UNIVERSITY OF COPENHAGEN
FACULTY OF SCIENCE

Enhancing Superconductivity by Disorder

Written by *Marie Ernø-Møller*

16.01.19

Supervised by *Brian Møller Andersen*

UNIVERSITY OF COPENHAGEN
FACULTY OF SCIENCE

Faculty:	*Faculty of Science*
Institute:	*Niels Bohr Institute*
Author(s):	*Marie Ernø-Møller*
Email:	*bqh285@alumni.ku.dk*
Title:	*Enhancing Superconductivity by Disorder*
Supervisor(s):	*Brian Møller Andersen*
Handed in:	*16.01.19*
Defended:	*23.01.19*

Name: MARIE ERNØ-MØLLER

Signature: Marie Ern

Date: 15.01.19

Abstract

In this thesis an s-wave superconductor using the tight-binding model with nearest and next-nearest neighbour hopping terms on a 2D square lattice is investigated with the purpose of finding the effect of dense disorder on the critical temperature T_c. An introduction to second quantization and the microscopic BCS theory of superconductivity is given. The gap equation has then been solved numerically in momentum space. The Bogouliubov-de Gennes equations are derived and subsequently solved numerically for a 50x50 system with 15% impurity of varying impurity strength. This has been found to establish regions of finite energy gap Δ even for temperatures well above the critical temperature of the system if the impurity potential is strong enough.

Contents

1 Introduction

Superconductivity was discovered in 1911 by Heike Kamerlingh Onnes. The microscopic theory of superconductivity, BCS theory, was proposed in 1957. Ever since then superconductivity has been a very active and broad field of research. An interesting question is what happens to the critical temperature as a result of disorder? Normally this is understood with respect to the Anderson theorem which states that T_c remains unchanged in the presence of impurity. However, this is under the assumption that the impurity is dilute and the order parameter and the density of states are both spatially uniform [1].
In this thesis we will try and reproduce the results of Gastiasoro and Andersen [2] of enhanced T_c by impurities. This is done by examining an s-wave superconductor in the tight-binding model with nearest and next nearest neightbour hopping on a 2D square lattice. Impurities have been added to 15% of the lattice sites and the superconducting gap Δ have then been calculated.

2 Theory

2.1 Second quantization

[1] Second quantization, also known as occupation number representation, is a useful way of describing many-particle systems. As the name suggests, the N-particle basis state simply lists the occupation number of each state:

$$|n_{\nu_1}, n_{\nu_2}, n_{\nu_3}, ...\rangle \quad ; \sum_j n_{\nu_j} = N \tag{1}$$

where n_{ν_j} is the number of particles in state ν_j. The occupation number n_{ν_j} can be any non-negative integer value for bosons and either 0 or 1 for fermions - the latter is due to Pauli's exclusion principle.
Since in this thesis be we will dealing with electrons we will only introduce the operator algebra for fermions. This is done by introducing the fermionic creation operator $\hat{c}^\dagger_{\nu_j}$ and annihilation operator $c_{\nu_j} \equiv (\hat{c}^\dagger_{\nu_j})^\dagger$. The creation operator raises the occupation number in state ν_j by one while the annihilation operator lowers the occupation number by one. When dealing with fermions it is crucial that the antisymmetry is maintained meaning that not only the occupation number but also the order of the states has significance:

$$|..., n_{\nu_j} = 1, ..., n_{\nu_k} = 1, ...\rangle = -|..., n_{\nu_k} = 1, ..., n_{\nu_j} = 1\rangle \tag{2}$$

This means that $\hat{c}^\dagger_{\nu_j}$ and $\hat{c}^\dagger_{\nu_k}$ anti-commute which in turn means that also c_{ν_j} and c_{ν_k} anti-commute. As mentioned, n_{ν_j} can only be 0 or 1 for fermions. This implies

$$c^\dagger_{\nu_j}|1\rangle = c_{\nu_j}|0\rangle = 0 \tag{3}$$

[1] This section is based on chapter 1 of [3]

meaning that both the creation and annihilation operator can act at most twice on a state before the state is annihilated. The operator algebra for the fermionic creation and annihilation operators is defined by these anti-commutation relations:

$$\{c^\dagger_{\nu_j}, c^\dagger_{\nu_k}\} = 0, \;\; \{c_{\nu_j}, c_{\nu_k}\} = 0, \;\; \{c_{\nu_j}, c^\dagger_{\nu_k}\} = \delta_{\nu_j,\nu_k} \tag{4}$$

