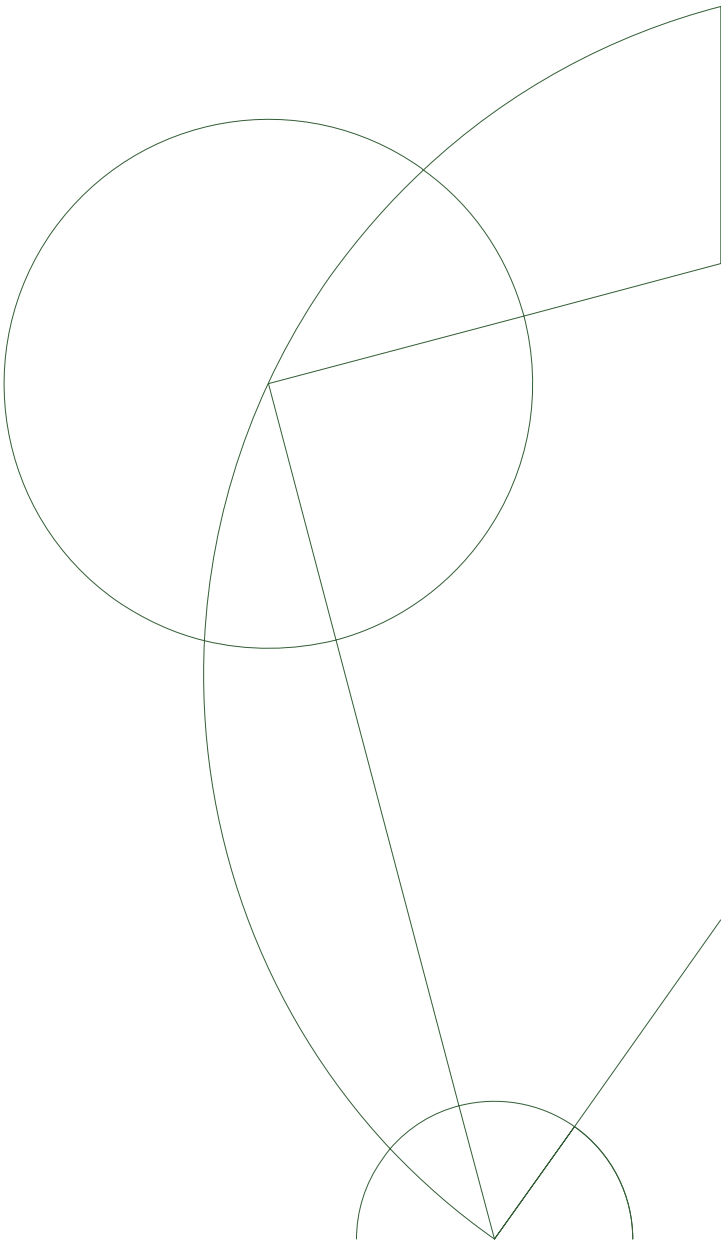
FACULTY OF SCIENCE
UNIVERSITY OF COPENHAGEN

# Master's Thesis in Physics

Junang Wang

# Superfluid Stiffness of Disordered Superconductor



Supervisors: Prof. Brian Møller Andersen

October 2, 2018

**Abstract**

Disordered supercondoctor is still a rich field, which is full of mysteries, to study. The essential mechanism behind them is the key to understand microscopic condensated particles' behaviors. In this thesis, we review the BCS theory and Bogoliubov-de Gennes equations and study the superfluid stiffness in a conventional disordered s-wave supercondoctor. We point out the criteria of a disordered supercondoctor and confirm the effect of $T_c$ enhancement by impurites. We also study unconventional high-$T_c$ d-wave supercondoctors, we try to examine a recent puzzling experiment data presented by Božović *et al*. Since lack of time, we can not make a conclusion yet not in the future we will try to resolve the discrepancy found in the d-wave case.

# Contents

# 1 Introduction

In this thesis, we will discuss conventional and unconventional superconductivity in metallic systems. Superconductivity was discovered by Heike Kamerlingh Onnes in 1911 as the disappearance of the DC eletrical resistance of mercury when cooling it below a critical temperature $T_c$. superconducting material do not only possess interesting electrical properties, but also present peculiar magnetic properties. In 1933 Messner and Ochsenfeld observed that metals in the superconducting state are perfect diamagnets, they expel magnetic field completely. In 1957 the first successful microscopic theory of superconductivity, the BCS theory, was presented by Bardeen, Cooper and Schrieffer. In this thesis, we will investigate an s-wave and d-wave superconductor using the tight-binding model with nearest neighbor hopping in a 2-D square lattice. Using Bogoliubov-de Gennes equations, we evaluate an important quantity called superfluid stiffness $D_s$, which is used to determine the criteria of superconductor in a disorder system [1]. We examine the effect of $T_c$-enhancement by disorder found by Gastiasoro and Andersen [2]. And we also shortly discuss d-wave superconductivity using Bogoliubov-de Gennes equations.

# 2 BCS theory

In the following, we brief introduce the BSC theory.

## 2.1 Cooper pairs

The analysis of Cooper from 1956 that the instability of the Fermi surface due to Cooper pair formation was a percursor of the BCS theory. Cooper found that any finite (and however small) attractive interaction may lead to a bound state pair. It seems rather bizarre to consider an attractive interaction between two apparently repulsive eletrons, but Cooper considered that in a medium they may end up with an effective attraction due to the slow-moving positive ions, we can call it phonons. The interaction between electrons and phonons may be attractive. Consider two electrons located right at the Fermi surface combine into an electron-pair state of zero momentum and zero spin. The Schrodinger equation for the two particle wavefunction is

$$-\frac{\hbar^2}{m}\frac{\partial^2\psi(r)}{\partial r^2} + V(r)\psi(r) = (\Delta + \frac{\hbar^2 k_F^2}{m})\psi(r). \tag{2.1}$$

Here $r = r_1 - r_2$ is relative coordinate, $V$ is a potential between two electrons, $k_F$ is Fermi vector, $m$ is electron mass and $\Delta$ is the energy of the electron pair measured with

respect to the energy of the two decoupled electrons with $\frac{\hbar^2 k_F^2}{m}$. And we can rewrite the Schrodinger equation in momentum space,

$$\frac{\hbar^2 k^2}{m}\psi(k) + \int \frac{d^3k'}{(2\pi)^3} V(k-k')\psi(k') = (\Delta + \frac{\hbar^2 k_F^2}{m})\psi(k), \tag{2.2}$$

where

$$\begin{aligned} \psi(k) &= \int d^3r \psi(r) e^{-ikr}, \\ V(k-k') &= \int d^3r e^{-i(k-k')r} V(r). \end{aligned} \tag{2.3}$$

Then the assumption for the potential was made that the electron-phonon interaction only exists if the eletrons are located with in $\hbar\omega_D$ from Fermi surface.

$$V(k-k') = \begin{cases} -|U| \quad for \quad E_F \leq \frac{\hbar^2 k^2}{2m}, \frac{\hbar^2 k'^2}{2m} \geq E_F + \hbar\omega_D \\ 0 \qquad\qquad\qquad\qquad\qquad\quad \text{otherwise} \end{cases} \tag{2.4}$$

With this form of $V(k-k')$ we have that

$$(\frac{\hbar^2(k^2 - k_F^2)}{m} - \Delta)\psi(k) = |U| \int \frac{d^3k'}{(2\pi)^3}\psi(k'). \tag{2.5}$$

Introducing the density of states $N(\zeta)$, we can change momentum summations to energy integrals. Here, $\zeta$ denotes the energy measured from Fermi level, i.e. $\zeta = \frac{\hbar^2 k^2}{2m} - E_F$. Also, we assume that $N(\zeta)$ varies barely between $[0, \hbar\omega_D]$. Then

$$(2\zeta - \Delta)\psi(k) = |U|N(0) \int_0^{\hbar\omega_D} d\zeta' \psi(k'). \tag{2.6}$$

Finally, we arrive at (see Appendix A)

$$\Delta = -2\hbar\omega_D \exp(-\frac{2}{|U|N(0)}). \tag{2.7}$$

Thus we get an important conclusion that the electron pair will form a lower energy state, or we call it bound state, since $\Delta < 0$. And we did not make any assumption of the value of $|U|$ , thus it shows that this happens for any attractive interaction no matter how small it is. Finally note there is nothing special about the two electrons we selected from the beginning of the calculation, so it really shows that the entire Fermi surface is unstable when subjected to attractive electron-electron interaction. After Cooper discovered the unstability of electron gas below a certain critical temperature $T_c$, it soon led Bardeen, Cooper and Schrieffer(BCS) to develop the microscopic theory explaining superconductivity. And we will briefly discuss BCS theory below.

## 2.2 Tight-binding model and BCS theory

In this thesis, tight-binding model is applied to analyze superconductivity. In tight-binding model, free electrons in lattice are constrained to discrete positions corresponding to the atoms at crystal lattice (the eletrons are considered to be 'tightly bound' to atoms). However, the electrons can hop from one atom to another, which allows electrons to travel through the lattice, which enable normal eletrical conduction. Hopping between nearest-neighbors is controlled by a hopping parameter $t$.

In order to develop our model, we introduce second quantization formalism, which is well used in many body systems. In this formalism, we have the so-called creation operators($c^{\dagger}_{i\sigma}$) and annihilation operators($c_{i\sigma}$), which means an electron with spin $\sigma$ is added or removed from the lattice site $i$. The electron number operator, which gives the number of electrons with spin $\sigma$ on site $i$ is

$$n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}. \tag{2.8}$$

Therefore, the kinetic energy Hamiltonian for free electrons in tight-binding model can be written as

$$\begin{aligned} H_0 =& -t \sum_{<ij>,\sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + H.c) \\ =& \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}. \end{aligned} \tag{2.9}$$

Here $\mathbf{k}$ is momentum, $\varepsilon_{\mathbf{k}} = -2t(\cos(k_x) + \cos(k_y))$ for two-dimensional square lattice system.

Then considering about the electron-electron attractive interaction(Cooper pairs), the Hamiltonian of BCS theory is given by [3]:

$$H_{BCS} = \sum_{\mathbf{k},\sigma} (\varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}) + \sum_{\mathbf{kk'}} V_{\mathbf{kk'}} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} c_{\mathbf{-k'}\downarrow} c_{\mathbf{k'}\uparrow} \tag{2.10}$$

where $V_{\mathbf{kk'}} = -|U|$ for $|\varepsilon_{\mathbf{k}}| < \hbar\omega_D$. The second term is an interaction term which describes scattering of Cooper pairs with momenta($\mathbf{k'}, -\mathbf{k'}$ into another pair with momenta $(\mathbf{k}, -\mathbf{k})$. However, this interaction term cannot be diagonalized. Hence, we apply a mean-field decoupling of the interation term;

$$c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} c_{\mathbf{-k'}\downarrow} c_{\mathbf{k'}\uparrow} \approx \langle c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} \rangle c_{-\mathbf{k'}\downarrow} c_{\mathbf{k'}\uparrow} + c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} \langle c_{-\mathbf{k'}\downarrow} c_{\mathbf{k'}\uparrow} \rangle. \tag{2.11}$$

Here Hartree shift is absorbed into the chemical potential.

Then we define a parameter

$$\Delta = -|U| \sum_{\mathbf{k}} \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle. \tag{2.12}$$

The BCS mean-field Hamiltonian is obtained:

$$H_{BCS}^{mf} = \sum_{\mathbf{k},\sigma} (\varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma}) + \sum_{\mathbf{k}} (\Delta c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger} + \Delta^{*} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}), \tag{2.13}$$

which we can write in matrix form as

$$H_{BCS}^{mf} = \sum_{\mathbf{k}} \begin{pmatrix} c_{\mathbf{k}\uparrow}^{\dagger} & c_{-\mathbf{k}\downarrow} \end{pmatrix} \begin{pmatrix} \varepsilon_{\mathbf{k}} & \Delta \\ \Delta^{*} & -\varepsilon_{-\mathbf{k}} \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c_{-\mathbf{k}\downarrow}^{\dagger} \end{pmatrix}. \tag{2.14}$$

Here we assume the crystal exhibits inversion symmetry then the spectrum in invariant under $\mathbf{k} \to -\mathbf{k}$, i.e. $\varepsilon_{-\mathbf{k}} = \varepsilon_{\mathbf{k}}$. Now we diagonalize the Hamiltonian by introducing the unitary transformation $U$

$$U = \begin{pmatrix} u_{\mathbf{k}} & -v_{\mathbf{k}}^{*} \\ v_{\mathbf{k}} & u_{\mathbf{k}}^{*} \end{pmatrix}, \tag{2.15}$$

and demand that it diagonalizes $H_{BCS}^{mf}$,

$$U^{\dagger} \begin{pmatrix} \varepsilon_{\mathbf{k}} & \Delta \\ \Delta^{*} & -\varepsilon_{\mathbf{k}} \end{pmatrix} U = \begin{pmatrix} E_{\mathbf{k}} & 0 \\ 0 & -E_{\mathbf{k}} \end{pmatrix}. \tag{2.16}$$

In homogeneous case, $\mathbf{k}$ is a good quantum number and $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ can be taken to be real. Using that $U$ is unitary, so that $|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1$, then we get that:

$$E_{\mathbf{k}} = \sqrt{\varepsilon_{\mathbf{k}}^2 + |\Delta|^2}, \tag{2.17}$$

$$|u_{\mathbf{k}}| = \sqrt{\frac{1}{2}(1 + \frac{\varepsilon_{\mathbf{k}}}{E_{\mathbf{k}}})}, |v_{\mathbf{k}}| = \sqrt{\frac{1}{2}(1 - \frac{\varepsilon_{\mathbf{k}}}{E_{\mathbf{k}}})}. \tag{2.18}$$

Diagonlization also means performing a transformation, the Bogoliubov transformation, of the original operators to a set of new fermionic creation and annihilation operators:

$$\begin{pmatrix} \gamma_{\mathbf{k}\uparrow} \\ \gamma_{-\mathbf{k}\downarrow}^{\dagger} \end{pmatrix} = U^{\dagger} \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c_{-\mathbf{k}\downarrow}^{\dagger} \end{pmatrix} \tag{2.19}$$

and the Hamiltonian is diagonal in these new operators:

$$H_{BCS}^{mf} = E_0 + \sum_{\mathbf{k}\sigma} E_{\mathbf{k}} \gamma_{\mathbf{k}\sigma}^{\dagger} \gamma_{\mathbf{k}\sigma}. \tag{2.20}$$

The new quasiparticles described by the number operator $\gamma^\dagger_{\mathbf{k}\sigma}\gamma_{\mathbf{k}\sigma}$ are called Bogoliubons after the Bogoliubov transformation spawning them. As is evident from Eq.2.17, there are no fermion excitation possible with energy less than $|\Delta|$. Then the mean-field parameter $|\Delta|$ provides an energy gap denoted the superconducting gap.

The self-consistent solution for $\Delta$ is given by using Eq.2.15, 2.18 and 2.19:

$$\begin{aligned}
\Delta &= -|U|\sum_{\mathbf{k}}\langle c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}\rangle \\
&= -|U|\sum_{\mathbf{k}}\langle(u_{\mathbf{k}}\gamma_{\mathbf{k}\downarrow}+v^*_{\mathbf{k}}\gamma^\dagger_{\mathbf{k}\uparrow})\times(u_{\mathbf{k}}\gamma_{\mathbf{k}\uparrow}-v^*_{\mathbf{k}}\gamma^\dagger_{\mathbf{k}\downarrow})\rangle \\
&= |U|\sum_{\mathbf{k}}u_{\mathbf{k}}v^*_{\mathbf{k}}(1-f(E_{\mathbf{k}})-f(E_{\mathbf{k}})) \\
&= |U|\sum_{\mathbf{k}}u_{\mathbf{k}}v^*_{\mathbf{k}}(1-2f(E_{\mathbf{k}})) \\
&= |U|\sum_{\mathbf{k}}\frac{\Delta}{2E_{\mathbf{k}}}\tanh(\frac{E_{\mathbf{k}}}{2k_BT})
\end{aligned} \tag{2.21}$$

where in the third step it was used that the Bogoliubons are free fermions so that $\langle\gamma^\dagger_{\mathbf{k}\sigma}\gamma_{\mathbf{k}\sigma}\rangle = f(E_{\mathbf{k}})$, here the Fermi distribution $f(E_{\mathbf{k}}) = \frac{1}{\exp(E_{\mathbf{k}}/k_BT)+1}$. The mean-field assumption made by BCS is that due to the presence of cooper pairs, causes the expection value $\langle c^\dagger_{-\mathbf{k}\downarrow}c^\dagger_{\mathbf{k}\uparrow}\rangle \neq 0$, and its fluctuations around the average value are small. In finite temperature situation, as the temperature rises, Cooper pairs are split and leave the cooper-pair condensate as ordinary electrons. The critical temperature is the temperature where all Cooper-pair break into ordinary electrons(and $\Delta$ vanishes). Below the critical temperature the thermodynamic average of $c^\dagger_{-\mathbf{k}\downarrow}c^\dagger_{\mathbf{k}\uparrow}$ is non-zero, which violates gauge invariance [4].

## 2.3 Gauge invariance breaking

As we know, when a phase transition appear, there is always one kind of symmetry broken. For metal-superconductor transition, below critical temperature the gauge symmetry is broken spontaneously. The gauge transformation can be written as:

$$\begin{aligned}
\mathbf{A} \to \tilde{\mathbf{A}} = \mathbf{A} + \bigtriangledown\chi, \\
c_{\mathbf{k}\sigma} \to \tilde{c}_{\mathbf{k}\sigma} = c_{\mathbf{k}\sigma}e^{-i\chi}.
\end{aligned} \tag{2.22}$$

Here $\mathbf{A}$ is vector potential and $\chi$ is scalar potential. For superconductors, physical quantities may change after performing the gauge transformation. For instance, in the case of the Meissner effect, the London equation $J_e = -\frac{e^2\rho_s(r)}{m}\mathbf{A}$ is not gauge invariant any more. If we perform the gauge transformation Eq.2.22 a physical quantity, current

$J_e$, changes. But we can still argue that the calculation unchange for the transverse part of $\mathbf{A}$ fulfiling $\bigtriangledown \cdot \mathbf{A} = 0$. However, the longitudinal part $\bigtriangledown \chi$ appearing in $\mathbf{A}$ by the gauge transformation affects the order parameter $\Delta$,

$$\Delta_{\mathbf{k}} = -|U| \sum_{\mathbf{k}} \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle \rightarrow \tilde{\Delta}_{\mathbf{k}} = \Delta_{\mathbf{k}} e^{-2i\chi}. \tag{2.23}$$

This result indicates that the Messiner-effect calculation should have been done self-consistently with $\tilde{\Delta}$. So in the gauge $\bigtriangledown \cdot \mathbf{A} = 0$, gauge transformation may not effects the transverse part of physical quantities, but the longitudinal part would change. More details will be discussed later. And in next chapter inhomogeneous case will be considered, we will introduce Bogoliubov-de Gennes equation and focus on the disorder dependence of various physically interesting quantities, such as superfluid density, energy gap.

