(\tilde{G}^{-1}(k, i\omega_n))} \sin(k_{1z}c),
\]

(C.18)

\[
\Sigma_{2}^{(3)}(i\omega_n) = -4\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{\Delta + \Sigma_2}{\det(\tilde{G}^{-1}(k, i\omega_n))} \cos(k_{1z}c) \cos(k_{1x}a),
\]

(C.19)

\[
\Sigma_{2}^{(4)}(i\omega_n) = -4\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{\Delta + \Sigma_2}{\det(\tilde{G}^{-1}(k, i\omega_n))} \cos(k_{1z}c) \cos(k_{1y}a),
\]

(C.20)
Appendix C. The self-energy in the superconducting state

\[ \Sigma_2^{(5)}(i\omega_n) = -4\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{\Delta + \Sigma_2}{\det(\hat{G}^{-1}(k,i\omega_n))} \sin(k_{1z}c) \sin(k_{1z}a), \]  
\[ \Sigma_2^{(6)}(i\omega_n) = -4\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{\Delta + \Sigma_2}{\det(\hat{G}^{-1}(k,i\omega_n))} \sin(k_{1z}c) \sin(k_{1y}a), \]  
\[ \Sigma_2^{(7)}(i\omega_n) = 4\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{\Delta + \Sigma_2}{\det(\hat{G}^{-1}(k,i\omega_n))} \cos(k_{1z}c) \sin(k_{1z}a), \]  
\[ \Sigma_2^{(8)}(i\omega_n) = 4\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{\Delta + \Sigma_2}{\det(\hat{G}^{-1}(k,i\omega_n))} \cos(k_{1z}c) \sin(k_{1y}a), \]  
\[ \Sigma_2^{(9)}(i\omega_n) = 4\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{\Delta + \Sigma_2}{\det(\hat{G}^{-1}(k,i\omega_n))} \sin(k_{1z}c) \cos(k_{1z}a), \]  
\[ \Sigma_2^{(10)}(i\omega_n) = 4\gamma^2 \int \frac{d^3k_1}{(2\pi)^3} \frac{\Delta + \Sigma_2}{\det(\hat{G}^{-1}(k,i\omega_n))} \sin(k_{1z}c) \cos(k_{1y}a). \]  

For the above equations, the following assumptions are self-consistent

\[ \Sigma_1^j(i\omega_n) = 0, j = 1, 2...10, \]  
\[ \Sigma_2^j(i\omega_n) = 0, j = 0, 1...10. \]  

So the self-energy is momentum-independent and satisfies the following equation

\[ \Sigma(i\omega_n) = -2\left(\gamma^2 + 4\gamma^2\right) \int \frac{d^3k_1}{(2\pi)^3} \frac{i\omega_n + \xi_{k_1} - \Sigma_2(i\omega_n)}{\det(\hat{G}^{-1}(i\omega_n))}. \]
Appendix D

Gap equation

The gap equation is

$$\frac{1}{VN_F} = \pi T \sum_n \left[ \left\langle \frac{\phi_k^2}{\sqrt{\omega_n^2 + \Delta_k^2}} \right\rangle_{FS} - \frac{1}{|\omega_n|} \right] + \pi T \sum_n \frac{1}{|\omega_n|}. \quad (D.1)$$

The second term can be manipulated as follows

$$\pi T \sum_n \frac{1}{|\omega_n|} = \pi T \sum_n \frac{1}{|(2n + 1) \pi T|}$$

$$= \frac{1}{2} \sum_n \frac{1}{|n + 1/2|} = \sum_{n=0}^{n_c} \frac{1}{n + 1/2} = \ln \left( 4e^C n_c \right), \quad (D.2)$$

where $C$ is the Euler’s constant and

$$n_c = \frac{\omega_c}{2\pi T} \gg 1. \quad (D.3)$$

Then we have

$$\ln \left( 4e^C n_c \right) = \ln \left( \frac{2e^C \omega_c}{\pi \frac{\Delta}{T}} \right) = \ln \left( \frac{2e^C \omega_c}{\pi} \frac{T_c^{(0)}}{T} \right). \quad (D.4)$$

So (D.2) changes into

$$\pi T \sum_n \frac{1}{|\omega_n|} = \ln \left( \frac{2e^C \omega_c T_c^{(0)}}{\pi T_c^{(0)} T} \right). \quad (D.5)$$
Bibliography