2.2 Cooper pairs

A precursor to the Bardeen-Cooper-Schrieffer theory was the discovery made by L. N. Cooper that a pair of electrons near the Fermi surface would form a bound state, a so-called Cooper pair.
Consider the case of a filled Fermi sea with two electrons located exactly at the Fermi surface, that is $k = k_F$. Let these two electrons interact via a potential $V(r_1 - r_2)$. The Schrödinger equation is then [5]:

$$\frac{-\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2)\psi(r_1, r_2) + V(r_1 - r_2)\psi(r_1, r_2) = \left(\Delta + \frac{\hbar^2 k_F^2}{m}\right)\psi(r_1, r_2) \tag{5}$$

Choosing the case of $k = -k'$ and rewriting in terms of relative position $r = r_1 - r_2$ gives us:

$$\frac{-\hbar^2}{m}\frac{\partial^2\psi(r)}{\partial r^2} + V(r)\psi(r) = \left(\Delta + \frac{\hbar^2 k_F^2}{2m}\right)\psi(r) \tag{6}$$

Rewrite the Schrödinger equation in momentum space:

$$\frac{\hbar^2 k^2}{m}g(k) + \int \frac{d^3k'}{(2\pi)^3}V(k - k')g(k') = \left(\Delta + \frac{\hbar^2 k_F^2}{2m}\right)g(k) \tag{7}$$

where

$$g(k) = \int d^3r\psi(r)\mathrm{e}^{-ikr} \tag{8}$$

and

$$V(k - k') = \int d^3r\mathrm{e}^{-i(k-k')r}V(r) \tag{9}$$

The potential $V(k-k')$ scatters a pair of electrons with momentum $(k', -k')$ into another pair with momentum $(k, -k)$. It may be approximated in the following way [5]:

$$V(k - k') = \begin{cases} -V & \text{for } \; E_F < \frac{\hbar^2 k^2}{2m}, \frac{\hbar^2 k'^2}{2m} < E_F + \hbar\omega_D \\ 0 & \text{otherwise} \end{cases} \tag{10}$$

With this approximation we now have

$$\left(\frac{\hbar^2(k^2 - k_F^2)}{2m} - \Delta\right)g(k) = V\int \frac{d^3k}{(2\pi)^3}g(k') \tag{11}$$

Letting ξ be the energy measured from the Fermi level and $N(\xi)$ the density of states we can write

$$(2\xi - \Delta)g(k) = V\int_0^{\hbar\omega_D} d\xi' N(\xi')g(k') \tag{12}$$

$$= VN(0)\int_0^{\hbar\omega_D} d\xi' g(k') \tag{13}$$

where the last equality assumes that the density of states does not vary significantly in the interval $[0, \hbar\omega_D]$. Integrating with respect to the energy gives us:

$$\int_0^{\hbar\omega_D} d\xi g(k) = \int_0^{\hbar\omega_D} d\xi \frac{VN(0)\int_0^{\hbar\omega_D} d\xi' g(k')}{2\xi - \Delta} \tag{14}$$

$$1 = \int_0^{\hbar\omega_D} d\xi \frac{VN(0)}{2\xi - \Delta} \tag{15}$$

$$= \frac{VN(0)}{2}\ln\left(\frac{2\hbar\omega_D - \Delta}{-\Delta}\right) \tag{16}$$

In the weak coupling limit where $VN(0) \ll 1$ this can be solved to give [5]:

$$\Delta = -2\hbar\omega_D \exp\left(\frac{-2}{VN(0)}\right) \tag{17}$$

2.3 BCS theory

The microscopic theory of superconductivity was named BSC theory in 1957 after J. Bardeen, L. N. Cooper and J. R. Schrieffer. BCS theory describes how the Fermi surface is unstable against the formation of bound electron pairs, so called Cooper pairs. This is due to an attractive electron-electron interaction for electrons located near the Fermi surface. The interaction is caused by coupling with the phonons of the crystal lattice [4] and is attractive for electrons located within $\hbar\omega_D$ of the Fermi surface (ω_D is the Debye frequency).
The BCS Hamiltonian is given by [5]:

$$H_{BCS} = \sum_{k\sigma} \xi_k c^\dagger_{k\sigma} c_{k\sigma} - V\sum_{kk'} c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} c_{-k'\downarrow} c_{k'\uparrow} \tag{18}$$