# 3 Inhomogeneous BCS theory

For clean supercondoctors, just like a peaceful, boring openwater, if we want to know the mysteries beneath the water, we need to throw some rocks in it and see what is happening. Disorder is just like rocks, if we want to know the mechanism for superconductors, the inhomogeneous system is our rough sea.

For homogeneous system, as we know $\mathbf{k}$ is a good quantum number, the unitary transformation(Bogoliubov transformation) is rather easy to obtain as previous chapter shows. However, for inhomogenous system, there are some random impurities sprinkled in the crystal, therefore $\mathbf{k}$ is no longer a good quantum number. We need a more powerful tool: the Bogoliubov-de Gennes equations.

## 3.1 Bogoliubov-de Gennes equations

The purpose of solving the Bogoliubov-de Gennes equations is to find the unitary transformation which diagonalizes the Hamiltonian. The Hamiltonian describling s-wave superconductivity in a two-dimensional square lattice using tight-binding model is given by

$$H = -t \sum_{\langle ij \rangle, \sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + H.c.) + \sum_{i,\sigma} (V_i - \mu) n_{i\sigma} - |U| \sum_i n_{i\uparrow} n_{i\downarrow}. \tag{3.1}$$

Here $c^{\dagger}_{i\sigma}(c_{i\sigma})$ is the electron creation(annihilation) operator with spin $\sigma$ on a site $r_i$ of a square lattice, t is nearest-neighbor hopping, $V_i$ is real space disorder strength, $\mu$ is the chemical potential, $|U|$ is pairing interation, and $n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$.
Then we apply mean-field approximation, which means

$$n_{i\uparrow} n_{i\downarrow} \approx \langle c_{i\uparrow} c_{i\downarrow} \rangle c^{\dagger}_{i\uparrow} c^{\dagger}_{i\downarrow} + c_{i\uparrow} c_{i\downarrow} \langle c^{\dagger}_{i\uparrow} c^{\dagger}_{i\downarrow} \rangle, \tag{3.2}$$

and we define the local pairing amplitude(order parameter)

$$\Delta_i = |U| \langle c_{i\uparrow} c_{i\downarrow} \rangle. \tag{3.3}$$

The Hamiltonian can be rewriten as

$$H = -t \sum_{\langle ij \rangle, \sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + H.c.) + \sum_{i,\sigma} (V_i - \mu) n_{i\sigma} + \sum_i [\Delta^*_i c_{i\uparrow} c_{i\downarrow} + c^{\dagger}_{i\uparrow} c^{\dagger}_{i\downarrow} \Delta_i]. \tag{3.4}$$

The Hamiltonian can be written in matrix form:

$$H = \sum_{ij} \begin{pmatrix} c^{\dagger}_{i\uparrow} \\ c_{i\downarrow} \end{pmatrix} \begin{pmatrix} -t\delta_{\langle ij \rangle} + (V_i - \mu)\delta_{ij} & \Delta_i \delta_{ij} \\ \Delta^*_i \delta_{ij} & t\delta_{\langle ij \rangle} - (V_i - \mu)\delta_{ij} \end{pmatrix} \begin{pmatrix} c_{j\uparrow} \\ c^{\dagger}_{j\downarrow} \end{pmatrix}, \tag{3.5}$$

Here

$$\delta_{ij} = \begin{cases} 1 & \text{for} \quad i = j \\ 0 & \text{otherwise} \end{cases}, \tag{3.6}$$

$$\delta_{\langle ij \rangle} = \begin{cases} 1 & \text{for} \quad i \quad \text{and} \quad j \quad \text{are nearest neighbor} \\ 0 & \text{otherwise} \end{cases}. \tag{3.7}$$

The Hamiltonian can be diagonalized by the transformation

$$\begin{aligned} H &= E_0 + \sum_{n\sigma} E_{n\sigma} \gamma^\dagger_{n\sigma} \gamma_{n\sigma}, \\ c^\dagger_{i\uparrow} &= \sum_n (u^*_{ni\uparrow} \gamma^\dagger_{n\uparrow} - v_{ni\uparrow} \gamma_{n\downarrow}), \\ c^\dagger_{i\downarrow} &= \sum_n (u^*_{ni\downarrow} \gamma^\dagger_{n\downarrow} + v_{ni\downarrow} \gamma_{n\uparrow}). \end{aligned} \tag{3.8}$$

here $\gamma$ and $\gamma^\dagger$ are quasiparticle operators, which are linear combinations of the original $c$ operator. As well as we only care about the excitation above the superconducting ground state, thus the summation is over positive eigenvalues only($E_{n\sigma} > 0$). The matrix form for the transformation can be expressed in this way:

$$\begin{pmatrix} c^\dagger_{i\uparrow} \\ c_{i\downarrow} \end{pmatrix} = \sum_n \begin{pmatrix} u^*_{ni\uparrow} & -v_{ni\uparrow} \\ v^*_{ni\downarrow} & u_{ni\downarrow} \end{pmatrix} \begin{pmatrix} \gamma^\dagger_{n\uparrow} \\ \gamma_{n\downarrow} \end{pmatrix}, \tag{3.9}$$

which the unitary matrix can be defined by

$$U = \sum_n \begin{pmatrix} u^*_{ni\uparrow} & -v_{ni\uparrow} \\ v^*_{ni\downarrow} & u_{ni\downarrow} \end{pmatrix}, \tag{3.10}$$

and it satisfies $U^\dagger U = 1$, which means $u_{ni}$ and $v_{ni}$ satisfy the relationship $\sum_n |u_{ni}|^2 + |v_{ni}|^2 = 1$.

Using the form of $H$ given by Eq. 3.4(more details seen in Appendix **B**), we have

$$\begin{aligned} [H, c_{i\uparrow}] &= t \sum_{\langle j \rangle} c_{j\uparrow} - (V_i - \mu) c_{i\uparrow} - \Delta_i c^\dagger_{i\downarrow}, \\ [H, c_{i\downarrow}] &= t \sum_{\langle j \rangle} c_{j\downarrow} - (V_i - \mu) c_{i\downarrow} + \Delta_i c^\dagger_{i\uparrow}. \end{aligned} \tag{3.11}$$

Here $\langle j \rangle$ means nearest neighbor. Similarly, using the form of $H$ given by Eq. 3.8 and $[\gamma_n, \gamma^\dagger_n] = 1$, we have

$$\begin{aligned} [H, c_{i\uparrow}] &= [H, \sum_n (u_{ni\uparrow} \gamma_{n\uparrow} - v^*_{ni\uparrow} \gamma^\dagger_{n\downarrow})] = \sum_n (-E_{n\uparrow} u_{ni\uparrow} \gamma_{n\uparrow} - E_{n\downarrow} v^*_{ni\uparrow} \gamma^\dagger_{n\downarrow}), \\ [H, c_{i\downarrow}] &= [H, \sum_n (u_{ni\downarrow} \gamma_{n\downarrow} + v^*_{ni\downarrow} \gamma^\dagger_{n\uparrow})] = \sum_n (-E_{n\downarrow} u_{ni\downarrow} \gamma_{n\downarrow} + E_{n\uparrow} v^*_{ni\downarrow} \gamma^\dagger_{n\uparrow}). \end{aligned} \tag{3.12}$$

By substituting the transformation in Eq. 3.8 into Eq. 3.11 demanding the commutators in Eq.3.11 and 3.12 to be equal, we can obtain the Bogoliubov-de Gennes equations

$$\begin{aligned}
E_{n\uparrow}u_{ni\uparrow} &= -t\sum_{\langle j\rangle} u_{nj\uparrow} + (V_i-\mu)u_{ni\uparrow} + \Delta_i v_{ni\downarrow},\\
E_{n\downarrow}v^*_{ni\uparrow} &= \quad t\sum_{\langle j\rangle} v^*_{nj\uparrow} - (V_i-\mu)v^*_{ni\uparrow} + \Delta_i u^*_{ni\downarrow},\\
E_{n\downarrow}u_{ni\downarrow} &= -t\sum_{\langle j\rangle} u_{nj\downarrow} + (V_i-\mu)u_{ni\downarrow} + \Delta_i v_{ni\uparrow},\\
E_{n\uparrow}v^*_{ni\downarrow} &= \quad t\sum_{\langle j\rangle} v^*_{nj\downarrow} - (V_i-\mu)v^*_{ni\downarrow} + \Delta_i u^*_{ni\uparrow},
\end{aligned} \tag{3.13}$$

these four formula can be written in matrix form:

$$\begin{pmatrix} \hat{K} & \hat{\Delta} \\ \hat{\Delta}^* & -\hat{K}^* \end{pmatrix} \begin{pmatrix} u_{ni\uparrow} \\ v_{ni\downarrow} \end{pmatrix} = E_{n\uparrow} \begin{pmatrix} u_{ni\uparrow} \\ v_{ni\downarrow} \end{pmatrix}, \tag{3.14}$$

$$\begin{pmatrix} \hat{K} & \hat{\Delta} \\ \hat{\Delta}^* & -\hat{K}^* \end{pmatrix} \begin{pmatrix} u_{ni\downarrow} \\ v_{ni\uparrow} \end{pmatrix} = E_{n\downarrow} \begin{pmatrix} u_{ni\downarrow} \\ v_{ni\uparrow} \end{pmatrix}. \tag{3.15}$$

Where $\hat{K}u_{ni\sigma} = -t\sum_{<j>} u_{nj\sigma} + (V_i-\mu)u_{ni\sigma}$ and $\hat{\Delta}u_{ni\sigma} = \Delta_i u_{ni\sigma}$, and similarly for $v_{ni\sigma}$. And it is only necessary to solve one of the Eq. 3.14 and 3.15, because it's clear to see if $(u_{ni\uparrow}, v_{ni\downarrow})$ is an eigenvector of matrix with eignenergy $E_{n\uparrow}$, then $(u_{ni\downarrow}, v_{ni\uparrow})$ is the eigenvector with same eigenenergy $E_{n\downarrow}$, thus the spin index can be suppressed. And we only want to consider the excitation eigenvalues $E_n \geq 0$. The self-consistency conditions are given by

$$\begin{aligned}
\Delta_i &= |U|\langle c_{i\uparrow}c_{i\downarrow}\rangle \\
&= |U|\langle \sum_n (u_{ni}\gamma_{n\uparrow} - v^*_{ni}\gamma^\dagger_{n\downarrow}) \times \sum_{n'} (u_{n'i}\gamma_{n'\downarrow} + v^*_{n'i}\gamma^\dagger_{n'\uparrow})\rangle \\
&= |U|\sum_n u_{ni}v^*_{ni}(1-f(E_n)-f(E_n)) \\
&= |U|\sum_n u_{ni}v^*_{ni}(1-2f(E_n)).
\end{aligned} \tag{3.16}$$

$$\begin{aligned}
\langle n_i\rangle = \sum_\sigma \langle c^\dagger_{i\sigma}c_{i\sigma}\rangle &= \sum_{n\sigma} (u^*_{ni}u_{ni}\gamma^\dagger_{n\sigma}\gamma_{n\sigma} + v^*_{ni}v_{ni}\gamma_{n\bar{\sigma}}\gamma^\dagger_{n\bar{\sigma}}) \\
&= 2\sum_n u^2_{ni}f(E_n) + v^2_{ni}(1-f(E_n)).
\end{aligned} \tag{3.17}$$

Here the summation is over positive eigenvalues only. Then we solve the BdG equations as follows; Starting with setting a finite lattice of $N$ sites with periodic boundary conditions and define all kinds of parameters, nearest-neighbor hopping $t$, disorder strength

$V_i$, pairing interation $|U|$ and average density $\langle n \rangle = \sum_i \langle n_i \rangle$ . Guess an initial set of order parameter $\{\Delta_i\}$ and an initial chemical potential $\mu$, which is determined by average density $\langle n \rangle$. Then we solve the BdG equations 3.14, determine the eigenvalues $E_n$ and eigenvectors $\{u_{ni}, v_{ni}\}$. Using Eq. 3.16 and Eq. 3.17, compute $\{\Delta_i\}$ and $\{n_i\}$. If these values differ from the initial ones, the whole process will be iterated with these new values until the results are self-consistent.

## 3.2 Disorder and impurity

Disorder is always an important issue for superconductivity. So what happens to the superconductivity, or we can say critical temperature $T_c$, upon increasing the amount of disorder in a material? From lots of previous studies, the well acceptable answer is that critical temperature $T_c$ drops or remains unaffected. In strong-disorder regime, when the coherence length $\xi$ is longer than the inter-impurity distance, the electron-electron interaction is affected by impurities, electrons of Cooper pair may hitting into impurity causes SC order parameter reducing dramatically and Cooper-pairs breaking [5] [6] [7]. Thus critical temperature $T_c$ drops. In week-disorder regime, when the coherence length $\xi$ is not longer than the inter-impurity distance, disorder may not affect superconductivity. Anderson's theorem [8] states that nonmagnetic week disorder does not affect $T_c$ for conventional superconductors. But Anderson's theorem does not work in unconventional superconductors, this is a complicated and unsovled problem. We are not going to discuss about it in this thesis.

However, we may ask, is it possible to enhance superconductivity by disorder? At least, there is no fundamental principle preventing it. In the following section, using the Bogoliubov-de Gennes approach, we demonstrate that disorder-generated $T_c$ enhancements and try to figure out the criteria for superconductivity.

# 4 Superfluid stiffness

In this section, we will discuss superconductivity of inhomogenous systems. But first we have to figure out the critical line between superconductors and metals. Apparently, the appearance of the excitation gap($\Delta$) is not the reason for the superconductivity itself. The superconductivity is due to the lack of gauge invariance. The superconductors spontaneously break the gauge invariance by picking a particular phase $\phi$ below $T_c$. In other word, the superconductor prefers to sustain a constant phase $\phi$ everywhere in lattice in order to minimize the free energy. And in fact, gapless superconductors do exist. So we need a physical quantity to determine whether a system is metallic or superconducting.

## 4.1 Theory of superfluid Stiffness

In this section, we will introduce an important physical quantity, superfluid stiffness. Superfluid stiffness can be used to examine the criteria for superconductivity.

First, let's consider the electrical current in our model. The x component of the paramagnetic current density can be written as:

$$j^p_{xi} = \sum_\sigma [\Psi^\dagger_\sigma(r_i + x)(\bigtriangledown \Psi_\sigma(r_i)) - (\bigtriangledown \Psi^\dagger_\sigma(r_i))\Psi_\sigma(r_i + x)] = it \sum_\sigma (c^\dagger_{i+x\sigma} c_{i\sigma} - c^\dagger_{i\sigma} c_{i+x\sigma}), \tag{4.1}$$

and $K_{xi}$ is the kinetic-energy density along with the x-oriented links:

$$K_{xi} = \sum_\sigma [\Psi^\dagger_\sigma(r_i + x)\Psi_\sigma(r_i) + \Psi^\dagger_\sigma(r_i)\Psi_\sigma(r_i + x)] = t \sum_\sigma (c^\dagger_{i+x\sigma} c_{i\sigma} + c^\dagger_{i\sigma} c_{i+x\sigma}). \tag{4.2}$$

The total current-density $j_{xi}$ is obtained by

$$j_{xi} = e j^p_{xi} + e^2 K_{xi} A_{xi}, \tag{4.3}$$

here $A$ is vector potential. More details can be seen in Appendix **D**.

Apply the Kubo linear response formula, we obtain

$$\langle j_x(q, \omega) \rangle = -e^2 [\langle -K_x \rangle - \Lambda_{xx}(q, \omega)] A_x(q, \omega). \tag{4.4}$$

Here $\Lambda_{xx}(q, \omega)$ is obtained from

$$\Lambda_{xx}(q, i\omega_n) = \frac{1}{N} \int_0^\beta d\tau e^{i\omega_n \tau} \langle j^p_x(q, \tau) j^p_x(-q, 0) \rangle, \tag{4.5}$$

with $iw_n = 2\pi nT$, by the usual analytic continuation in which $\omega_n \to \omega + i\delta$, and

$$j_x^p(q) = it \sum_{i\sigma} e^{-iqr_i}(c_{i+x\sigma}^\dagger c_{i\sigma} - c_{i\sigma}^\dagger c_{i+x\sigma}). \tag{4.6}$$

As is well known, the Meissner effect can be expressed by London equations. When a superconductor in a static, $\omega = 0$, long wavelength $q_y \to 0$, vector potential, the London equation can be written in a transverse gauge $\mathbf{q} \cdot \mathbf{A} = 0$ as

$$j_x(q) = -\frac{1}{4\pi}\frac{1}{\lambda^2}A_x(q_y). \tag{4.7}$$

In this case, the magnetic field would be expelled except within a penetration depth $\lambda$, with

$$\frac{1}{\lambda^2} = \frac{4\pi n_s e^2}{mc^2}. \tag{4.8}$$

Here $n_s$ is the superfluid density and $m$ the electron mass. And the linear relation between electrical current and vector potential is

$$j_\alpha(\mathbf{q}) = \Lambda_{\alpha\beta}(\mathbf{q})A_\beta(\mathbf{q}), \tag{4.9}$$

$$\Lambda_{\alpha\beta} = (\delta_{\alpha\beta} - \frac{q_\alpha q_\beta}{q^2})\Lambda^T + \frac{q_\alpha q_\beta}{q^2}\Lambda^L. \tag{4.10}$$

Here $\Lambda^T$ is the transverse part of $\Lambda$ and $\Lambda^L$ longitudinal part. And we here apply Einstein summation convention. For a superconductor, from Eqs. 4.7 and 4.9 one has

$$-\frac{\Lambda_{\alpha\beta}(\mathbf{q} \to 0)}{e^2} = (\frac{n_s}{m})^* = \frac{D_s}{\pi e^2}. \tag{4.11}$$

Where $D_s$ is superfluid stiffness which measures the ratio of the superfluid density to the mass. Now from the linear response relation, Eq. 4.4, and Eqs. 4.10 and 4.11, we have

$$\frac{D_s}{\pi e^2} = \langle -K_x \rangle - \Lambda_{xx}(q_x = 0, q_y \to 0, i\omega_n = 0), \tag{4.12}$$

and

$$0 = \langle -K_x \rangle - \Lambda_{xx}(q_x \to 0, q_y = 0, i\omega_n = 0). \tag{4.13}$$

And we can expect that $D_s$ goes to 0 for a metal or insulator, and $D_s$ remains finite for a superconductor. More details will be discussed in Appendix **D**.