The first term with $\xi_k = \frac{\hbar^2 k^2}{2m} - \mu$ counts the single particle energy depending on whether the state is occupied or not. The second term describes the scattering of a Cooper pair with momentum $(k', -k')$ into another pair with momentum $(k, -k)$. V is the amplitude with which the scattering occurs. In order to treat this problem further we perform a mean-field decoupling of the last term:

$$c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} c_{-k'\downarrow} c_{k'\uparrow} \simeq \langle c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}\rangle c_{-k'\downarrow} c_{k'\uparrow} + c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} \langle c_{-k'\downarrow} c_{k'\uparrow}\rangle \tag{19}$$

We can now write the BCS mean-field Hamiltonian as

$$H_{BCS}^{mf} = \sum_{k\sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma} - \sum_k (\Delta c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger + \Delta^* c_{-k\downarrow} c_{k\uparrow}) \tag{20}$$

where $\Delta = V \sum_k \langle c_{-k\downarrow} c_{k\uparrow} \rangle$. Furthermore, it is reasonable to assume that the crystal exhibits inversion symmetry meaning $\xi_k = \xi_{-k}$ and the Hamiltonian can then be written in matrix form as

$$H_{BCS}^{mf} = \sum_k \begin{pmatrix} c_{k\uparrow}^\dagger \\ c_{-k\downarrow} \end{pmatrix} \begin{pmatrix} \xi_k & -\Delta \\ -\Delta^* & -\xi_k \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c_{-k\downarrow}^\dagger \end{pmatrix} \tag{21}$$

The next step is to diagonalize the Hamiltonian. This is done by introducing a unitary transformation U and demanding that this transformation diagonalizes the Hamiltonian, that is

$$U^\dagger \begin{pmatrix} \xi_k & -\Delta \\ -\Delta^* & -\xi_k \end{pmatrix} U = \begin{pmatrix} E_k & 0 \\ 0 & -E_k \end{pmatrix} \tag{22}$$

where

$$U = \begin{pmatrix} u_k & v_k^* \\ -v_k & u_k^* \end{pmatrix} \tag{23}$$

Parametrizing with $u_k = \cos t$ and $v_k = \sin t$ and assuming u_k, v_k are real this set of equations can be solved to give the following results:

$$E_k = \sqrt{\xi_k^2 + |\Delta|^2} \tag{24}$$

$$|u_k|^2 = \frac{1}{2}\left(1 + \frac{\xi_k}{E_k}\right) \text{ and } |v_k|^2 = \frac{1}{2}\left(1 - \frac{\xi_k}{E_k}\right) \tag{25}$$

The physical interpretation of u_k and v_k is that $|u_k|^2$ is the probability of measuring a hole and $|v_k|^2$ is the probability of measuring an electron if the charge of the excitation is measured. [4].
The diagonalization is really just a rotation of the original fermionic creation/annihilation operators to a new set of fermionic creation/annihilation operators in which the Hamiltonian is diagonal, that is:

$$H = \sum_{k\sigma} E_k \gamma_{k\sigma}^\dagger \gamma_{k\sigma} \tag{26}$$

where

$$\begin{pmatrix} \gamma_{k\uparrow} \\ \gamma_{-k\downarrow}^\dagger \end{pmatrix} = U^\dagger \begin{pmatrix} c_{k\uparrow} \\ c_{-k\downarrow}^\dagger \end{pmatrix} \tag{27}$$

The new γ-operators still represent fermions and so their thermal averages are given by

$$\langle \gamma_{k\sigma}^\dagger \gamma_{k'\sigma'} \rangle = f(E_k) \delta_{kk'} \delta_{\sigma\sigma'} \text{ and } \langle \gamma_{k\sigma}^\dagger \gamma_{k'\sigma'}^\dagger \rangle = 0 \tag{28}$$

Subsituting the obtained expressions for u_k, v_k we can write the following expression for the superconducting order parameter Δ:

$$\Delta = V \sum_k u_k v_k^* (1 - 2f(E_k)) \tag{29}$$

$$= V \sum_k \frac{\Delta}{2E_k} \tanh \frac{E_k}{2k_B T} \tag{30}$$

where $f(E_k) = \frac{1}{\exp(E_k/(k_B T))+1}$ This equation is the BCS gap equation which is a self-consistency equation for Δ.