## 4.2 Calculation of the Superfluid Stiffness by BdG

In this section, we want to calculate the superfluid stiffness $D_s$ and some physically interesting quantities. Once the BdG iteration process is done, a self-consistent set of

$\{\Delta_i\}$ and $\{n_i\}$ are obtained. Using Bogoliubov transformation Eq. 3.8, some physically interesting quantities can be demonstrated.

Using Eq. 4.2, the kinetic-energy density along with x-oriented bonds can be expressed by:

$$\langle -K_x\rangle = \langle t\sum_{i,n,\sigma}[(u^{n*}_{i+x\sigma}u^n_{i\sigma} + u^{n*}_{i\sigma}u^n_{i+x\sigma})f(E_{n\sigma}) + \bar{\sigma}^2(v^{n*}_{i+x\sigma}v^n_{i\sigma} + v^{n*}_{i\sigma}v^n_{i+x\sigma})f(-E_{n\bar{\sigma}})]\rangle, \tag{4.14}$$

here summation over all $n$ with $E_n > 0$. For a spin-less case we can drop the spin index and write simply as we argue in previous chapter. And since $\bar{\sigma}^2 = 1$, the above formula can be rewritten as:

$$\langle -K_x\rangle = 2t\langle\sum_{i,n}[(u^{n*}_{i+x}u^n_i + u^{n*}_i u^n_{i+x})f(E_n) + (v^{n*}_{i+x}v^n_i + v^{n*}_i v^n_{i+x})f(-E_n)]\rangle. \tag{4.15}$$

In homogeneous case($E_n = E_k$), applying Fourier transformation yields

$$\begin{aligned}\langle -K_x\rangle &= 2t\langle\sum_{k,k',n}[(u^{n*}_{i+x}u^n_i e^{-ik(r_i+x)}e^{ik'r_i} + u^{n*}_i u^n_{i+x}e^{-ik'(r_i+x)}e^{ikr_i})f(E_n)\\ &\quad + (v^{n*}_{i+x}v^n_i e^{-ik(r_i+x)}e^{ik'r_i} + v^{n*}_i v^n_{i+x}e^{-ik'(r_i+x)}e^{ikr_i})f(-E_n)]\rangle\\ &= 4t\sum_k(u_k^2\cos(k_x)f(E_k) + v_k^2\cos(k_x)f(-E_k)).\end{aligned} \tag{4.16}$$

Then turning to the current-current correlation function, using Eqs. 4.5 and 4.6, this is then

$$\begin{aligned}\Lambda_{xx}(q_x, i\omega_n) = \frac{-t^2}{N}\sum_{ij\sigma\sigma'}\int_0^\beta d\tau e^{i\omega_n\tau}e^{iq(r_j-r_i)}(c^\dagger_{i+x\sigma}(\tau)c_{i\sigma}(\tau) - c^\dagger_{i\sigma}(\tau)c_{i+x\sigma}(\tau))\\ \times(c^\dagger_{j+x\sigma'}(0)c_{j\sigma'}(0) - c^\dagger_{j\sigma'}(0)c_{j+x\sigma'}(0)),\end{aligned} \tag{4.17}$$

Fourier transform it to the real space gives

$$\begin{aligned}\Lambda_{xx}(i,j,i\omega_n) = \frac{-t^2}{N}\sum_{\sigma\sigma'}\int_0^\beta d\tau e^{i\omega_n\tau}(c^\dagger_{i+x\sigma}(\tau)c_{i\sigma}(\tau) - c^\dagger_{i\sigma}(\tau)c_{i+x\sigma}(\tau))\\ \times(c^\dagger_{j+x\sigma'}(0)c_{j\sigma'}(0) - c^\dagger_{j\sigma'}(0)c_{j+x\sigma'}(0)),\end{aligned} \tag{4.18}$$

so that

$$\Lambda_{xx}(\mathbf{q}, i\omega_n) = \sum_{ij} e^{i\mathbf{q}(r_j-r_i)}\Lambda_{xx}(i,j,i\omega_n), \tag{4.19}$$

we have to evaluate the four correlators

$$\langle c^\dagger_{i+x\sigma}(\tau)c_{i\sigma}(\tau)c^\dagger_{j+x\sigma'}(0)c_{j\sigma'}(0)\rangle, \tag{4.20}$$

$$\langle c^\dagger_{i+x\sigma}(\tau)c_{i\sigma}(\tau)c^\dagger_{j\sigma'}(0)c_{j+x\sigma'}(0)\rangle, \tag{4.21}$$

$$\langle c^\dagger_{i\sigma}(\tau)c_{i+x\sigma}(\tau)c^\dagger_{j+x\sigma'}(0)c_{j\sigma'}(0)\rangle, \tag{4.22}$$

$$\langle c^\dagger_{i\sigma}(\tau)c_{i+x\sigma}(\tau)c^\dagger_{j\sigma'}(0)c_{j+x\sigma'}(0)\rangle. \tag{4.23}$$

Applying Wick's theorem

$$\begin{aligned}\langle c^\dagger_{i+x\sigma}(\tau)c_{i\sigma}(\tau)c^\dagger_{j+x\sigma'}(0)c_{j\sigma'}(0)\rangle = &- \langle c_{j\sigma'}(0)c^\dagger_{i+x\sigma}(\tau)\rangle\langle c_{i\sigma}(\tau)c^\dagger_{j+x\sigma'}(0)\rangle \\ &- \langle c^\dagger_{i+x\sigma}(\tau)c^\dagger_{j+x\sigma'}(0)\rangle\langle c_{i\sigma}(\tau)c_{j\sigma'}(0)\rangle,\end{aligned} \tag{4.24}$$

$$\begin{aligned}\langle c^\dagger_{i+x\sigma}(\tau)c_{i\sigma}(\tau)c^\dagger_{j\sigma'}(0)c_{j+x\sigma'}(0)\rangle = &- \langle c_{j+x\sigma'}(0)c^\dagger_{i+x\sigma}(\tau)\rangle\langle c_{i\sigma}(\tau)c^\dagger_{j\sigma'}(0)\rangle \\ &- \langle c^\dagger_{i+x\sigma}(\tau)c^\dagger_{j\sigma'}(0)\rangle\langle c_{i\sigma}(\tau)c_{j+x\sigma'}(0)\rangle,\end{aligned} \tag{4.25}$$

$$\begin{aligned}\langle c^\dagger_{i\sigma}(\tau)c_{i+x\sigma}(\tau)c^\dagger_{j+x\sigma'}(0)c_{j\sigma'}(0)\rangle = &- \langle c_{j\sigma'}(0)c^\dagger_{i\sigma}(\tau)\rangle\langle c_{i+x\sigma}(\tau)c^\dagger_{j+x\sigma'}(0)\rangle \\ &- \langle c^\dagger_{i\sigma}(\tau)c^\dagger_{j+x\sigma'}(0)\rangle\langle c_{i+x\sigma}(\tau)c_{j\sigma'}(0)\rangle,\end{aligned} \tag{4.26}$$

$$\begin{aligned}\langle c^\dagger_{i\sigma}(\tau)c_{i+x\sigma}(\tau)c^\dagger_{j\sigma'}(0)c_{j+x\sigma'}(0)\rangle = &- \langle c_{j+x\sigma'}(0)c^\dagger_{i\sigma}(\tau)\rangle\langle c_{i+x\sigma}(\tau)c^\dagger_{j\sigma'}(0)\rangle \\ &- \langle c^\dagger_{i\sigma}(\tau)c^\dagger_{j\sigma'}(0)\rangle\langle c_{i+x\sigma}(\tau)c_{j+x\sigma'}(0)\rangle.\end{aligned} \tag{4.27}$$

Plugging in the Bogoliubov transformation Eq. 3.8, one gets for the first term in Eq. 4.24 that

$$\begin{aligned}&-\langle c_{j\sigma'}(0)c^\dagger_{i+x\sigma}(\tau)\rangle\langle c_{i\sigma}(\tau)c^\dagger_{j+x\sigma'}(0)\rangle \\ &\quad= -\sum_n (u^n_{j\sigma'}u^{n*}_{i+x\sigma}\delta_{\sigma\sigma'}\langle\gamma_{n\sigma'}(0)\gamma^\dagger_{n\sigma}(\tau)\rangle + \bar\sigma\bar\sigma' v^{n*}_{j\sigma'}v^n_{i+x\sigma}\delta_{\bar\sigma\bar\sigma'}\langle\gamma^\dagger_{n\bar\sigma'}(0)\gamma_{n\bar\sigma}(\tau)\rangle)\times \\ &\quad\sum_m (u^m_{i\sigma}u^{m*}_{j+x\sigma'}\delta_{\sigma\sigma'}\langle\gamma_{m\sigma}(\tau)\gamma^\dagger_{m\sigma'}(0)\rangle + \bar\sigma\bar\sigma' v^{m*}_{i\sigma}v^m_{j+x\sigma'}\delta_{\bar\sigma\bar\sigma'}\langle\gamma^\dagger_{m\bar\sigma}(\tau)\gamma_{m\bar\sigma'}(0)\rangle),\end{aligned} \tag{4.28}$$

and from the second term in Eq. 4.24

$$\begin{aligned}&-\langle c^\dagger_{i+x\sigma}(\tau)c^\dagger_{j+x\sigma'}(0)\rangle\langle c_{i\sigma}(\tau)c_{j\sigma'}(0)\rangle \\ &\quad= -\sum_n (\bar\sigma' u^{n*}_{i+x\sigma}v^n_{j+x\sigma'}\delta_{\sigma\bar\sigma'}\langle\gamma^\dagger_{n\sigma}(\tau)\gamma_{n\bar\sigma'}(0)\rangle + \bar\sigma v^n_{i+x\sigma}u^{n*}_{j+x\sigma'}\delta_{\bar\sigma\sigma'}\langle\gamma_{n\bar\sigma}(\tau)\gamma^\dagger_{n\sigma'}(0)\rangle)\times \\ &\quad\sum_m (\bar\sigma' u^m_{i\sigma}v^{m*}_{j\sigma'}\delta_{\sigma\bar\sigma'}\langle\gamma_{m\sigma}(\tau)\gamma^\dagger_{m\bar\sigma'}(0)\rangle + \bar\sigma v^{m*}_{i\sigma}u^m_{j\sigma'}\delta_{\bar\sigma\sigma'}\langle\gamma^\dagger_{m\bar\sigma}(\tau)\gamma_{m\sigma'}(0)\rangle).\end{aligned} \tag{4.29}$$

The other three terms can be obtained by interchanges of $i \leftrightarrow i+x$ and/or $j \leftrightarrow j+x$ indices. Using that

$$\begin{aligned}\langle\gamma_{n\sigma}(\tau)\gamma^\dagger_{n\sigma}(0)\rangle &= (1-f(E_{n\sigma}))e^{-E_{n\sigma}\tau}, \\ \langle\gamma^\dagger_{n\sigma}(\tau)\gamma_{n\sigma}(0)\rangle &= f(E_{n\sigma})e^{E_{n\sigma}\tau}, \\ \langle\gamma_{n\sigma}(0)\gamma^\dagger_{n\sigma}(\tau)\rangle &= -f(E_{n\sigma})e^{E_{n\sigma}\tau}, \\ \langle\gamma^\dagger_{n\sigma}(0)\gamma_{n\sigma}(\tau)\rangle &= -(1-f(E_{n\sigma}))e^{-E_{n\sigma}\tau}.\end{aligned} \tag{4.30}$$

One can infer that the first part (of the normal part) contributes to the correlator with

$$\begin{aligned}\Lambda^{1n}_{xx}(i,j,i\omega_n) =&\frac{t^2}{N}\sum_{nm\sigma}\int_0^\beta d\tau e^{i\omega_n\tau}(u^n_{j\sigma}u^{n*}_{i+x\sigma}u^m_{i\sigma}u^{m*}_{j+x\sigma}(-f(E_{n\sigma}))(1-f(E_{m\sigma}))e^{(E_{n\sigma}-E_{m\sigma})\tau}\\&+\bar{\sigma}^2u^n_{j\sigma}u^{n*}_{i+x\sigma}v^{m*}_{i\sigma}v^m_{j+x\sigma}(-f(E_{n\sigma}))(f(E_{m\bar{\sigma}}))e^{(E_{n\sigma}+E_{m\bar{\sigma}})\tau}\\&+\bar{\sigma}^2v^{n*}_{j\sigma}v^n_{i+x\sigma}u^m_{i\sigma}u^{m*}_{j+x\sigma}(-(1-f(E_{n\bar{\sigma}})))(1-f(E_{m\sigma}))e^{(-E_{n\bar{\sigma}}-E_{m\sigma})\tau}\\&+\bar{\sigma}^4v^{n*}_{j\sigma}v^n_{i+x\sigma}v^{m*}_{i\sigma}v^m_{j+x\sigma}(-(1-f(E_{n\bar{\sigma}})))(f(E_{m\bar{\sigma}}))e^{(-E_{n\bar{\sigma}}+E_{m\bar{\sigma}})\tau}),\end{aligned}\tag{4.31}$$

which $\bar{\sigma}^2=1$ Performing the $\tau$-integration gives

$$\begin{aligned}\Lambda^{1n}_{xx}(i,j,i\omega_n) =& \frac{t^2}{N}\sum_{nm\sigma}(u^n_{j\sigma}u^{n*}_{i+x\sigma}u^m_{i\sigma}u^{m*}_{j+x\sigma}\frac{f(E_{n\sigma})-f(E_{m\sigma})}{i\omega_n+E_{n\sigma}-E_{m\sigma}}\\&+u^n_{j\sigma}u^{n*}_{i+x\sigma}v^{m*}_{i\sigma}v^m_{j+x\sigma}\frac{f(E_{n\sigma})+f(E_{m\bar{\sigma}})-1}{i\omega_n+E_{n\sigma}+E_{m\bar{\sigma}}}\\&+v^{n*}_{j\sigma}v^n_{i+x\sigma}u^m_{i\sigma}u^{m*}_{j+x\sigma}\frac{1-f(E_{n\bar{\sigma}})-f(E_{m\sigma})}{i\omega_n-E_{n\bar{\sigma}}-E_{m\sigma}}\\&+v^{n*}_{j\sigma}v^n_{i+x\sigma}v^{m*}_{i\sigma}v^m_{j+x\sigma}\frac{f(E_{m\bar{\sigma}})-f(E_{n\bar{\sigma}})}{i\omega_n-E_{n\bar{\sigma}}+E_{m\bar{\sigma}}}),\end{aligned}\tag{4.32}$$

likewise one can find that the first part of the superconducting part contributes with

$$\begin{aligned}\Lambda^{1s}_{xx}(i,j,i\omega_n) =&\frac{t^2}{N}\sum_{nm\sigma}\int_0^\beta d\tau e^{i\omega_n\tau}(u^{n*}_{i+x\sigma}v^n_{j+x\bar{\sigma}}u^m_{i\sigma}v^{m*}_{j\bar{\sigma}}f(E_{n\sigma})(1-f(E_{m\sigma}))e^{(E_{n\sigma}-E_{m\sigma})\tau}\\&+\sigma\bar{\sigma}u^{n*}_{i+x\sigma}v^n_{j+x\bar{\sigma}}v^{m*}_{i\sigma}u^m_{j\bar{\sigma}}f(E_{n\sigma})f(E_{m\bar{\sigma}})e^{(E_{n\sigma}+E_{m\bar{\sigma}})\tau}\\&+\sigma\bar{\sigma}v^n_{i+x\sigma}u^{n*}_{j+x\bar{\sigma}}u^m_{i\sigma}v^{m*}_{j\bar{\sigma}}(1-f(E_{n\bar{\sigma}}))(1-f(E_{m\sigma}))e^{(-E_{n\bar{\sigma}}-E_{m\sigma})\tau}\\&+\bar{\sigma}^2\sigma^2v^n_{i+x\sigma}u^{n*}_{j+x\bar{\sigma}}v^{m*}_{i\sigma}u^m_{j\bar{\sigma}}(1-f(E_{n\bar{\sigma}}))(f(E_{m\bar{\sigma}}))e^{(-E_{n\bar{\sigma}}+E_{m\bar{\sigma}})\tau}),\end{aligned}\tag{4.33}$$

which $\bar{\sigma}\sigma=-1$, Performing $\tau$-integration of this monster gives

$$\begin{aligned}\Lambda^{1n}_{xx}(i,j,i\omega_n) =& \frac{t^2}{N}\sum_{nm\sigma}(-u^{n*}_{i+x\sigma}v^n_{j+x\bar{\sigma}}u^m_{i\sigma}v^{m*}_{j\bar{\sigma}}\frac{f(E_{n\sigma})-f(E_{m\sigma})}{i\omega_n+E_{n\sigma}-E_{m\sigma}}\\&+u^{n*}_{i+x\sigma}v^n_{j+x\bar{\sigma}}v^{m*}_{i\sigma}u^m_{j\bar{\sigma}}\frac{f(E_{n\sigma})+f(E_{m\bar{\sigma}})-1}{i\omega_n+E_{n\sigma}+E_{m\bar{\sigma}}}\\&+v^n_{i+x\sigma}u^{n*}_{j+x\bar{\sigma}}u^m_{i\sigma}v^{m*}_{j\bar{\sigma}}\frac{1-f(E_{n\bar{\sigma}})-f(E_{m\sigma})}{i\omega_n-E_{n\bar{\sigma}}-E_{m\sigma}}\\&-v^n_{i+x\sigma}u^{n*}_{j+x\bar{\sigma}}v^{m*}_{i\sigma}u^m_{j\bar{\sigma}}\frac{f(E_{m\bar{\sigma}})-f(E_{n\bar{\sigma}})}{i\omega_n-E_{n\bar{\sigma}}+E_{m\bar{\sigma}}}).\end{aligned}\tag{4.34}$$