While the above holds for homogeneous systems, things get slightly more complicated when the system is not spatially uniform, e.g. in the presence of impurities. The Hamiltonian describing s-wave superconductivity on a two-dimensional square lattice in the tight-binding model is given by:

$$H = -\sum_{<ij>,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i\sigma} (V_{i\sigma}^{imp} - \mu) c_{i\sigma}^\dagger c_{i\sigma} - V \sum_i c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} = H_1 + H_2 + H_3 \tag{31}$$

where $c_{i\sigma}^\dagger$ and $c_{i\sigma}$ are the fermionic creation and annihilation operators at site i. The first term is the kinetic energy with hopping integral t_{ij}. This includes both nearest neighbour hopping $t_{ij} = t$ and next-nearest neighbour hopping $t_{ij} = t'$. The second term is the onsite energy with impurity strength $V_{i\sigma}^{imp}$ and chemical potential μ. The third term is the BCS term from which the superconductivity arises. Since this term is not quadratic in the creation/annihilation operators we again perform a mean-field decoupling of the term in order to be able to diagonalize the Hamiltonian [5]:

$$H_3^{mf} = -\sum_i \left(\Delta_i^* c_{i\downarrow} c_{i\uparrow} + \Delta_i c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \right) \tag{32}$$

where $\Delta_i = V \langle c_{i\downarrow} c_{i\uparrow} \rangle$ and $\Delta_i^* = V \langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \rangle$. Now that the Hamiltonian can be diagonalized, it is time to introduce the Bogoliubov-de Gennes equations. Solving these equations is equivalent to diagonalizing the Hamiltonian.

2.4 Bogoliubov-de Gennes equations

In the case of a homogeneous system, the transformation that diagonalizes the Hamiltonian is just the Bogoliubov transformation used in the previous section. However, when the system is inhomogeneous, k is no longer a good quantum number and we need a different transformation. This is where the Bogoliubov-de Gennes equations come into play. We start by introducing a more general transformation:

$$c_{i\sigma} = \sum_n \left(u_{ni\sigma} \gamma_{n\sigma} + v_{ni\sigma} \gamma_{i\sigma'}^\dagger \right) \tag{33}$$

We again demand that the Hamiltonian is diagonal in these new operators:

$$H = E_0 + \sum_{n\sigma} \gamma^\dagger_{n\sigma}\gamma_{n\sigma} \tag{34}$$

From the anti-commutation relations in eq. [**?**] we easily get:

$$[H, \gamma_{n\sigma}] = -E_{n\sigma}\gamma_{n\sigma} \tag{35}$$

$$[H, \gamma^\dagger_{n\sigma}] = E_{n\sigma}\gamma^\dagger_{n\sigma} \tag{36}$$

The Bogoliubov-de Gennes equations can now be found by calculating the commutators of the Hamiltonians in eq. 31 and 34 and the fermionic creation/annihilation operators. The γ-operators are still fermionic operators and thus obey eq. 4. The commutators are calculated using the identity

$$[AB, C] = A\{B, C\} - \{A, C\}B \tag{37}$$

. First term:

$$\begin{aligned}
[H_1, c_{i\uparrow}] &= -\sum_{ij,\sigma} t_{ij}[c^\dagger_{i\sigma}c_{j\sigma}, c_{i\uparrow}] \\
&= -\sum_{j\sigma} t_{ij}(c^\dagger_{i\sigma}\{c_{j\sigma}, c_{i\uparrow}\} - \{c^\dagger_{i\sigma}, c_{i\uparrow}\}c_{j\sigma}) \\
&= \sum_{j\sigma} t_{ij}\delta_{\sigma\uparrow}c_{j\sigma} \\
&= \sum_{j} t_{ij}c_{j\uparrow}
\end{aligned} \tag{38}$$