Combining it all together, we get $\Lambda^1_{xx}(i,j,i\omega_n) = \Lambda^{1n}_{xx}(i,j,i\omega_n) + \Lambda^{1s}_{xx}(i,j,i\omega_n)$,

$$\begin{aligned}\Lambda^1_{xx}(i,j,i\omega_n) = \frac{t^2}{N}\sum_{nm\sigma}([u^n_{j\sigma}u^{n*}_{i+x\sigma}u^m_{i\sigma}u^{m*}_{j+x\sigma} - u^{n*}_{i+x\sigma}v^n_{j+x\bar{\sigma}}u^m_{i\sigma}v^{m*}_{j\bar{\sigma}}]\frac{f(E_{n\sigma})-f(E_{m\sigma})}{i\omega_n + E_{n\sigma} - E_{m\sigma}} + \\ [u^n_{j\sigma}u^{n*}_{i+x\sigma}v^{m*}_{i\sigma}v^m_{j+x\sigma} + u^{n*}_{i+x\sigma}v^n_{j+x\bar{\sigma}}v^{m*}_{i\sigma}u^m_{j\bar{\sigma}}]\frac{f(E_{n\sigma})+f(E_{m\bar{\sigma}})-1}{i\omega_n + E_{n\sigma} + E_{m\bar{\sigma}}} + \\ [v^{n*}_{j\sigma}v^n_{i+x\sigma}u^m_{i\sigma}u^{m*}_{j+x\sigma} + v^n_{i+x\sigma}u^{n*}_{j+x\bar{\sigma}}u^m_{i\sigma}v^{m*}_{j\bar{\sigma}}]\frac{1-f(E_{n\bar{\sigma}})-f(E_{m\sigma})}{i\omega_n - E_{n\bar{\sigma}} - E_{m\sigma}} + \\ [v^{n*}_{j\sigma}v^n_{i+x\sigma}v^{m*}_{i\sigma}v^m_{j+x\sigma} - v^n_{i+x\sigma}u^{n*}_{j+x\bar{\sigma}}v^{m*}_{i\sigma}u^m_{j\bar{\sigma}}]\frac{f(E_{m\bar{\sigma}})-f(E_{n\bar{\sigma}})}{i\omega_n - E_{n\bar{\sigma}} + E_{m\bar{\sigma}}}).\end{aligned} \tag{4.35}$$

With this notation the total function is

$$\Lambda_{xx}(i,j,i\omega_n) = \Lambda^1_{xx}(i,j,i\omega_n) - \Lambda^2_{xx}(i,j,i\omega_n) - \Lambda^3_{xx}(i,j,i\omega_n) + \Lambda^4_{xx}(i,j,i\omega_n), \tag{4.36}$$

where $\Lambda^2_{xx}(i,j,i\omega_n)$ is obtained from the above explicit expression for $\Lambda^1_{xx}(i,j,i\omega_n)$ by simply interchanging the indices $j \leftrightarrow j+x$. $\Lambda^3_{xx}(i,j,i\omega_n)$ is obtained from $\Lambda^1_{xx}(i,j,i\omega_n)$ by interchanging the indices $i \leftrightarrow i+x$, and $\Lambda^4_{xx}(i,j,i\omega_n)$ is obtained by interchanging both $i \leftrightarrow i+x$ and $j \leftrightarrow j+x$ in $\Lambda^1_{xx}(i,j,i\omega_n)$. Then the final expression is

$$\begin{aligned}\Lambda_{xx}(q,i\omega_n) = \frac{t^2}{N}\sum_{nmij\sigma} e^{iq(r_j-r_i)}(a^{ij}_{nm}(u,v)\frac{f(E_{n\sigma})-f(E_{m\sigma})}{i\omega_n + E_{n\sigma} - E_{m\sigma}} \\ + b^{ij}_{nm}(u,v)\frac{f(E_{n\sigma})+f(E_{m\bar{\sigma}})-1}{i\omega_n + E_{n\sigma} + E_{m\bar{\sigma}}} \\ + c^{ij}_{nm}(u,v)\frac{1-f(E_{n\bar{\sigma}})-f(E_{m\sigma})}{i\omega_n - E_{n\bar{\sigma}} - E_{m\sigma}} \\ + d^{ij}_{nm}(u,v)\frac{f(E_{m\bar{\sigma}})-f(E_{n\bar{\sigma}})}{i\omega_n - E_{n\bar{\sigma}} + E_{m\bar{\sigma}}}).\end{aligned} \tag{4.37}$$

with

$$\begin{aligned}a^{ij}_{nm}(u,v) = u^n_{j\sigma}u^{n*}_{i+x\sigma}u^m_{i\sigma}u^{m*}_{j+x\sigma} - u^{n*}_{i+x\sigma}v^n_{j+x\bar{\sigma}}u^m_{i\sigma}v^{m*}_{j\bar{\sigma}} - u^n_{j+x\sigma}u^{n*}_{i+x\sigma}u^m_{i\sigma}u^{m*}_{j\sigma} + u^{n*}_{i+x\sigma}v^n_{j\bar{\sigma}}u^m_{i\sigma}v^{m*}_{j+x\bar{\sigma}} \\ - u^n_{j\sigma}u^{n*}_{i\sigma}u^m_{i+x\sigma}u^{m*}_{j+x\sigma} + u^{n*}_{i\sigma}v^n_{j+x\bar{\sigma}}u^m_{i+x\sigma}v^{m*}_{j\bar{\sigma}} + u^n_{j+x\sigma}u^{n*}_{i\sigma}u^m_{i+x\sigma}u^{m*}_{j\sigma} - u^{n*}_{i\sigma}v^n_{j\bar{\sigma}}u^m_{i+x\sigma}v^{m*}_{j+x\bar{\sigma}},\end{aligned} \tag{4.38}$$

$$\begin{aligned}b^{ij}_{nm}(u,v) = u^n_{j\sigma}u^{n*}_{i+x\sigma}v^{m*}_{i\sigma}v^m_{j+x\sigma} + u^{n*}_{i+x\sigma}v^n_{j+x\bar{\sigma}}v^{m*}_{i\sigma}u^m_{j\bar{\sigma}} - u^n_{j+x\sigma}u^{n*}_{i+x\sigma}v^{m*}_{i\sigma}v^m_{j\sigma} - u^{n*}_{i+x\sigma}v^n_{j\bar{\sigma}}v^{m*}_{i\sigma}u^m_{j+x\bar{\sigma}} \\ - u^n_{j\sigma}u^{n*}_{i\sigma}v^{m*}_{i+x\sigma}v^m_{j+x\sigma} - u^{n*}_{i\sigma}v^n_{j+x\bar{\sigma}}v^{m*}_{i+x\sigma}u^m_{j\bar{\sigma}} + u^n_{j+x\sigma}u^{n*}_{i\sigma}v^{m*}_{i+x\sigma}v^m_{j\sigma} + u^{n*}_{i\sigma}v^n_{j\bar{\sigma}}v^{m*}_{i+x\sigma}u^m_{j+x\bar{\sigma}},\end{aligned} \tag{4.39}$$

$$\begin{aligned}c^{ij}_{nm}(u,v) = v^{n*}_{j\sigma}v^n_{i+x\sigma}u^m_{i\sigma}u^{m*}_{j+x\sigma} + v^n_{i+x\sigma}u^{n*}_{j+x\bar{\sigma}}u^m_{i\sigma}v^{m*}_{j\bar{\sigma}} - v^{n*}_{j+x\sigma}v^n_{i+x\sigma}u^m_{i\sigma}u^{m*}_{j\sigma} - v^n_{i+x\sigma}u^{n*}_{j\bar{\sigma}}u^m_{i\sigma}v^{m*}_{j+x\bar{\sigma}} \\ - v^{n*}_{j\sigma}v^n_{i\sigma}u^m_{i+x\sigma}u^{m*}_{j+x\sigma} - v^n_{i\sigma}u^{n*}_{j+x\bar{\sigma}}u^m_{i+x\sigma}v^{m*}_{j\bar{\sigma}} + v^{n*}_{j+x\sigma}v^n_{i\sigma}u^m_{i+x\sigma}u^{m*}_{j\sigma} + v^n_{i\sigma}u^{n*}_{j\bar{\sigma}}u^m_{i+x\sigma}v^{m*}_{j+x\bar{\sigma}},\end{aligned} \tag{4.40}$$

$$d^{ij}_{nm}(u,v) = v^{n*}_{j\sigma}v^{n}_{i+x\sigma}v^{m*}_{i\sigma}v^{m}_{j+x\sigma} - v^{n}_{i+x\sigma}u^{n*}_{j+x\bar{\sigma}}v^{m*}_{i\sigma}u^{m}_{j\bar{\sigma}} - v^{n*}_{j+x\sigma}v^{n}_{i+x\sigma}v^{m*}_{i\sigma}v^{m}_{j\sigma} + v^{n}_{i+x\sigma}u^{n*}_{j\bar{\sigma}}v^{m*}_{i\sigma}u^{m}_{j+x\bar{\sigma}}$$
$$- v^{n*}_{j\sigma}v^{n}_{i\sigma}v^{m*}_{i+x\sigma}v^{m}_{j+x\sigma} + v^{n}_{i\sigma}u^{n*}_{j+x\bar{\sigma}}v^{m*}_{i+x\sigma}u^{m}_{j\bar{\sigma}} + v^{n*}_{j+x\sigma}v^{n}_{i\sigma}v^{m*}_{i+x\sigma}v^{m}_{j\sigma} - v^{n}_{i\sigma}u^{n*}_{j\bar{\sigma}}v^{m*}_{i+x\sigma}u^{m}_{j+x\bar{\sigma}}. \tag{4.41}$$

which in the relevant limit $i\omega_n = 0$ and $q_x = 0$ case, can be written as

$$\Lambda_{xx}(q_x = 0, q_y, i\omega_n = 0) = \frac{t^2}{N}\sum_{nmij\sigma} e^{iq_y(r_j - r_i)}([a^{ij}_{nm}(u,v) + d^{ij}_{nm}(u,v)]\frac{f(E_{n\sigma}) - f(E_{m\sigma})}{E_{n\sigma} - E_{m\sigma}} +$$
$$[b^{ij}_{nm}(u,v) + c^{ij}_{nm}(u,v)]\frac{f(E_{n\sigma}) + f(E_{m\bar{\sigma}}) - 1}{E_{n\sigma} + E_{m\bar{\sigma}}}), \tag{4.42}$$

Next, we consider the Green function for superconductor:

$$\begin{aligned} G(\tau) &= -\langle T_\tau c_{i\sigma}(\tau)c^\dagger_{i\sigma}(\tau')\rangle \\ &= -\langle T_\tau((\sum_{ni\sigma} u_{ni\sigma}\gamma_{n\sigma}(\tau) + \bar{\sigma}v^*_{ni\sigma}\gamma^\dagger_{n\bar{\sigma}}(\tau)) \times (\sum_{n'i\sigma} u^*_{n'i\sigma}\gamma^\dagger_{n'\sigma}(\tau') + \bar{\sigma}v_{n'i\sigma}\gamma^\dagger_{n'\bar{\sigma}}(\tau')))\rangle \end{aligned}$$

since$\gamma_{n\sigma}(\tau) = e^{-E_n\tau}\gamma_n$

$$\begin{aligned} &= -\sum_{ni\sigma}[(\theta(\tau - \tau')(u^2_{ni\sigma}\langle\gamma_n\gamma^\dagger_n\rangle e^{-E_n(\tau-\tau')} + v^2_{ni\sigma}\langle\gamma^\dagger_n\gamma_n\rangle e^{E_n(\tau-\tau')}) + \\ &\qquad (\theta(\tau' - \tau)(u^2_{ni\sigma}\langle\gamma^\dagger_n\gamma_n\rangle e^{E_n(\tau-\tau')} + v^2_{ni\sigma}\langle\gamma_n\gamma^\dagger_n\rangle e^{-E_n(\tau-\tau')})]. \end{aligned} \tag{4.43}$$

$$\begin{aligned} G(iw_n) &= \int_0^\beta d\tau e^{iw_n\tau}G(v,\tau) \\ &= -\sum_{ni\sigma}(u^2_{ni\sigma}(1 - f(E_n))\int_0^\beta d\tau e^{iw_n\tau}e^{-E_n\tau} + v^2_{ni\sigma}f(E_n)\int_0^\beta d\tau e^{iw_n\tau}e^{E_n\tau}) \\ &= -\sum_{ni\sigma}(u^2_{ni\sigma}(1 - f(E_n))\frac{e^{iw_n\beta}e^{-E_n\beta} - 1}{iw_n - E_n} + v^2_{ni\sigma}f(E_n)\frac{e^{iw_n\beta}e^{E_n\beta} - 1}{iw_n + E_n}) \\ &\text{since} \quad e^{iw_n\beta} = -1 \\ &= \sum_{ni\sigma}(\frac{u^2_{ni\sigma}}{iw_n - E_n} - \frac{v^2_{ni\sigma}}{iw_n + E_n}) \end{aligned} \tag{4.44}$$

Then the density of states is

$$\begin{aligned} N(w) &= -2ImG(iw_n) \\ &= -2\sum_{ni\sigma}\mathrm{Im}(\frac{u^2_{ni\sigma}}{iw_n - E_n} - \frac{v^2_{ni\sigma}}{iw_n + E_n}) \\ &\text{since} \quad iw_n \to w + i\eta \\ &= \sum_{ni\sigma}(u^2_{ni\sigma}\delta(w - E_n) - v^2_{ni\sigma}\delta(w + E_n)). \end{aligned} \tag{4.45}$$

## 4.3 Numerical calculations

### 4.3.1 Homogeneous case

Using Eq. 4.37, the correlation function can be calculated directly no matter if the system is homogeneous or inhomogenous, normal metallic or superconducting. However, since the formula has 4-indices summation, the whole calculation is time-consuming for large systems. Fortunately, in homogenous case, we can simplify this formula. And we set $t = 1$ from now on.

In the homogeneous case, $k$ is a good quantum number, we can replace $n$ with $k$. With $u_k^2 = \frac{1}{2}(1 + \frac{\epsilon_k}{E_k})$ , $v_k^2 = \frac{1}{2}(1 - \frac{\epsilon_k}{E_k})$ and $E_k = \sqrt{\epsilon_k^2 + \Delta^2}$. In the normal state, the correlation function reduces to($\Delta = 0$, $E \to \epsilon$, $v_k^2 = \frac{1}{2}(1 - \frac{\epsilon_k}{E_k}) = 0$ )

$$\Lambda_{xx}(\mathbf{q}, i\omega_n) = 2\frac{t^2}{N}\sum_{nmij} e^{i\mathbf{q}(r_j - r_i)}\tilde{a}_{nm}^{ij}(u)\frac{f(\epsilon_n) - f(\epsilon_m)}{i\omega_n + \epsilon_n - \epsilon_m}, \tag{4.46}$$

with

$$a_{nm}^{ij}(u,v) = u_{j\sigma}^n u_{i+x\sigma}^{n*} u_{i\sigma}^m u_{j+x\sigma}^{m*} - u_{j+x\sigma}^n u_{i+x\sigma}^{n*} u_{i\sigma}^m u_{j\sigma}^{m*} - u_{j\sigma}^n u_{i\sigma}^{n*} u_{i+x\sigma}^m u_{j+x\sigma}^{m*} + u_{j+x\sigma}^n u_{i\sigma}^{n*} u_{i+x\sigma}^m u_{j\sigma}^{m*}. \tag{4.47}$$

Replace $n$ with $k$, we get

$$\Lambda_{xx}(\mathbf{q}, i\omega_n) = 2\frac{t^2}{N}\sum_{kk'ij} e^{i\mathbf{q}(r_j - r_i)}\tilde{a}_{kk'}^{ij}(u)\frac{f(\epsilon_k) - f(\epsilon_k')}{i\omega_n + \epsilon_k - \epsilon_k'}. \tag{4.48}$$

Applying a Fourier transformation

$$u_i^n = \sum_k e^{ikx} u_k, \tag{4.49}$$

we obtain

$$\Lambda_{xx}(\mathbf{q}, i\omega_n) = 2\frac{t^2}{N}\sum_k (e^{-2ik_x - iq_x} - 2 + e^{2ik_x + iq_x})\frac{f(\epsilon_k) - f(\epsilon_{k+q})}{i\omega_n + \epsilon_k - \epsilon_{k+q}}. \tag{4.50}$$

Therefore for $q_x = 0$ we have

$$\Lambda_{xx}(\mathbf{q}, i\omega_n) = -8\frac{t^2}{N}\sum_k \sin^2(k_x)\frac{f(\epsilon_k) - f(\epsilon_{k+q})}{i\omega_n + \epsilon_k - \epsilon_{k+q}}. \tag{4.51}$$

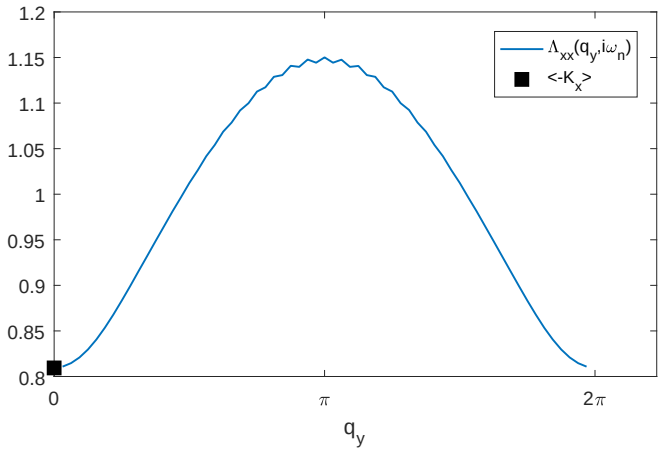



Figure 1: $\Lambda_{xx}(q_y, \omega_n = 0)$ vs $q_y$ for a 2-D 64×64 clean lattice. Here average charge density $\langle n \rangle = 0.85, |U| = 0, \beta = \frac{1}{k_B T} = 20$, while the solid square marks $\langle -K_x \rangle$.

We examine Eq. 4.51 in a 2-D 64×64 clean metal lattice(self-consistent result $\Delta_i = 0$ in the whole real space) with $\langle n \rangle = 0.85, |U| = 0.8, \beta = \frac{1}{k_B T} = 20$. See in Figure. 1, when $q_y$ goes to a small value($q_y \to 0$), $\Lambda_{xx}(q_y \to 0, \omega_n = 0) = \langle -K_x \rangle$, which means that the superfluid density $D_s = 0$. Thus the system is a normal metal.