Similarly

$$[H_1, c_{i\downarrow}] = \sum_{j} t_{ij}c_{j\downarrow} \tag{39}$$

Second term:

$$\begin{aligned}
[H_2, c_{i\uparrow}] &= \sum_{i\sigma}(V^{imp}_{i\sigma} - \mu)[c^\dagger_{i\sigma}c_{i\sigma}, c_{i\uparrow}] \\
&= \sum_{\sigma}(V^{imp}_{i\sigma} - \mu)(c^\dagger_{i\sigma}\{c_{i\sigma}, c_{i\uparrow}\} - \{c^\dagger_{i\sigma}, c_{i\uparrow}\}c_{i\sigma}) \\
&= -\sum_{\sigma}(V^{imp}_{i\sigma} - \mu)\delta_{\sigma\uparrow}c_{i\sigma} \\
&= -(V^{imp}_{i\sigma} - \mu)c_{i\uparrow}
\end{aligned} \tag{40}$$

Similarly

$$[H_2, c_{i\downarrow}] = -(V^{imp}_{i\sigma} - \mu)c_{i\downarrow} \tag{41}$$

Third term:

$$\begin{aligned}[H_3, c_{i\uparrow}] &= -\sum_i (\Delta_i^*[c_{i\downarrow}c_{i\uparrow}, c_{i\uparrow}] + \Delta_i[c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger, c_{i\uparrow}]) \\ &= -\big(\Delta_i^*(c_{i\downarrow}\{c_{i\uparrow}, c_{i\uparrow}\} - \{c_{i\downarrow}, c_{i\uparrow}\}) + \Delta_i(c_{i\uparrow}\{c_{i\downarrow}^\dagger, c_{i\uparrow}\} - \{c_{i\uparrow}^\dagger, c_{i\uparrow}\}c_{i\downarrow}^\dagger)\big) \\ &= \Delta_i c_{i\downarrow}^\dagger \end{aligned} \tag{42}$$

And

$$[H_3, c_{i\downarrow}] = -\Delta c_{i\uparrow}^\dagger \tag{43}$$

Combining the terms we now have:

$$\begin{aligned}[H, c_{i\uparrow}] &= [H, \sum_n u_{ni\uparrow}\gamma_{n\uparrow} + v_{ni\uparrow}^*\gamma_{n\downarrow}^\dagger] \\ &= -E_{n\uparrow}u_{ni\uparrow}\gamma_{n\uparrow} + E_{n\downarrow}v_{ni\uparrow}^*\gamma_{n\downarrow}^\dagger \\ &= \sum_j t_{ij}\big(\sum_n u_{nj\uparrow}\gamma_{n\uparrow} + v_{nj\uparrow}^*\gamma_{n\downarrow}^\dagger\big) \\ &- (V_{i\uparrow}^{imp} - \mu)\big(\sum_n u_{ni\uparrow}\gamma_{n\uparrow} + v_{ni\uparrow}^*\gamma_{n\downarrow}^\dagger\big) \\ &+ \Delta_i\big(\sum_n u_{ni\downarrow}^*\gamma_{n\downarrow}^\dagger + v_{ni\downarrow}\gamma_{n\uparrow}\big) \end{aligned} \tag{44}$$

$$\begin{aligned}[H, c_{i\downarrow}] &= [H, \sum_n u_{ni\downarrow}\gamma_{n\downarrow} + v_{ni\downarrow}^*\gamma_{n\uparrow}^\dagger] \\ &= -E_{n\downarrow}u_{ni\downarrow}\gamma_{n\downarrow} + E_{n\uparrow}v_{ni\downarrow}^*\gamma_{n\uparrow}^\dagger \\ &= -\sum_j t_{ij}\big(\sum_n u_{nj\downarrow}\gamma_{n\downarrow} + v_{nj\downarrow}^*\gamma_{n\uparrow}^\dagger\big) \\ &- (V_{i\downarrow}^{imp} - \mu)\big(\sum_n u_{ni\downarrow}\gamma_{n\downarrow} + v_{ni\downarrow}^*\gamma_{n\uparrow}^\dagger\big) \\ &- \Delta_i\big(\sum_n u_{ni\uparrow}^*\gamma_{n\uparrow}^\dagger + v_{ni\uparrow}\gamma_{n\downarrow}\big) \end{aligned} \tag{45}$$