In the superconducting state, one gets

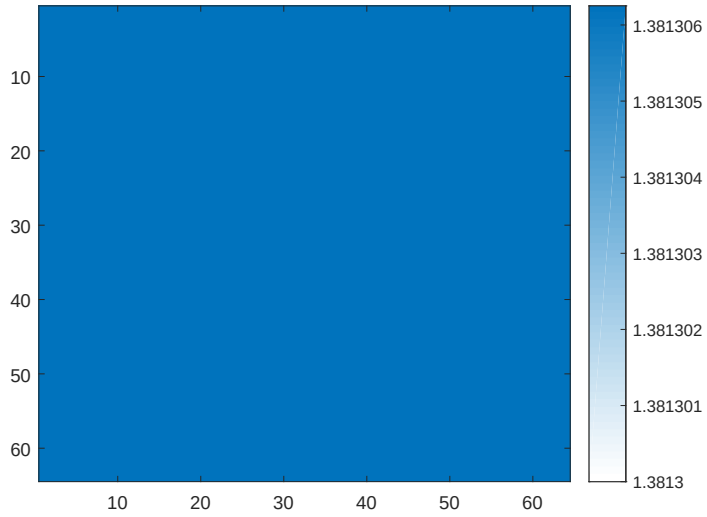



Figure 2: Self-consistent $\Delta$ map for a 2-D 64×64 clean lattice, here average charge density $\langle n\rangle = 1, |U| = 4, \beta = \frac{1}{k_B T} = 200$.

$$\Lambda_{xx}(q_x = 0, q_y, i\omega_n = 0) = -\frac{4t^2}{N}\sum_{k\sigma}\sin^2(k_x)([a_{k,k+q}(u,v) + d_{k,k+q}(u,v)]\frac{f(E_{k\sigma}) - f(E_{k+q_y\sigma})}{E_{k\sigma} - E_{k+q_y\sigma}} + [b_{k,k+q}(u,v) + c_{k,k+q}(u,v)]\frac{f(E_{k\sigma}) + f(E_{k+q_y\bar{\sigma}}) - 1}{E_{k\sigma} + E_{k+q_y\bar{\sigma}}}), \tag{4.52}$$

One gets

$$a_{k,k+q}(u,v) = u_k^2 u_{k+q}^2 + u_k v_k u_{k+q} v_{k+q} = \frac{1}{4}(1 + \frac{\epsilon_k}{E_k} + \frac{\epsilon_{k+q}}{E_{k+q}} + \frac{\epsilon_k\epsilon_{k+q}}{E_k E_{k+q}} + \frac{\Delta_k\Delta_{k+q}}{E_k E_{k+q}}), \tag{4.53}$$

$$d_{k,k+q}(u,v) = v_k^2 v_{k+q}^2 + v_k u_k u_{k+q} v_{k+q} = \frac{1}{4}(1 - \frac{\epsilon_k}{E_k} - \frac{\epsilon_{k+q}}{E_{k+q}} + \frac{\epsilon_k\epsilon_{k+q}}{E_k E_{k+q}} + \frac{\Delta_k\Delta_{k+q}}{E_k E_{k+q}}), \tag{4.54}$$

$$b_{k,k+q}(u,v) = u_k^2 v_{k+q}^2 - u_k v_k u_{k+q} v_{k+q} = \frac{1}{4}(1 + \frac{\epsilon_k}{E_k} - \frac{\epsilon_{k+q}}{E_{k+q}} - \frac{\epsilon_k\epsilon_{k+q}}{E_k E_{k+q}} - \frac{\Delta_k\Delta_{k+q}}{E_k E_{k+q}}), \tag{4.55}$$

$$c_{k,k+q}(u,v) = v_k^2 u_{k+q}^2 - u_k v_k u_{k+q} v_{k+q} = \frac{1}{4}(1 - \frac{\epsilon_k}{E_k} + \frac{\epsilon_{k+q}}{E_{k+q}} - \frac{\epsilon_k\epsilon_{k+q}}{E_k E_{k+q}} - \frac{\Delta_k\Delta_{k+q}}{E_k E_{k+q}}). \tag{4.56}$$

Defining $p^2(k,k+q) = \frac{1}{2}(1 - \frac{\epsilon_k\epsilon_{k+q} + \Delta_k\Delta_{k+q}}{E_k E_{k+q}})$, and $l^2(k,k+q) = \frac{1}{2}(1 + \frac{\epsilon_k\epsilon_{k+q} + \Delta_k\Delta_{k+q}}{E_k E_{k+q}})$,

finally we have that

$$\Lambda_{xx}(q_x=0,q_y,i\omega_n=0)$$
$$=\frac{4t^2}{N}\sum_{k\sigma}\sin^2(k_x)[l^2(k,k+q)(\frac{1}{i\omega_n+E_{k\sigma}-E_{k+q_y\sigma}}+\frac{1}{-i\omega_n+E_{k\sigma}-E_{k+q_y\sigma}})(f(E_{k\sigma})-f(E_{k+q_y\sigma}))$$
$$+p^2(k,k+q)(\frac{1}{i\omega_n+E_{k\sigma}+E_{k+q_y\sigma}}+\frac{1}{-i\omega_n+E_{k\sigma}+E_{k+q_y\sigma}})(1-f(E_{k\sigma})-f(E_{k+q_y\sigma}))], \tag{4.57}$$

analogously, in the limit $q_y=0$, thus can be written as

$$\Lambda_{xx}(q_x,q_y=0,i\omega_n=0)$$
$$=\frac{4t^2}{N}\sum_{k\sigma}(\sin^2(k_x)+\frac{q_x}{2})\times$$
$$[l^2(k,k+q)(\frac{1}{i\omega_n+E_{k\sigma}-E_{k+q_x\sigma}}+\frac{1}{-i\omega_n+E_{k\sigma}-E_{k+q_x\sigma}})(f(E_{k\sigma})-f(E_{k+q_x\sigma}))$$
$$+p^2(k,k+q)(\frac{1}{i\omega_n+E_{k\sigma}+E_{k+q_x\sigma}}+\frac{1}{-i\omega_n+E_{k\sigma}+E_{k+q_x\sigma}})(1-f(E_{k\sigma})-f(E_{k+q_x\sigma}))]. \tag{4.58}$$

As we discussed in previous chapter, the transverse part($\Lambda_{xx}(q_x,q_y=0,i\omega_n=0)$) violates gauge invariance, which gives incorrect value. However, it is well known that vertex corrections fix this difficulty.

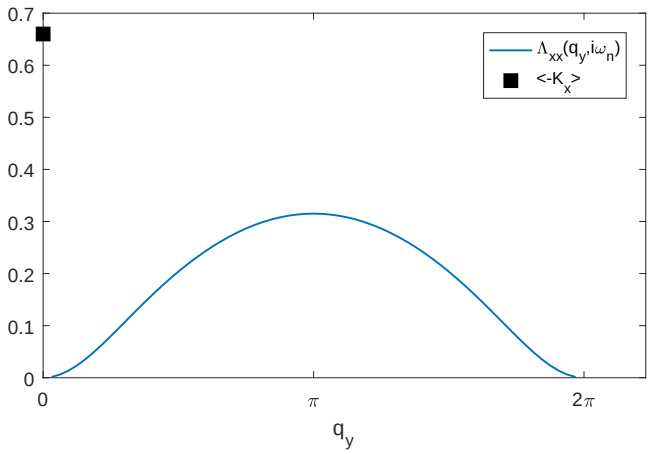



Figure 3: $\Lambda_{xx}(q_y,\omega_n=0)$ vs $q_y$ for a 2-D 64×64 clean lattice. Here average charge density $\langle n\rangle=1, |U|=4, \beta=\frac{1}{k_BT}=200$, while the solid square marks $\langle -K_x\rangle$.

Once the BdG equations are solved, a set of self-consistent result can be obtained. Using Eqs. 4.16 and 4.57 , the homogeneous superfluid density can be calculated. See

Figure. 2 for self-consistent $\Delta_i$ in a square lattice of size 64×64, where average charge density $\langle n \rangle = 1, |U| = 4, \beta = \frac{1}{k_B T} = 200$. Since the system is homogeneous, $\Delta_i$ is uniform in the real space, which is consistent. The correlation function $\Lambda_{xx}(q_y, \omega_n = 0)$ and kinetic density $\langle -K_x \rangle$ is showed in Figure. 3. And we demand $q_y$ goes to a small value($q_y \to 0$), using Eq. 4.12, in this case, we get a finite $\rho_s = \frac{D_s}{\pi e^2} = 0.6600$, which indicates this system is a superconductor. And the finite $\Delta_i$ in Figure. 2 agrees with this result. In figure 4, we evaluate the critical temperature $T_c$ for a 2-D 22×22 lattice. It is noticed that the superfluid density $\rho_s$ and the order parameter $\Delta$ goes to zero at the same temperature, which indicates our result is consistent.

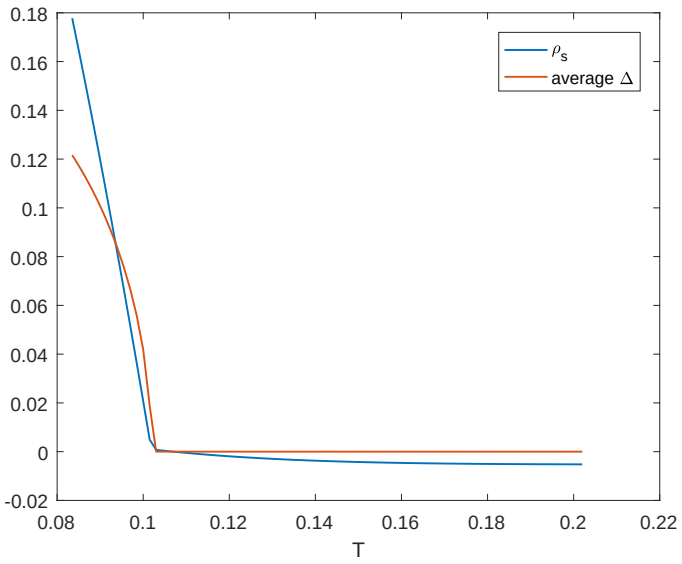
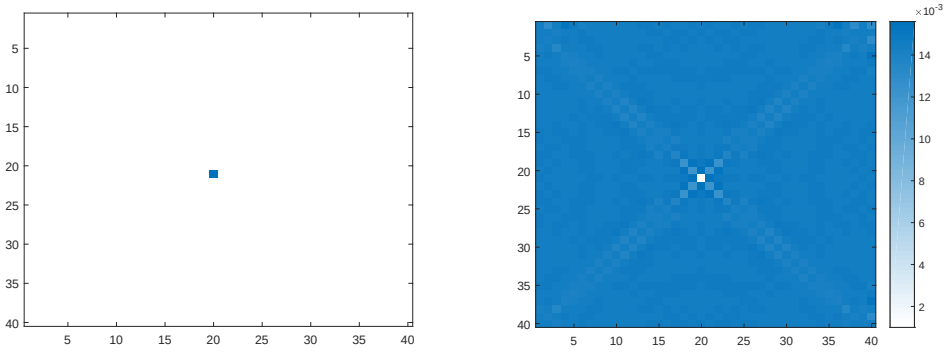



Figure 4: $\rho_s$ vs $T$(blue curve) and average $\Delta$ vs $T$(red curve) for a 2-D 22×22 clean lattice. Here average charge density $\langle n \rangle = 0.85, |U| = 0.8$

### 4.3.2 Inhomogeneous case

The following paragraphs will demonstrate the effect of disorder. When we consider about an inhomogeneous system, $k$ is no longer a good quantum number. We have no choice but use Eq. 4.37 to calculate correlation functions.

**A**. One impurity case; one impurity($V = 5.0$) is placed at the middle of lattice, shown in Figure. 5(a). As shown in Figure. 5(b), $\Delta_i$ has a strong suppression at the impurity sites. However, as seen in Figure. 6, the superfluid density in this case is still a finite number($\rho_s = 0.0594$), which indicates the system is in a superconducting state.



(a) Disorder map (b) $\Delta$ map

Figure 5: Disorder map and self-consistent $\Delta$ map for a 2-D 40×40 lattice with one impurity at the middle, here average charge density $\langle n \rangle = 0.85$, onsite attraction $|U| = 0.8$, disorder strength $V = 5.0$, $\beta = \frac{1}{k_B T} = 113$.

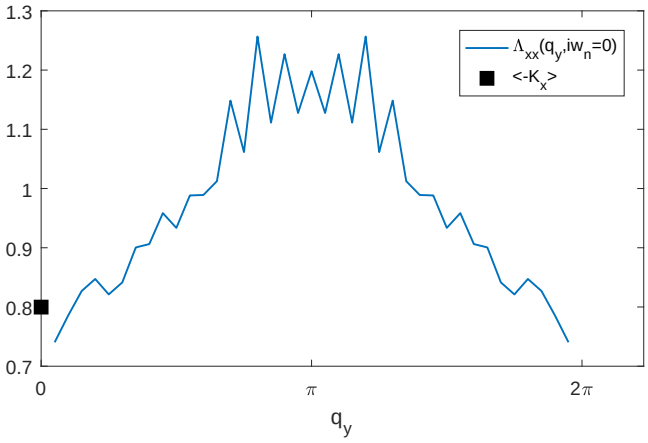



Figure 6: Self-consistent $\Lambda_{xx}(q_y, \omega_n = 0)$ vs $q_y$ for a 2-D 40×40 lattice with one impurity at the middle. Here average charge density $\langle n \rangle = 0.85, |U| = 0.8, \beta = \frac{1}{k_B T} = 113$, while the solid square marks $\langle -K_x \rangle$.

From Eq. 4.12, the first term is the kinetic energy along the $x$ direction divided by the number of lattice sites:

$$\langle -K_x \rangle = \frac{1}{N} \sum_i -\langle K_x^i \rangle. \tag{4.59}$$

Using Eq. 4.14, one has the local kinetic energy in the form:

$$\langle -K_x^i \rangle = \langle t \sum_{n,\sigma} [(u_{i+x\sigma}^{n*} u_{i\sigma}^n + u_{i\sigma}^{n*} u_{i+x\sigma}^n) f(E_{n\sigma}) + \bar{\sigma}^2 (v_{i+x\sigma}^{n*} v_{i\sigma}^n + v_{i\sigma}^{n*} v_{i+x\sigma}^n) f(-E_{n\bar{\sigma}})] \rangle. \quad (4.60)$$

From Eq. 4.12, the second term is the current-current correlation function with a double sum over lattice sites

$$\Lambda_{xx}(q_x = 0, q_y, i\omega_n = 0) = \frac{1}{N} \sum_{ij\sigma} e^{iq_y(r_j - r_i)} \Lambda_{xx}(i, j, i\omega_n = 0), \quad (4.61)$$

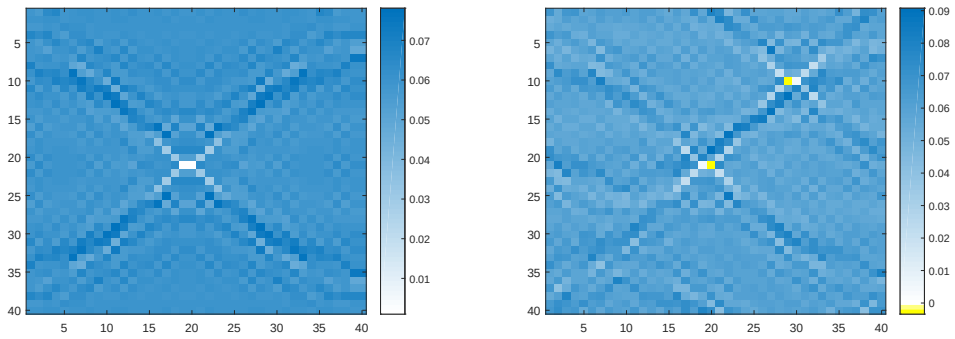
with $\Lambda_{xx}(i, j, i\omega_n = 0)$ shown in Eq. 4.36. The local current current correlation function can be written as:

$$\Lambda_{xx}^i(q_x = 0, q_y, i\omega_n = 0) = \sum_{j\sigma} e^{iq_y(r_j - r_i)} \Lambda_{xx}(i, j, i\omega_n = 0). \quad (4.62)$$

Then we can calculate the local superfluid density:

$$\rho_s^i = \langle -K_x^i \rangle - \Lambda_{xx}^i(q_x = 0, q_y, i\omega_n = 0). \quad (4.63)$$

The local superfluid density for the one impurity case is shown in Figure. 7(a). It is noticed that there is a suppression at the lattice site where impurity is located.

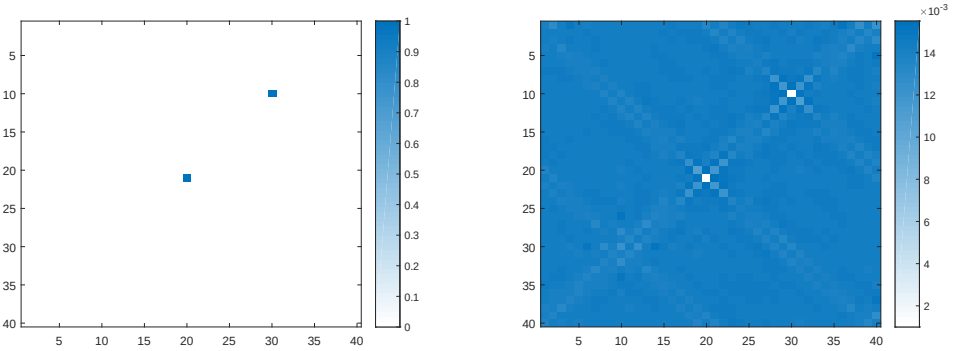



(a) Local superfluid density map of one impurity (b) Local superfluid density map of two impurities

Figure 7: Local superfluid density map for a 2-D 40×40 lattice, (a) is for one impurity and (b) is for two impurities, here average charge density $\langle n \rangle = 0.85$, onsite attraction $|U| = 0.8$, disorder strength $V = 5.0$, $\beta = \frac{1}{k_B T} = 113$.

**B**. Two impurities case; two impurities are placed in lattice as shown in Figure. 8(a). As seen in Figure. 8(b), $\Delta_i$ drops dramatically at the lattice site where impurites

are located. And we find similar curve and the superfluid density $\rho_s = 0.590$, shown by Figure. 9. The local superfluid density for two impurites case is shown in Figure. 7(b). It is noticed that there is a negative value at the lattice site where impurities locates, which means the onsite rigidity is negative and the coherence phase $\phi$ is easy to fluctuate. From Ginzburg-Landau equation, the free energy $F \sim \rho_s | \bigtriangledown \phi|^2 + a|\phi|^2 + b|\phi|^4$. To minimize the free energy, the negative local superfluid density means that the coherence phase $\phi$ does not want to remain as a constant instead to fluctuate strongly.



(a) Disorder map

(b) $\Delta$ map

Figure 8: Disorder map and self-consistent $\Delta$ map for a 2-D 40×40 lattice with two impurities, here average charge density $\langle n \rangle = 0.85$, onsite attraction $|U| = 0.8t$, disorder strength $V = 5.0$, $\beta = \frac{1}{k_B T} = 113$.

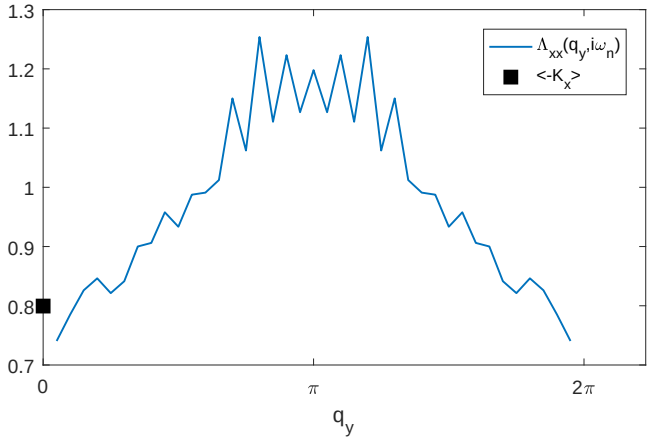
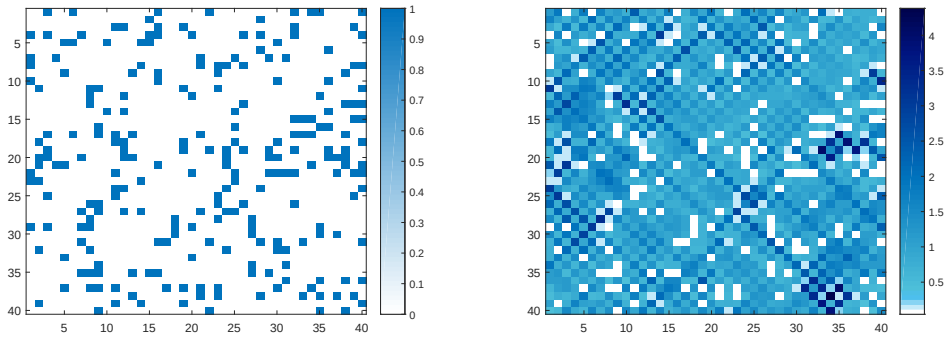



Figure 9: Self-consistent $\Lambda_{xx}(\mathbf{q}_y, \omega_n = 0)$ vs $\mathbf{q}_y$ for a 2-D 40×40 lattice with two impurities. Here average charge density $\langle n \rangle = 0.85$, onsite attraction $|U| = 0.8t$, disorder strength $V = 5.0$, $\beta = \frac{1}{k_B T} = 113$.

**C**. Many-impurities case. We use the same parameters in the numerical calculations as was used by **A** and **B**.( $\langle n \rangle = 0.85$, $|U| = 0.8t$, $V = 5.0$, $\beta = \frac{1}{k_B T} = 113$.). And we produce a $\Delta^0 = 0.0203$ at $T = 0$, and $T_c^0 = 0.0110$ for the clean case. Impurites are distributed randomly on 15% of the lattice sites, shown in Figure. 10(a). In Figure 10(b), $\Delta/\Delta^0$ drops dramatically at the lattice site where impurites are located, which we expect. However in some regions $\Delta/\Delta^0 > 1$, which indicates order parameter enhancement by disorder. Does it means superconductivity is enhanced by disorder?



(a) Disorder map

(b) $\Delta/\Delta^0$ map

Figure 10: Disorder map and self-consistent $\Delta/\Delta^0$ map for a 2-D 40×40 lattice with two impurities, here average charge density $\langle n\rangle = 0.85$, onsite attraction $|U| = 0.8$, disorder strength $V = 5.0$, $\beta = \frac{1}{k_B T} = 113$.

In the following paragraphs, we will demonstrate that the critical temperature of an s-wave superconductor can be enhanced in the presence of impurities. The reason for enhancement is that impurities make the density of states fluctuate, thus at some lattice sites the density of states may enhance. And it is difficult to define the critical temperature. In the homogeneous case, since the order parameter $\Delta$ is uniform, it is easy to define critical temperature when $\Delta$ drops to zero in all sites. However, in the inhomogeneous case, because of the density of states fluctuation, the $\Delta$ does not drop to zero everywhere in the superconductor at the same $T$. Instead, some regions still remain finite $\Delta$ while others drops to zero. Therefore, it is not crystal clear what are the criteria of superconductivity. How do we know whether an inhomogeneous system is a superconductor or not? Even the spatially average $\bar{\Delta}$, shown in Figure. 11, does not easily allow for a definition of the critical temperature $T_c$. In the very dilute disorder case, we dont need to bother with the problem that the order parameter may breaks up into disconnected regions at high temperature. But in the dense disorder situation, this problem need to be considered. Or can we define the critical temperature when all edges of the system are fully connected by finite $\Delta$ regions? But do we need to consider about the Josephson effect? In this paper, we will try to use another way, the superfluid stiffness $D_s$, to define the critical temperature. In Figure. 12, we show the $T$-dependence of real-space maps of $\Delta/\Delta^0$ for 15% disorder system with different impurity strengths $V$( $\langle n\rangle = 0.85$, $|U| = 0.8t$). As seen, for week impurity strength($V = 1.5$), $\Delta$ drops to zero even below $T_c$, nevertheless for strong enough impurity strengths($V = 5.0$), there are

large regions for finite $\Delta$ well above $T_c$. But the question is are they superconductors? Does the superconductivity enhancement by disorder really exist?

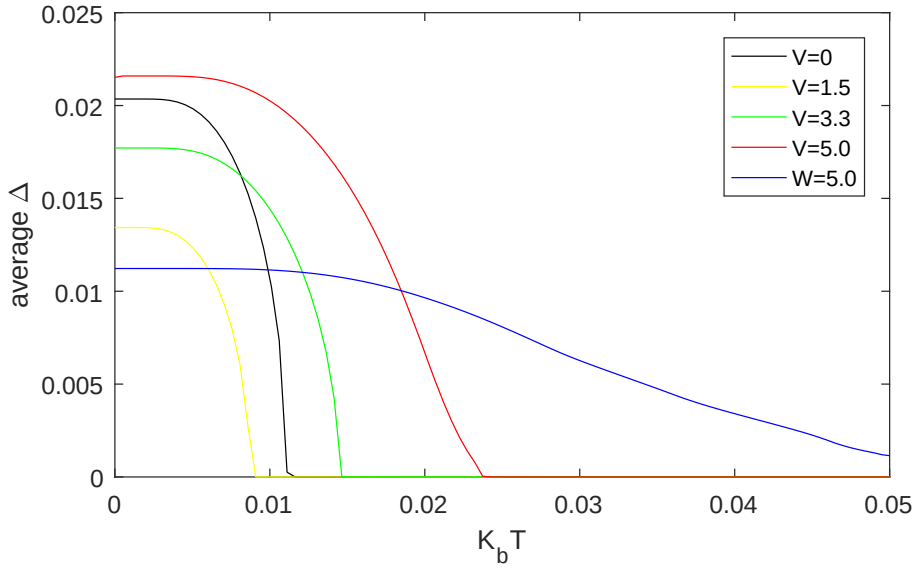



Figure 11: Spatially-averaged superconductor order parameter $\bar{\Delta}$ versus $T$ , and for Andersond disorder with $V_A = [-5, 5]$(blue curve)[1]. The clean case is shown by the black curve.

[1]disorder strength $V$ randomly distributed in [-5,5]

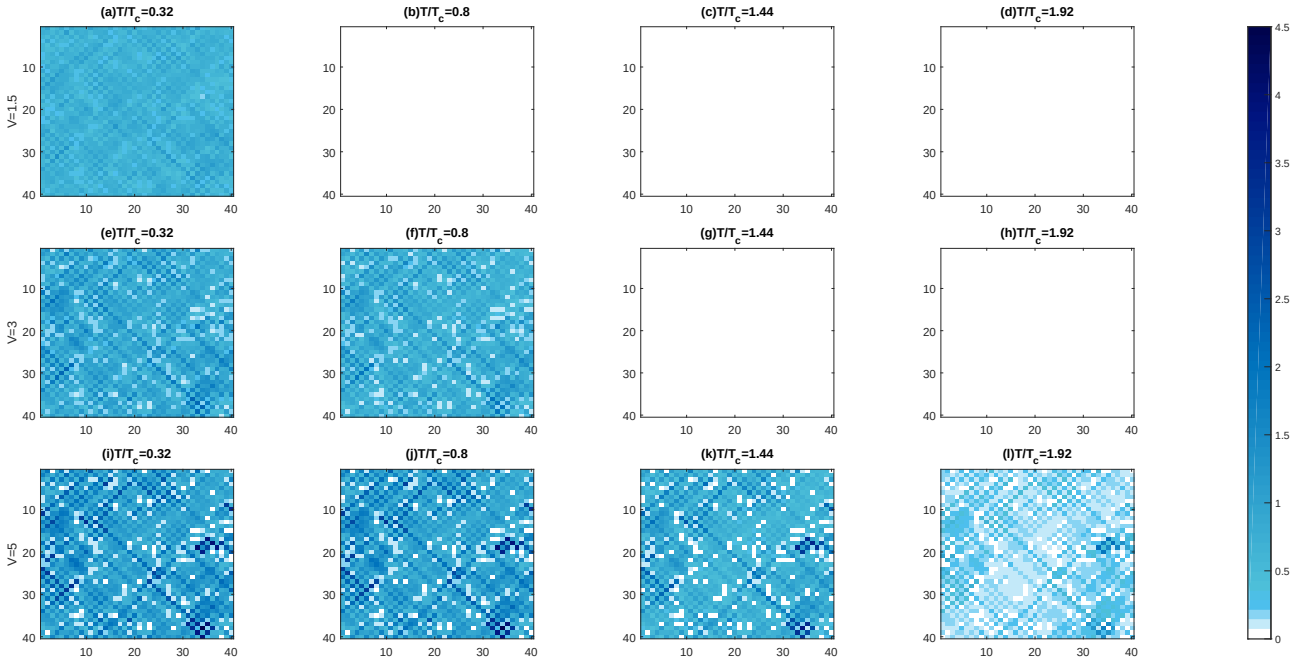
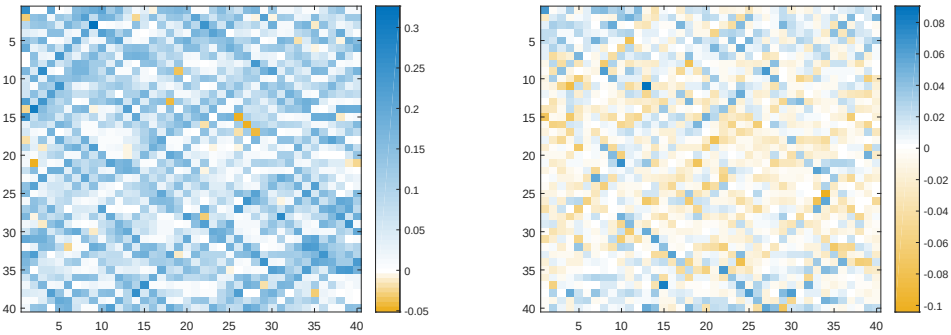



Figure 12: Real-space maps of $\Delta/\Delta^0$ versus $T$(rows) for a 15% disordered system with varing strength $V = 1.5, 3.0, 5.0$ for a conventional s-wave superconductor.



(a) Local superfluid density map of Figure. 12(j)

(b) Local superfluid density map of Figure. 12(g)

Figure 13: Local superfluid density map for a 2-D 40×40 lattice, (a) is for Figure. 12(j)($V = 5.0, T/T_c = 0.8$) and (b) is for 12(g)($V = 3.0, T/T_c = 1.44$), here average charge density $\langle n \rangle = 0.85$, onsite attraction $|U| = 0.8t$, disorder strength $V = 5.0$, $\beta = \frac{1}{k_B T} = 113$.

Using Eq. 4.12, we calculate the superfluid density $\rho_s$ seen in Figure. 14. It can

be noticed that the last two case(Figure.12(k),(l)) indeed have finite superfluid density $\rho_s$ even for temperatures are well above $T_c$. Therefore, this evidence indicates that the superconductivity enhancement by disorder exists. In this way, using the new criteria, superfluid stiffness $D_s$, we prove the superconductivity enhancement by disorder. And the local superfluid density is shown in Figure. 13. Where Figure. 13(a) is the local superfluid density map of Figure. 12(j), also we can see suppressions at the disorder lattice sites. And Figure. 13(b) is the local superfluid density map of Figure. 12(g), which has a big area of negative superfluid density. From Figure. 14(g), we know this is a normal state.

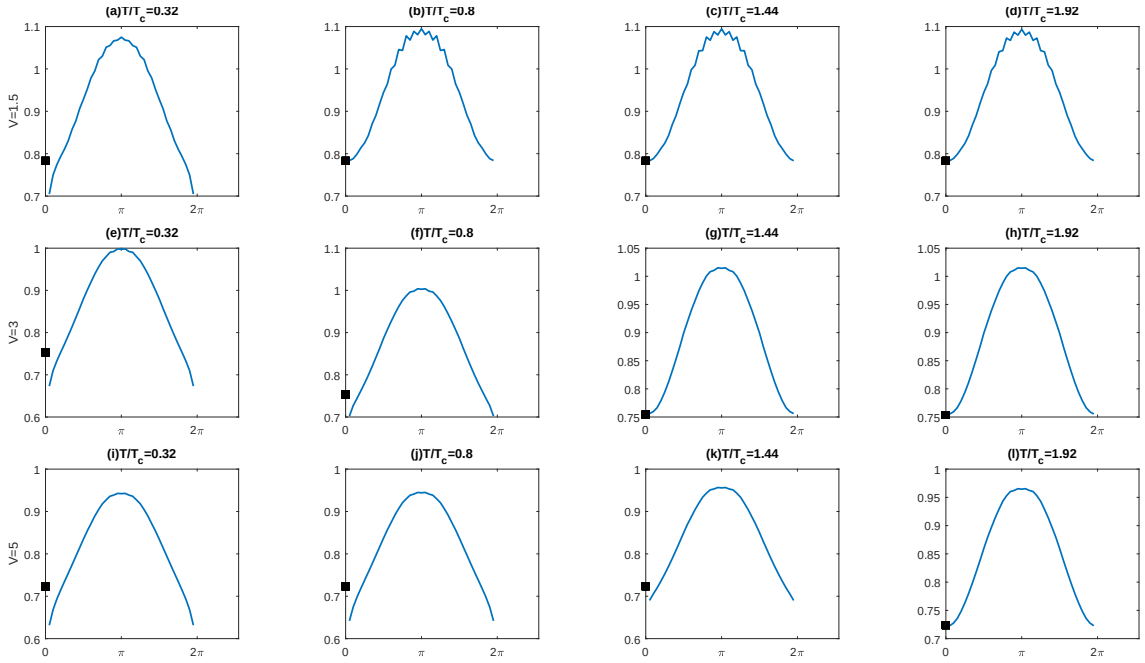



Figure 14: Self-consistent $\Lambda_{xx}(\mathbf{q}_y, \omega_n = 0)$ versus $T$(rows) for a 15% disordered system with varing strength $V = 1.5, 3.0, 5.0$ for a conventional s-wave superconductor.

# 5 d-wave superconductor

In this section, the d-wave superconductor will be discussed. The d-wave superconductor have different properties from the s-wave superconductor. For the d-wave superconductor, the Anderson's therom does not work any more, which means the robustness of superconductivity is weak, even a weak disorder may destroy its superconductivity. This makes the d-wave superconductor mysterious and interesting and studying them is essential to understand high-temperature supercondoctor.

## 5.1 d-wave BdG equations

Comparing to the s-wave superconductor, d-wave superconductor has a different Hamiltonian

$$\begin{aligned} H &= -t\sum_{\langle ij\rangle,\sigma}(c^\dagger_{i\sigma}c_{j\sigma}+H.c.)+\sum_{i,\sigma}(V_i-\mu)n_{i\sigma}-|U|\sum_{\langle ij\rangle}n_{i\uparrow}n_{j\downarrow} \\ &= -t\sum_{\langle ij\rangle,\sigma}(c^\dagger_{i\sigma}c_{j\sigma}+H.c.)+\sum_{i,\sigma}(V_i-\mu)n_{i\sigma}+|U|\sum_{\langle ij\rangle}c^\dagger_{i\uparrow}c^\dagger_{j\downarrow}c_{i\uparrow}c_{j\downarrow} \\ &= -t\sum_{\langle ij\rangle,\sigma}(c^\dagger_{i\sigma}c_{j\sigma}+H.c.)+\sum_{i,\sigma}(V_i-\mu)n_{i\sigma}+\sum_{\langle ij\rangle}[\Delta^*_{ij}c_{i\uparrow}c_{j\downarrow}+c^\dagger_{i\uparrow}c^\dagger_{j\downarrow}\Delta_{ij}], \end{aligned} \tag{5.1}$$

in the last line, we apply mean-field approximation, which means

$$c^\dagger_{i\uparrow}c^\dagger_{j\downarrow}c_{i\uparrow}c_{j\downarrow}\approx\langle c^\dagger_{i\uparrow}c^\dagger_{j\downarrow}\rangle c_{i\uparrow}c_{j\downarrow}+c^\dagger_{i\uparrow}c^\dagger_{j\downarrow}\langle c_{i\uparrow}c_{j\downarrow}\rangle, \tag{5.2}$$

and

$$\Delta_{ij}=|U|\langle c_{i\uparrow}c_{j\downarrow}\rangle. \tag{5.3}$$

The Hamiltonian can be diagonalized by the Bogoliubov transformation

$$\begin{aligned} H &= E_0+\sum_{n\sigma}E_{n\sigma}\gamma^\dagger_{n\sigma}\gamma_{n\sigma}, \\ c^\dagger_{i\uparrow} &= \sum_n(u^*_{ni\uparrow}\gamma^\dagger_{n\uparrow}-v_{ni\uparrow}\gamma_{n\downarrow}), \\ c^\dagger_{i\downarrow} &= \sum_n(u^*_{ni\downarrow}\gamma^\dagger_{n\downarrow}+v_{ni\downarrow}\gamma_{n\uparrow}). \end{aligned} \tag{5.4}$$

Considering the commutator(refer to Appendix **B**), one has

$$\begin{aligned} [H,c_{i\uparrow}] &= t\sum_{\langle j\rangle}c_{j\uparrow}-(V_i-\mu)c_{i\uparrow}-\sum_{\langle j\rangle}\Delta_{ij}c^\dagger_{j\downarrow}, \\ [H,c_{i\downarrow}] &= t\sum_{\langle j\rangle}c_{j\downarrow}-(V_i-\mu)c_{i\downarrow}+\sum_{\langle j\rangle}\Delta_{ij}c^\dagger_{j\uparrow}. \end{aligned} \tag{5.5}$$

Then subsituting Eq. 5.4 into the Hamiltonian Eq. 5.1, one gets

$$\begin{aligned}
[H, c_{i\uparrow}] &= [H, \sum_n (u_{ni\uparrow}\gamma_{n\uparrow} - v^*_{ni\uparrow}\gamma^\dagger_{n\downarrow})] = \sum_n (-E_{n\uparrow}u_{ni\uparrow}\gamma_{n\uparrow} - E_{n\downarrow}v^*_{ni\uparrow}\gamma^\dagger_{n\downarrow}), \\
[H, c_{i\downarrow}] &= [H, \sum_n (u_{ni\downarrow}\gamma_{n\downarrow} + v^*_{ni\downarrow}\gamma^\dagger_{n\uparrow})] = \sum_n (-E_{n\downarrow}u_{ni\downarrow}\gamma_{n\downarrow} + E_{n\uparrow}v^*_{ni\downarrow}\gamma^\dagger_{n\uparrow}).
\end{aligned} \tag{5.6}$$

Here $\gamma$ and $\gamma^\dagger$ are quasiparticle operators, which are linear combinations of the original $c$ operator. As well as we only care about the excitation above the superconducting ground state, thus the summation is over positive eigenvalues only($E_{n\sigma} > 0$).