We can now compare coefficients of the γ's to obtain the four Bogoliubov-de Gennes equations:

$$E_{n\uparrow}u_{ni\uparrow} = -\sum_j t_{ij}u_{nj\uparrow} + (V_{i\uparrow}^{imp} - \mu)u_{ni\uparrow} - \Delta_i v_{ni\downarrow} \tag{46}$$

$$E_{n\downarrow}v_{ni\uparrow}^* = \sum_j t_{ij}v_{nj\uparrow}^* - (V_{i\uparrow}^{imp} - \mu)v_{ni\uparrow}^* + \Delta_i u_{ni\downarrow}^* \tag{47}$$

$$E_{n\downarrow}u_{ni\downarrow} = -\sum_j t_{ij}u_{nj\downarrow} + (V_{i\downarrow}^{imp} - \mu)u_{ni\downarrow} + \Delta_i v_{ni\uparrow} \tag{48}$$

$$E_{n\uparrow}v_{ni\downarrow}^* = \sum_j t_{ij}v_{nj\downarrow}^* - (V_i^{imp}\downarrow - \mu)v_{ni\downarrow}^* - \Delta_i u_{ni\uparrow}^* \tag{49}$$

By defining an operator $h_\sigma u_{i\sigma} = -\sum_j t_{ij}u_{j\sigma} + (V_{i\sigma}^{imp} - \mu)u_{i\sigma}$ the four Bogoliubov-de Gennes equations can be written as eigenvalue problems:

$$E_{n\uparrow}\begin{pmatrix} u_{n\uparrow} \\ v_{n\downarrow} \end{pmatrix} = \begin{pmatrix} h_\uparrow & -\Delta_i \\ -\Delta_i^* & -h_\downarrow^* \end{pmatrix}\begin{pmatrix} u_{n\uparrow} \\ v_{n\downarrow} \end{pmatrix} \tag{50}$$

$$E_{n\downarrow}\begin{pmatrix} u_{n\downarrow} \\ v_{n\uparrow} \end{pmatrix} = \begin{pmatrix} h_\downarrow & \Delta_i \\ \Delta_i^* & -h_\uparrow^* \end{pmatrix}\begin{pmatrix} u_{n\downarrow} \\ v_{n\uparrow} \end{pmatrix} \tag{51}$$

We can also determine the order parameter in terms of $u_{ni\sigma}, v_{ni\sigma}$ by using the transformation in eq. 33 and the thermal averages in eq. 28:

$$\begin{aligned} \Delta_i = V\langle c_{i\downarrow}c_{i\uparrow}\rangle &= V\sum_n \left\langle \left(u_{ni\downarrow}\gamma_{n\downarrow} + v_{ni\downarrow}^*\gamma_{n\uparrow}^\dagger\right)\left(u_{ni\uparrow}\gamma_{n\uparrow} + v_{ni\uparrow}^*\gamma_{n\downarrow}^\dagger\right)\right\rangle \\ &= V\sum_n \left(u_{ni\downarrow}v_{ni\uparrow}^*\langle\gamma_{n\downarrow}\gamma_{n\downarrow}^\dagger\rangle + v_{ni\downarrow}^*u_{ni\uparrow}\langle\gamma_{n\uparrow}^\dagger\gamma_{n\uparrow}\rangle\right) \\ &= V\sum_n u_{ni\downarrow}v_{ni\uparrow}^*(1 - 2f(E_n)) \end{aligned} \tag{52}$$

3 Numerical calculations

3.1 Gap equation in momentum space

Equation 29 is a self-consistency equation for the superconducting order parameter Δ. It can be used to determine the gap numerically. This is done in the following way:

1. Guess a value for the gap Δ.
2. Use this value in eq. 29 to calculate a new value for Δ. This is done with the following code:

```
for n = 1:N
    for m = 1:N
        xik(n,m) = -2.0*(cos(kx(n))+cos(ky(m)))-mu;
    end
end

while abs(Delta_prev-Delta_new)>10^-6 % continue until Δ ...
    converges
```

```
Delta_prev = Delta_new;
Delta_new = 0.0;
    for i = 1:N
        for j = 1:N
            Delta_new = Delta_new+V_sc*(Delta_prev. ...
                /(2*sqrt(Delta_prev.^2+(xik(i,j)).^2))...
            *tanh(sqrt(Delta_prev.^2+(xik(i,j)).^2)...
            /(2*T(m)))/N^2;
        end
    end
end
```

3. Iterate over the previous step until Δ converges.

This has been done for a 2D square lattice in the tight-binding model. The dispersion relation is $\xi_k = -2t(\cos(k_x a) + \cos(k_y a))$ where k_x, k_y is in the first Brilluoin zone [6]. Figure 1 shows the resulting plot of the temperature dependence of the gap parameter Δ.