Demanding the commutators in Eq. 5.5 and Eq. 5.6 to be equal, one can obtain the Bogoliubov-de Gennes equations

$$\begin{aligned}
E_{n\uparrow}u_{ni\uparrow} &= -t\sum_{\langle j\rangle} u_{nj\uparrow} + (V_i - \mu)u_{ni\uparrow} + \sum_{\langle j\rangle}\Delta_{ij}v_{nj\downarrow}, \\
E_{n\downarrow}v^*_{ni\uparrow} &= \quad t\sum_{\langle j\rangle} v^*_{nj\uparrow} - (V_i - \mu)v^*_{ni\uparrow} + \sum_{\langle j\rangle}\Delta_{ij}u^*_{nj\downarrow}, \\
E_{n\downarrow}u_{ni\downarrow} &= -t\sum_{\langle j\rangle} u_{nj\downarrow} + (V_i - \mu)u_{ni\downarrow} + \sum_{\langle j\rangle}\Delta_{ij}v_{nj\uparrow}, \\
E_{n\uparrow}v^*_{ni\downarrow} &= \quad t\sum_{\langle j\rangle} v^*_{nj\downarrow} - (V_i - \mu)v^*_{ni\downarrow} + \sum_{\langle j\rangle}\Delta_{ij}u^*_{nj\uparrow},
\end{aligned} \tag{5.7}$$

these four formula can be written in matrix form:

$$\begin{pmatrix} \hat{K} & \hat{\Delta}_{ij} \\ \hat{\Delta}^*_{ij} & -\hat{K}^* \end{pmatrix} \begin{pmatrix} u_{ni\uparrow} \\ v_{ni\downarrow} \end{pmatrix} = E_{n\uparrow} \begin{pmatrix} u_{ni\uparrow} \\ v_{ni\downarrow} \end{pmatrix}, \tag{5.8}$$

$$\begin{pmatrix} \hat{K} & \hat{\Delta}_{ij} \\ \hat{\Delta}^*_{ij} & -\hat{K}^* \end{pmatrix} \begin{pmatrix} u_{ni\downarrow} \\ v_{ni\uparrow} \end{pmatrix} = E_{n\downarrow} \begin{pmatrix} u_{ni\downarrow} \\ v_{ni\uparrow} \end{pmatrix}. \tag{5.9}$$

Where $\hat{K}u_{ni\sigma} = -t\sum_{<j>} u_{nj\sigma} + (V_i - \mu)u_{ni\sigma}$ and $\hat{\Delta}_{ij}u_{ni\sigma} = \sum_{\langle j\rangle}\Delta_{ij}u_{nj\sigma}$, and similarly for $v_{ni\sigma}$. For the same reason we argued in section 2, it is only necessary to solve one of the Eqs. 5.8 and 5.9, thus the spin index can be suppressed. And we only want to consider the excitation eigenvalues $E_n \geq 0$.

The self-consistency conditions are given by

$$\begin{aligned}
\Delta_{ij} &= |U|\langle c_{i\uparrow}c_{j\downarrow}\rangle \\
&= |U|\langle \sum_n (u_{ni}\gamma_{n\uparrow} - v^*_{ni}\gamma^\dagger_{n\downarrow}) \times \sum_{n'} (u_{n'j}\gamma_{n'\downarrow} + v^*_{n'j}\gamma^\dagger_{n'\uparrow})\rangle \\
&= |U|\sum_n u_{ni}v^*_{nj}(1 - f(E_n)) - u_{nj}v^*_{ni}f(E_n)
\end{aligned} \tag{5.10}$$

$$\begin{aligned}\langle n_i\rangle &= \sum_\sigma \langle c^\dagger_{i\sigma} c_{i\sigma}\rangle = \sum_{n\sigma} (u^*_{ni} u_{ni} \gamma^\dagger_{n\sigma}\gamma_{n\sigma} + v^*_{ni} v_{ni}\gamma_{n\bar{\sigma}}\gamma^\dagger_{n\bar{\sigma}}) \\ &= 2\sum_n u^2_{ni} f(E_n) + v^2_{ni}(1 - f(E_n)).\end{aligned} \tag{5.11}$$

Here the summation is over positive eigenvalues only. In this paper, we will discuss $d_{x^2-y^2}$ superconductor, which means $\Delta_{i,i+\hat{x}} = -\Delta_{i,i+\hat{y}}$. Then we guess an initial set of order parameter $\{\Delta_i\}$ and an initial chemical potential $\mu$, which is determined by average density $\langle n\rangle$. And solve the Bogoliubov-de Gennes equations by a iteration process which was discussed in section 2.

## 5.2 d-wave superfluid stiffness

The formula of d-wave superfluid stiffness is same as s-wave superfluid stiffness, which is evaluated in section 3. In following paragraphs, we will demonstrate some numerical results for the d-wave superconductor.

### 5.2.1 Homogeneous case

We simulate a a 2-D 22×22 clean lattice. Because the system is homogeneous, the order parameter$\Delta$ is spatial isotrope. The local $d_{x^2-y^2}$ wave average order parameter is defined by $\bar{\Delta}_i = (\Delta_{i,i+\hat{x}} + \Delta_{i,i-\hat{x}} - \Delta_{i,i+\hat{y}} - \Delta_{i,i-\hat{y}})/4$. Then the average order parameter $\bar{\Delta} = \sum_i \Delta_i$. As shown in Figure. 15, $\bar{\Delta}$ and $\rho_s$ goes to zero at the same point, the critical temperture is $T_c = 0.0955$.

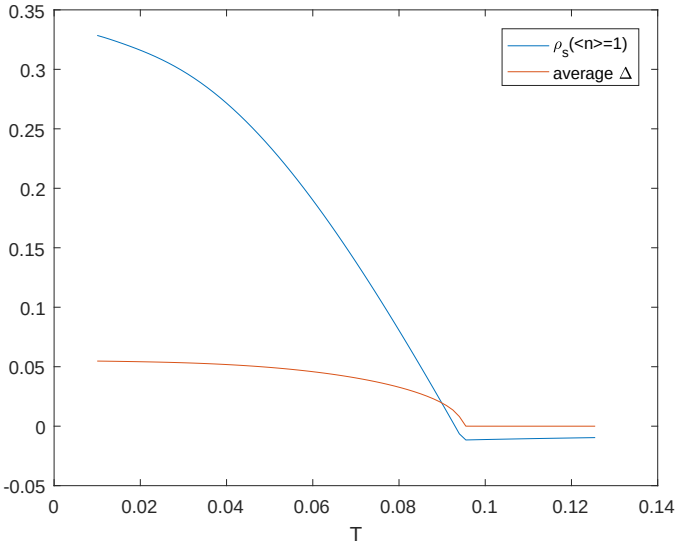



Figure 15: $\rho_s$ vs $T$(blue curve) and average $\Delta$ vs $T$(red curve) for a 2-D 22×22 clean lattice. Here average charge density $\langle n\rangle = 1, |U| = 0.8$

Using Eqs. 4.16 and 4.57 , the homogeneous superfluid density can be calculated. See in Figure. 16, when $T \to 0$, we have $\Lambda_{xx}(q_y, i\omega_n = 0)$ for a 2-D 64×64 clean lattice(blue curve) and $\langle -K_x\rangle$(solid square). Here average charge density $\langle n\rangle = 1, |U| = 4$, $T = 0.001$. We can obtain a finite superfluid density $\rho_s$, which indicates it is a superconductor.

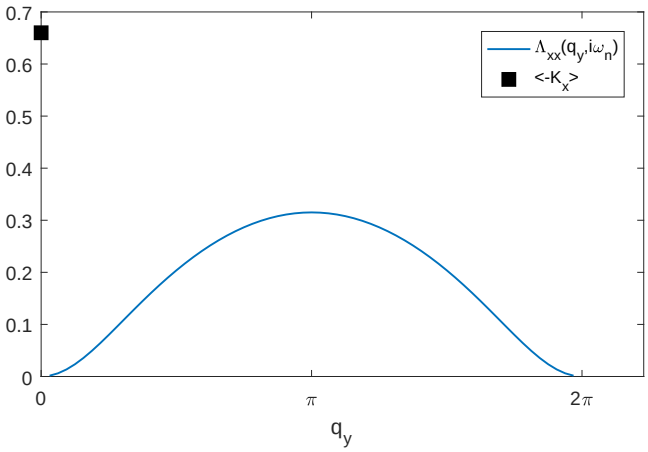
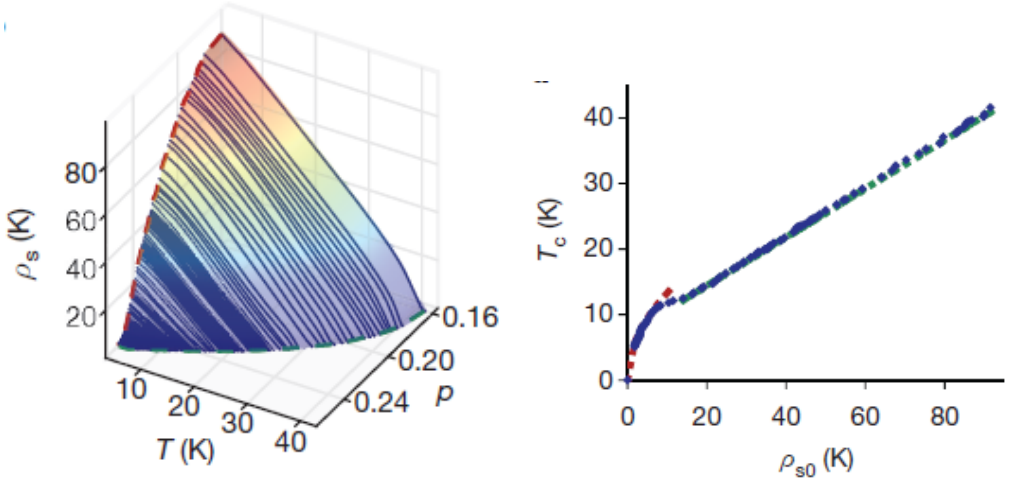



Figure 16: $\Lambda_{xx}(q_y, i\omega_n = 0)$ for a 2-D 64×64 clean lattice. Here average charge density $\langle n \rangle = 1, |U| = 4$, while the solid square marks $\langle -K_x \rangle$.

### 5.2.2 Inhomogeneous case

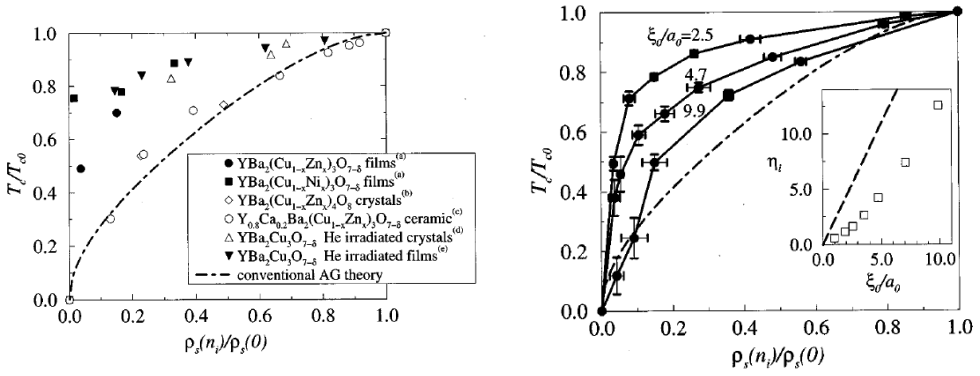
Recently, an experiment measured the superfluid density of a finely spaced set of high-quality epitaxial grown films of overdoped $La_{2-x}Sr_xCuO_4$ by Božović *et al* [9]. They showed that the superfluid density $\rho_s$ and the superconducting critical temperture $T_c$ approached zero together as a function of doping, shown in Figure. 17(a). This contradicts BCS theory, which predicts that the $T = 0$ superfluid density should be the carrier density independ of $T_c$ in a clean system. In a dirty superconductor, the superfluid density depends on $T_c$. However, in the lowest temperture, the $T$ dependence of the penetration depth reduces to a small value, which indicates that the sample is largely free of disorder. Under this assumption, the superfluid density $\rho_s$ should remain $T_c$ independent, the data shown in Figure 17(a) is inconsistent with the BCS theory.




(a) (b)

Figure 17: (a), superfluid density data measured on epitaxial grown $La_{2-x}Sr_xCuO_4$ thin films by Božović *et al.* (b), The dependence of $T_c$ on $\rho_{s0} = \rho_s(T \to 0)$ by Božović *et al.* The experiment data are represented by the blue diamonds; the green dashed line is the fit to $T_c = T_0 + \alpha\rho_s$ for $\rho_s > 15K$ and the red dashed line is the fit to $T_c = \gamma\sqrt{\rho_{s0}}$ for $\rho_{s0} < 12K$

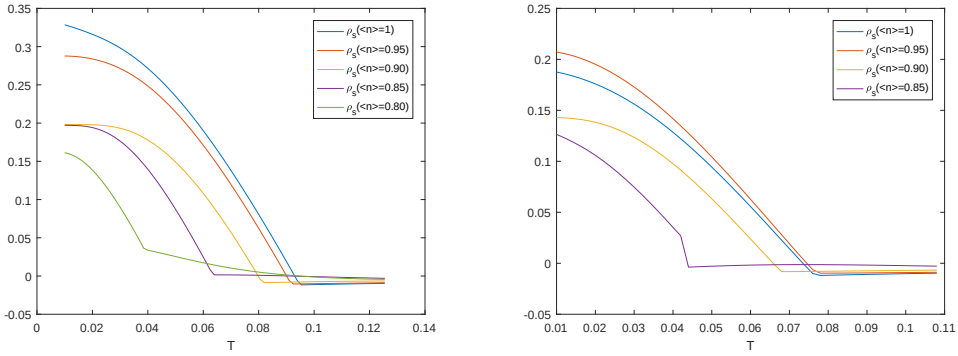
In Figure. 17(b), they show the scaling $T_c(\rho_{s0})$(The subscript 0 refers to the $T_0 \to 0$ limit). For $\rho_s > 15K$, they fit their data to a linear curve $T_c = T_0 + \alpha\rho_s$, and for $\rho_{s0} < 12K$, the curve fits closely to $T_c = \gamma\sqrt{\rho_{s0}}$. From their data and Homes' data [10], they argue that the scaling relation between $\rho_s$ and $T_c$ should be quadratic, the linear curve should not be shown by using BCS theory. Franz also got a quadratic relation instead linear relation by using BdG equations [11], shown in Figure 18.




(a) (b)

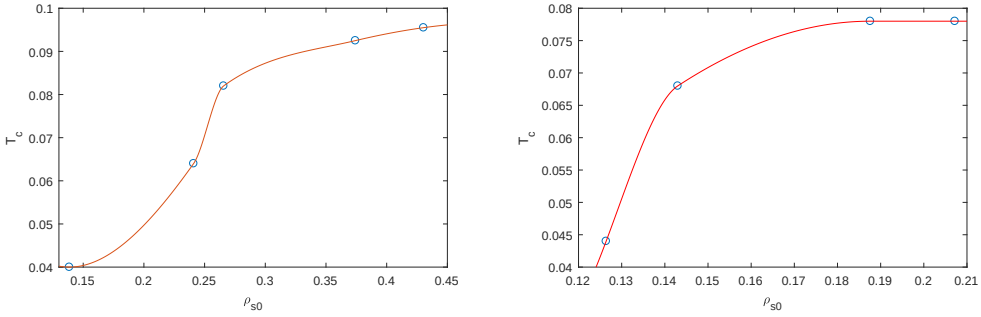
Figure 18: (a), critical temperture versus superfluid density from Franz's paper [11]. Dashed line is the theoretical curve for clean case. (b)critical temperture versus superfluid density [11] for a 2D 22×22 10% disorder system($V = -100$) and $|U| = (0.80, 1.05, 1.40)$ for coherence length $\xi = (9.9, 4.7, 2.5)$.

In order to examine this strange phenomenon, we use BdG equations to evaluate a 2-D d-wave superfluid density with varing charge density $\langle n \rangle$. We simulate a 2-D 22×22 lattice with 5% disorder(disorder strength $V = 1.5$). The superfluid density $\rho_s$ versus $T$ curve is shown in Figure 19(b). We also calculate curves for for a 2-D 22×22 clean lattice, shown in Figure. 19(a). And a critical temperture versus superfluid density curve is seen in Figure. 20(a) for clean case and Figure. 20(b) for disorder case. See in Figure. 20(a), the scaling relation in our calculation is not quadratic, we have an odd step like curve in the middle, and in Figure. 19(a), which is inconsistent with Franz' analysis(shown in Figure. 18(a)). It is noticed that the curve of $\rho_s(\langle n \rangle = 0.90$(orange) have a almost same $\rho_{s0}$ as the curve of $\rho_s(\langle n \rangle = 0.85$(purple), but have a large difference of $T_c$, which makes the step like curve appear. Since lack of time, we can not provide more data to discuss, thus we can not make a certain conclusion. But we would study the data carefully, get more data between $\langle n \rangle = [0.85, 0.90]$, simulate a bigger system, and try to fix the problem we concern above.




(a) (b)

Figure 19: (a), a 2-D 22×22 d-wave superfluid density with varing charge density $\langle n \rangle$ for avclean system. (b)a 2-D 22×22 d-wave superfluid density with varing charge density $\langle n \rangle$ for a 5% disorder system.




(a) (b)

Figure 20: (a), critical temperture versus superfluid density for a 2-D 22×22 clean lattice. (b)critical temperture versus superfluid density for a 2D 22×22 5% disorder system.