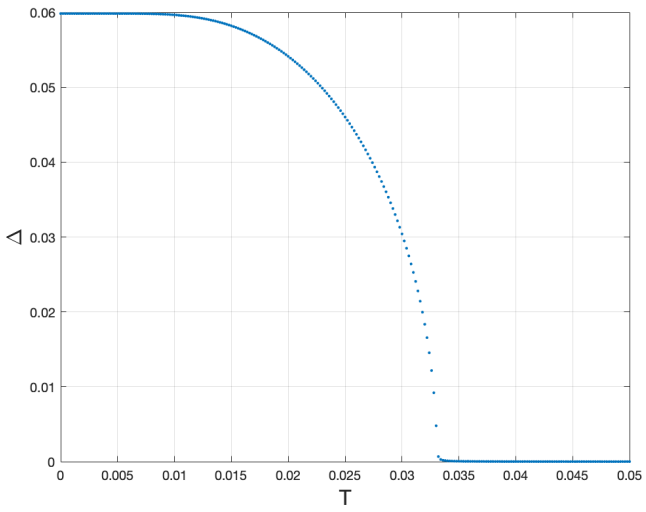

Figure 1: Gap parameter as a function of temperature

3.2 Gap equation in real space

1. Construct the Bogoliubov-de Gennes matrix $M = \begin{pmatrix} h_\uparrow & \Delta_i \\ \Delta_i^* & -h_\downarrow^* \end{pmatrix}$ with both nearest neighbour t and next-nearest neighbour t' hopping terms and with periodic boundary conditions.

2. Generate a set of random values to determine on which sites the impurities should be placed. Let the matrix elements of the form $M_{i,i}$ take the form $V_{imp} - \mu$ and elements of the form M_{N^2+i,N^2+i} take the form $-(V_{imp} - \mu)$.

3. Guess a value for the gap Δ and assign this value to all elements of the form $M_{N^2+i,i}$ and M_{i,N^2+i}.

4. Diagonalize the matrix M to find eigenvectors and eigenvalues.

5. Use the eigenvectors and eigenvalues to calculate the gap on site i:

```
[eigvecs,eigvals] = eig(bdg);

while abs(Delta_prev(1)-Delta_new(1))>10^-6 % continue ...
    until Δ converges
Delta_prev = Delta_new;
Delta_new = zeros(N^2,1);

for i = 1:N^2
    for n = 1:2*N^2
        Delta_new(i) = ...
            Delta_new(i)-V_sc*eigvecs(i,n)*conj(eigvecs(N^2+i,n))...
        *(exp(eigvals(n,n)/T(p))+1)^(-1);
    end
end
```

6. Iterate over the previous two steps until Δ converges.

This has been done for a system with 50x50 sites with filling 0.83. The following parameters have been used: nearest neighbour hopping $t = 1$, next nearest neighbour hopping $t' = -0.3t$ and on-site attraction $V_{sc} = 0.8t$. With these parameters we get $\Delta^0 = 0.025t$ at $T = 0$ and $k_B T_c^0 = 0.0148t$. The figures 2-4 show real space maps of $\Delta(r)/\Delta^0$ with 15% impurities for varying temperatures and impurity strengths. As seen from figure 2 the impurity potential of $1.5t$ is not strong enough to sustain regions of finite Δ above the critical temperature of the system. However, for both figure 3 and figure 4 we see disconnected regions of non-zero Δ even at $T/T_c^0 = 1.92$. This means that the superconductivity is not destroyed everywhere in the system and that regions of finite Δ can survive temperatures well above the critical temperature of the system if the impurity potential is strong enough. The regions of finite Δ are caused by an enhancement of the local density of states [2].