# 6 Conclusion and outlook

In this thesis, we review the background of tight-binding model and BCS theory, and by using BdG equations we study inhomogeneous BCS theory. Then a improtant physical quality, superfluid stiffness $D_s$, is introduced. Applying Bogoliubov transformation, we deduce the formula of superfluid stiffness step by step. Subsequently, we point out the criteria of superconducting by calculating superfluid stiffness in a s-wave 40×40 system, which prove that the $T_c$ enhancement by disorder exist. Also we discuss the local superfluid density, we find out in normal state some area have a negative local

superfluid density, which is not fully understood. Finally, a d-wave supercondoctor is concerned, first, we present the derivation of d-wave BdG equations, and consider about the puzzling experiment data presented by Božović *et al*. Since lack of time, our data is not convinced enough to make a certain conclusion. In the future, we are going to consider the deeper meaning of local superfluid density, the crystal clear definition of local superfluid density. And we will put effort to resolve the discrepancy found in the d-wave case.

## Acknowledgement

First and foremost, I would like to thank Brian Møller Andersen for significant guidance through out this project. And I would also like to thank Panagiotis Kotetes for technical discussion and Kristofer Bjornsson for computing assistance. Lastly, I thank my family and all my friends for their encouragement and their concerns.

# A Appendix A : Cooper pair

In this section the analytical derivation of the superconducting order parameter is presented. From Eq. 2.6

$$(2\xi - \Delta)\psi(k) = |U|N(0)\int_0^{\hbar\omega_D} d\xi'\psi(k'). \tag{A.1}$$

Then divide both sides by $2\xi - \Delta$, one gets

$$\psi(k) = \frac{|U|N(0)\int_0^{\hbar\omega_D} d\xi'\psi(k')}{(2\xi - \Delta)}. \tag{A.2}$$

And intergrate this on both sides with respect to $\xi$, one has

$$\int_0^{\hbar\omega_D} d\xi\psi(k) = \int_0^{\hbar\omega_D} d\xi\frac{|U|N(0)\int_0^{\hbar\omega_D} d\xi'\psi(k')}{(2\xi - \Delta)}. \tag{A.3}$$

It is noticed that $\int_0^{\hbar\omega_D} d\xi\psi(k)$ is just some number. We can divide it out on both sides to get

$$1 = \int_0^{\hbar\omega_D} d\xi\frac{|U|N(0)}{(2\xi - \Delta)} = \frac{|U|N(0)}{2}\ln(\frac{2\hbar\omega_D - \Delta}{-\Delta}). \tag{A.4}$$

In the so-called week-coupling limit where $VN(0) \ll 1$,

$$\begin{aligned} 1 &= \frac{|U|N(0)}{2}\ln(\frac{2\hbar\omega_D - \Delta}{-\Delta}) \\ -\frac{2}{|U|N(0)} &= \ln(\frac{-\Delta}{2\hbar\omega_D - \Delta}) \\ e^{-\frac{2}{|U|N(0)}} &= \frac{-\Delta}{2\hbar\omega_D - \Delta} \\ \Delta &= (-2\hbar\omega_D + \Delta)e^{-\frac{2}{|U|N(0)}} \\ \Delta &= -2\hbar\omega_D e^{-\frac{2}{|U|N(0)}}. \end{aligned} \tag{A.5}$$

Here we neglect the second at the last line. Then we are going to discuss a little bit about coherence length $\xi_0$ of Cooper pair. The coherence length shows the rough spatial extent of a Cooper pair. From Heisenberg's uncertainty principle, one has

$$\xi_0\delta k \sim 1, \tag{A.6}$$

and

$$\Delta \sim \frac{\hbar^2}{m}k_F\delta k \sim \hbar v_F\delta k. \tag{A.7}$$

Thus

$$\xi_0 \sim \frac{\hbar v_F}{\Delta}. \tag{A.8}$$

# B Appendix B: Commutators

In this section the details of the commutators in Eq. 3.11 are discussed. From Eq. 3.4, the Hamiltonian can be written in

$$H = -t \sum_{\langle ij \rangle, \sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + H.c.) + \sum_{i,\sigma} (V_i - \mu) n_{i\sigma} + \sum_{i} [\Delta^{*}_{i} c_{i\uparrow} c_{i\downarrow} + c^{\dagger}_{i\uparrow} c^{\dagger}_{i\downarrow} \Delta_i]. \tag{B.1}$$

Consider the first item in Eq. $(B.1)$, we have the commutator:

$$\begin{aligned} & -t \sum_{\langle ij \rangle, \sigma} [c^{\dagger}_{i\sigma} c_{j\sigma} + H.c., c_{i\uparrow}] \\ & = -t \sum_{\langle j \rangle, \sigma} (c^{\dagger}_{i\sigma} \{c_{j\sigma}, c_{i\uparrow}\} - \{c^{\dagger}_{i\sigma}, c_{i\uparrow}\} c_{j\sigma}) \\ & = t \sum_{\langle j \rangle, \sigma} \delta_{\sigma\uparrow} c_{j\sigma} \\ & = t \sum_{\langle j \rangle} c_{j\uparrow}, \end{aligned} \tag{B.2}$$

here

$$\delta_{\sigma\sigma'} = \begin{cases} 1 & \text{for} \quad \sigma = \sigma' \\ 0 & \quad \text{otherwise} \end{cases}. \tag{B.3}$$

Similarly

$$-t \sum_{\langle ij \rangle, \sigma} [c^{\dagger}_{i\sigma} c_{j\sigma} + H.c., c_{i\downarrow}] = t \sum_{\langle j \rangle} c_{j\downarrow}. \tag{B.4}$$

The second term in the Hamiltonian evaluates

$$\begin{aligned} & \sum_{i,\sigma} (V_i - \mu) [c^{\dagger}_{i\sigma} c_{i\sigma}, c_{i\uparrow}] \\ & = \sum_{\sigma} (V_i - \mu) (c^{\dagger}_{i\sigma} \{c_{i\sigma}, c_{i\uparrow}\} - \{c^{\dagger}_{i\sigma}, c_{i\uparrow}\} c_{i\sigma}) \\ & = - \sum_{\sigma} (V_i - \mu) \delta_{\sigma\uparrow} c_{i\sigma} \\ & = -(V_i - \mu) c_{i\uparrow}, \end{aligned} \tag{B.5}$$

Similarly

$$\sum_{i,\sigma} (V_i - \mu) [c^{\dagger}_{i\sigma} c_{i\sigma}, c_{i\downarrow}] = -(V_i - \mu) c_{i\downarrow} \tag{B.6}$$

For the last term in the Hamiltonian yields

$$\begin{aligned}
&\sum_{i,\sigma}(\Delta_i^*[c_{i\downarrow}c_{i\uparrow}, c_{i\uparrow}] + \Delta_i[c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger, c_{i\uparrow}] \\
&= \sum_{i,\sigma}(\Delta_i^*(c_{i\downarrow}\{c_{i\uparrow}, c_{i\uparrow}\} - \{c_{i\downarrow}, c_{i\uparrow}\}c_{i\uparrow}) + \Delta_i(c_{i\uparrow}^\dagger\{c_{i\downarrow}^\dagger, c_{i\uparrow}\} - \{c_{i\uparrow}^\dagger, c_{i\uparrow}\}c_{i\downarrow}^\dagger)) \\
&= -\Delta_i c_{i\downarrow}^\dagger.
\end{aligned} \tag{B.7}$$

And:

$$\sum_{i,\sigma}(\Delta_i^*[c_{i\downarrow}c_{i\uparrow}, c_{i\downarrow}] + \Delta_i[c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger, c_{i\downarrow}] = \Delta_i c_{i\uparrow}^\dagger. \tag{B.8}$$

By combining all expressions above one has Eq. 3.11

$$\begin{aligned}
[H, c_{i\uparrow}] &= t\sum_{\langle j\rangle} c_{j\uparrow} - (V_i - \mu)c_{i\uparrow} - \Delta_i c_{i\downarrow}^\dagger, \\
[H, c_{i\downarrow}] &= t\sum_{\langle j\rangle} c_{j\downarrow} - (V_i - \mu)c_{i\downarrow} + \Delta_i c_{i\uparrow}^\dagger.
\end{aligned} \tag{B.9}$$

Similarly, we can easily get the expression for d-wave(Eq. 5.5)

# C Appendix C: The general Kubo formula

Consider a quantum system described by the time independent Hamiltonian $H_0$ in thermodynamic equilibrium. An expectation value of a physical quantity, described by the operator $A$, can be evaluated as

$$\langle A\rangle = \frac{1}{Z_0}\sum_n \langle n|A|n\rangle e^{-\beta E_n}, \tag{C.1}$$

here $|n\rangle$ is a complete set of eigenstates $\{|n\rangle\}$ of the Hamiltonian $H_0$ with eigenenergies $\{E_n\}$. Suppose now that at some time, an external time dependence is applied to the system. Then the whole Hamiltonian can be rewritten as

$$H(t) = H_0 + H'(t). \tag{C.2}$$

The system is described by the same distribution of eigenstates but the states are now time-dependent and they have evolved according to the new Hamiltonian. we can obtain a new complete set of eigenstates $\{|n(t)\rangle\}$ of the Hamiltonian $H$. Then the time-dependent expection value of the operator $A$ can be shown as:

$$\langle A(t)\rangle = \frac{1}{Z_0}\sum_n \langle n(t)|A|n(t)\rangle e^{-\beta E_n}. \tag{C.3}$$

In the interation picture, we have

$$|n(t)\rangle = e^{-iH_0 t}|\hat{n}(t)\rangle = e^{iH_0(t-0)}\hat{U}(t,0)|n\rangle, \tag{C.4}$$

with the time-evolution operator $\hat{U}(t,0) = 1 - i\int_o^t dt'\hat{H}'(t')$. Then one obtains the expection value of $A$ up to linear order in the perturbation.

$$\begin{aligned}\langle A(t)\rangle &= \langle A\rangle_0 - i\int_0^t dt' \frac{1}{Z_0}\sum_n e^{-\beta E_n}\langle n|\hat{A}(t)\hat{H}'(t') - \hat{H}'(t')\hat{A}(t)|n\rangle. \\ &= \langle A\rangle_0 - i\int_0^t dt'\langle[\hat{A}(t),\hat{H}'(t')]\rangle_0.\end{aligned} \tag{C.5}$$

The brackets $\langle\rangle_0$ mean an equilibrium average with respect to the Hamiltonian $H_0$. We can rewrite the linear response result as

$$\delta\langle A\rangle(t) = \langle A(t)\rangle - \langle A\rangle_0 = \int_0^\infty dt' C^R_{AH'}(t,t'), \tag{C.6}$$

where the retarded response function is

$$C^R_{AH'}(t,t') = -i\theta(t-t')\langle[\hat{A}(t),\hat{H}'(t')]\rangle_0. \tag{C.7}$$

And if the external perturbation has the form

$$H'_B(t) = Bf(t), \tag{C.8}$$

where $B$ is a time-independent operator and the time-dependent function $f(t)$ is not an operator. The response function $C^R_{AH'_B}(t,t')$ becomes

$$C^R_{AH'_B}(t,t') = C^R_{AB}(t-t')f(t'). \tag{C.9}$$

Insert Eq. C.9 to Eq. C.6, we have

$$\delta\langle A\rangle(t) = \langle A(t)\rangle - \langle A\rangle_0 = \int_0^\infty dt' C^R_{AB}(t-t')f(t'). \tag{C.10}$$

# D Appendix D: Kubo formula in conductivity

In this section we will show the derivation for Eqs. 4.4, 4.12 and 4.13; Consider our system of charged particles, electrons, which is subjected to an external electronmagentic field. We can write down the Hamiltonian;

$$H(t) = H_0 + H'(t), \tag{D.1}$$

$$H'(t) = -e\int dr\rho(\mathbf{r})\phi_{ext}(\mathbf{r},t) + e\int \mathbf{J}(\mathbf{r})A_{ext}(\mathbf{r},t). \tag{D.2}$$

where $H_0$ is kinetic energy, $H'$ is the perturbation term. $\phi_{ext}$ is external potential and $A_{ext}$ vector potential, $\rho(\mathbf{r})$ particles density operator and $\mathbf{J}(\mathbf{r})$ current operator. We can choose a gauge transformation, let $\phi_{ext} = 0$. Then

$$H'(t) = e\int \mathbf{J}(\mathbf{r})A_{ext}(\mathbf{r},t). \tag{D.3}$$

Apply the Kubo formal(Eq. C.10), the linear relation between current and vector potential is

$$\langle \mathbf{J}(\mathbf{r})\rangle(t) = e\int d\mathbf{r}'\int dt'\sum_{\beta} C^R_{\mathbf{J}(\mathbf{r})J(\mathbf{r}')^\beta}(t-t')A^\beta_{ext}(\mathbf{r}',t'). \tag{D.4}$$

Fourier transform it

$$\langle \mathbf{J}(\mathbf{r})\rangle(\omega) = e\int d\mathbf{r}'\sum_{\beta} C^R_{\mathbf{J}(\mathbf{r})J(\mathbf{r}')^\beta}(\omega)A^\beta_{ext}(\mathbf{r}',\omega), \tag{D.5}$$

here the correlation function $C^R_{\mathbf{J}(\mathbf{r})J(\mathbf{r}')^\beta}(\omega) = \int e^{-i\omega t}\langle[\mathbf{J}(\mathbf{r},t), J(\mathbf{r}',t')^\beta]\rangle$ Then the total current operator can be read as

$$\mathbf{J}_{tot}(\mathbf{r},t) = \mathbf{J}(\mathbf{r}) + \mathbf{J}_{ext}(\mathbf{r}) = \mathbf{J}(\mathbf{r}) + \frac{e}{m}A_{ext}(\mathbf{r},t)\rho(\mathbf{r}). \tag{D.6}$$

The expection value $\mathbf{J}^{tot}_e = e\langle \mathbf{J}_{tot}\rangle$, namely

$$\mathbf{J}^{tot}_e(\mathbf{r},\omega) = e^2\sum_{\beta} C^R_{\mathbf{J}(\mathbf{r})J(\mathbf{r}')^\beta}(\omega)A^\beta_{ext}(\mathbf{r}',\omega) + \sum_{\beta}\frac{e^2}{m}A^\beta_{ext}(\mathbf{r},\omega)\rho(\mathbf{r}). \tag{D.7}$$

Fourier transform it,

$$\mathbf{J}^{tot}_e(q,\omega) = e^2\sum_{\beta} C^R_{\mathbf{J}J^\beta}(q,\omega)A^\beta_{ext}(q,\omega) + \sum_{\beta}\frac{e^2}{m}A^\beta_{ext}(q,\omega)\langle\rho(q)\rangle, \tag{D.8}$$

$$\begin{aligned}\mathbf{J}^{tot}_{e,\alpha}(q,\omega) &= e^2\sum_\beta C^R_{J^\alpha J^\beta}(q,\omega)A^\beta_{ext}(q,\omega) + \sum_\beta \frac{e^2}{m}A^\beta_{ext}(q,\omega)\langle\rho(q)\rangle\delta_{\alpha\beta} \\ &= -e^2\sum_\beta(-C^R_{J^\alpha J^\beta}(q,\omega) - \frac{1}{m}\langle\rho(q)\rangle\delta_{\alpha\beta})A^\beta_{ext}(q,\omega),\end{aligned} \tag{D.9}$$

here

$$\delta_{\alpha\beta} = \begin{cases} 1 & \text{for} \quad \alpha = \beta \\ 0 & \quad \text{otherwise} \end{cases}. \tag{D.10}$$

If we substitute $it$ by $\tau$, Eq. D.9 is exactly the same formula as Eq. 4.4. Now from Eqs. 4.4, 4.10 and 4.11, we have

$$\frac{D_s}{\pi e^2}(\delta_{x\beta} - \frac{q_x q_\beta}{q^2})A_\beta(q,\omega) = [\langle -K_x\rangle - \Lambda_{xx}(q, i\omega_n = 0)]A_x(q,\omega), \tag{D.11}$$

if $q_x = 0, q_y \to 0$,

$$\frac{D_s}{\pi e^2}[(\delta_{xx} - \frac{q_x q_x}{q^2})A_x(q,\omega) + (\delta_{xy} - \frac{q_x q_y}{q^2})A_y(q,\omega)] = [\langle -K_x\rangle - \Lambda_{xx}(q, i\omega_n = 0)]A_x(q,\omega), \tag{D.12}$$

$$\frac{D_s}{\pi e^2} = \langle -K_x\rangle - \Lambda_{xx}(q_x = 0, q_y \to 0, i\omega_n = 0). \tag{D.13}$$

If $q_y = 0, q_x \to 0$,

$$\frac{D_s}{\pi e^2}[(\delta_{xx} - \frac{q_x q_x}{q^2})A_x(q,\omega) + (\delta_{xy} - \frac{q_x q_y}{q^2})A_y(q,\omega)] = [\langle -K_x\rangle - \Lambda_{xx}(q, i\omega_n = 0)]A_x(q,\omega), \tag{D.14}$$

$$0 = \langle -K_x\rangle - \Lambda_{xx}(q_y = 0, q_x \to 0, i\omega_n = 0). \tag{D.15}$$

# References


[1] Douglas J Scalapino, Steven R White, and Shoucheng Zhang. Insulator, metal, or superconductor: The criteria. *Physical Review B*, 47(13):7995, 1993.

[2] Maria N Gastiasoro and Brian M Andersen. Enhancing superconductivity by disorder. *arXiv preprint arXiv:1712.02656*, 2017.

[3] Karsten Flensberg Henrik Bruus. *Many-Body Quantum Theory in Condensed Matter Physics*. Oxford University Press 2007, 2011.

[4] Fetter and Walecka. *Quantum Theory of Many-Particle Systems*. Dover Publication, 2003.

[5] Tanmoy Das, Jian-Xin Zhu, and Matthias J Graf. Local suppression of the superfluid density of pucoga 5 by strong onsite disorder. *Physical Review B*, 84(13):134510, 2011.

[6] RT Scalettar, N Trivedi, and C Huscroft. Quantum monte carlo study of the disordered attractive hubbard model. *Physical Review B*, 59(6):4364, 1999.

[7] Amit Ghosal, Mohit Randeria, and Nandini Trivedi. Inhomogeneous pairing in highly disordered s-wave superconductors. *Physical Review B*, 65(1):014501, 2001.

[8] P.W.Anderson. Enhancing superconductivity by disorder. *Phys.Rev.*, 3:325, 1959.

[9] I Božović, X He, J Wu, and AT Bollinger. Dependence of the critical temperature in overdoped copper oxides on superfluid density. *Nature*, 536(7616):309, 2016.

[10] CC Homes, SV Dordevic, M Strongin, DA Bonn, Ruixing Liang, WN Hardy, Seiki Komiya, Yoichi Ando, G Yu, N Kaneko, et al. A universal scaling relation in high-temperature superconductors. *Nature*, 430(6999):539, 2004.

[11] M Franz, C Kallin, AJ Berlinsky, and MI Salkola. Critical temperature and superfluid density suppression in disordered high-t c cuprate superconductors. *Physical Review B*, 56(13):7882, 1997.