A lot of studies, both experimental and theoretical, has been done on the effect of disorder on the critical temperature. Mostly it has been found that disorder makes the critical temperature drop, or at best does not affect the critical temperature (this is understood with respect to the Anderson theorem). However, there have also been experimental examples of enhanced T_c by disorder [2]. In this particular case it has been found that impurities causes areas of non-zero Δ for temperatures above the critical temperature of the system. This is caused by areas of reinforced density of states. This means that super-

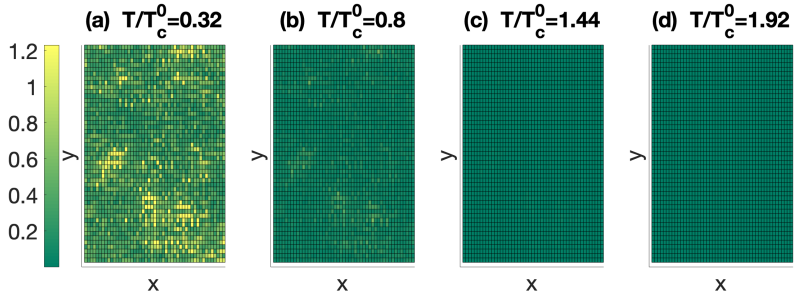

Figure 2: Impurity strength $V_{imp} = 1.5t$.

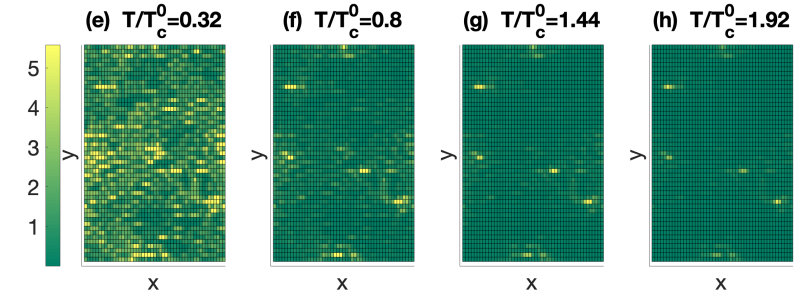

Figure 3: Impurity strength $V_{imp} = 3.3t$

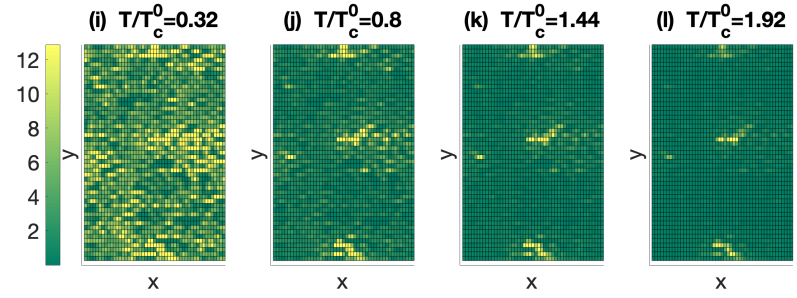

Figure 4: Impurity strength $V_{imp} = 5t$

conductivity is not destroyed everywhere at once, but rather some areas remain superconducting while other areas revert back to the normal state.

4 Conclusion

In this thesis the effect of disorder on the critical temperature on a conventional s-wave superconductor has been studied. This has been done by solving the Bogoliubov-de Gennes equations numerically on a 2D square lattice with 15% impurities. It has been found that there are regions of finite gap parameter Δ even for temperatures well above the critical temperature of the system, meaning that there remains regions of superconductivity. This is caused by a local enhancement of the local density of states [2].
If the time had permitted so, it would have been interesting to investigate the conditions on the coherence length or the typical inter-impurity distance in order to better understand what makes T_c grow.

References

[1] P. W. Anderson. *Theory of Dirty Superconductors*. J. Phys. Chem. Solids vol. 11, 03/03/59.

[2] Maria N. Gastiasoro and Brian M. Andersen. *Enhancing Superconductivity by Disorder*. 08/12/17. arXiv:1712.02656v1 [cond-mat.supr-con].

[3] Henrik Bruus and Karsten Flensberg. *Many-Body Quantum Theory in Condensed Matter Physics*. Oxford University Press, 2004.

[4] James F. Annett. *Superconductivity, Superfluids, and Condensates*. Oxford University Press, 2004.

[5] Brian M. Andersen. *Lecture notes for the course CMP2*. Niels Bohr Institute, 2017.

[6] Carl J. Chandler, Christian Prosko and F. Marsiglio. *The Effect of Next-Nearest Neighbour Hopping in the One, Two, and Three Dimensional Holstein Model*. Nature Scientific Reports, 02/09/16.