



Suppression of the critical temperature in s-wave superconductors by magnetic and non-magnetic impurities

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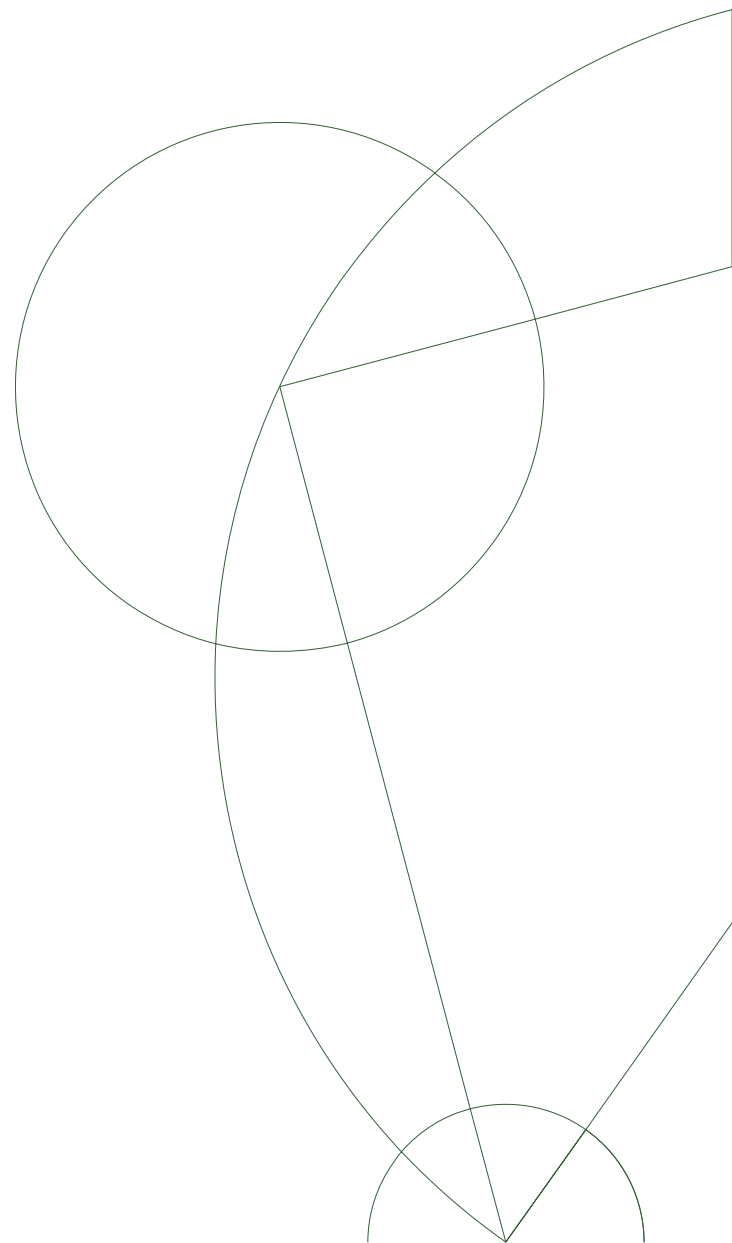
Bachelor's thesis in physics

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Abstract

In this Bachelor's thesis we investigate the temperature dependence of the superconducting gap parameter, as well as its response to magnetic and non-magnetic impurities. We formulate self-consistent gap equations in real space and in momentum space. We treat impurities by applying Abrikosov-Gor'kov theory in momentum space and by randomly distributing localised impurities on the lattice sites in the real space formulation. Both magnetic and non-magnetic impurities are found to suppress the critical temperature. The dependence of the critical temperature on impurity concentration is found for certain concentrations and compared to the theoretically expected values.

Contents

1	Introduction	1
2	A brief look at second quantisation	1
3	BCS theory in momentum space	2
4	BCS theory with Matsubara Green's functions	3
5	Abrikosov Gor'kov theory	5
6	BCS theory in real space	7
7	Numerical calculations	11
7.1	Note on parameters	11
7.2	Gap equation in momentum space	11
7.3	Gap equation with Matsubara Green's functions	12
7.4	Gap equation in real space	16
8	Discussion	18
9	Conclusion	20
10	References	20
	Appendix	21
A	Calculation of $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$	21
B	Proof of commutator identities	22
C	Fourier transformation of the BCS mean-field Hamiltonian	22
D	Anticommutation of Bogoliubov-transformed operators	22
E	An example of the \mathbf{M} -matrix	23

1 Introduction

In 1957, close to half a century after Onnes first discovered superconductivity, Bardeen, Cooper and Schrieffer proposed the first microscopic theory of the phenomenon. Since the mid-fifties, the study of the effect of impurities in superconductors has garnered much interest. In the BCS theory, superconductivity is understood as the correlation between electrons with opposite spin and momentum, which are seen as time-reversed states. [1] [2] Anderson [3] and Abrikosov and Gor'kov [4] considered conventional s-wave superconductors and argued that non-magnetic impurities would not break the time-reversal symmetry of the Cooper-pairs and thus would not affect the transition temperature. Shortly after, Abrikosov and Gor'kov examined the effect of magnetic impurities, and found that these would locally break the time-reversal symmetry and suppress the critical temperature. [5]

The purpose of this Bachelor's thesis is to investigate, through numerical simulation, the effect of magnetic and non-magnetic impurities in a superconductor, by use of two approaches, one of which is the theory developed by Abrikosov and Gor'kov (AG). The other approach is to Fourier transform the BCS Hamiltonian to real space and set up a two-dimensional lattice with periodic boundary conditions, in order to see the effect of randomly distributed, localised impurities on the superconducting gap parameter.

The critical temperatures for different impurity concentrations will be numerically computed using AG theory, and compared to the theoretically predicted values. For the real space lattice, the value for the gap parameter on the different sites will be plotted to see how impurities affect the gap and how the gap parameter is suppressed in the area surrounding the impurities.

2 A brief look at second quantisation

For an N -particle system in the second quantisation representation, or occupation number representation, the basis states are found by listing the occupation numbers of each basis state [6]. Thus an N -particle basis state can be written

$$|n_{\nu_1}, n_{\nu_2}, n_{\nu_3}, \dots\rangle, \quad \sum_j n_{\nu_j} = N \quad (2.1)$$

The occupation number n_{ν_j} is then the number of particles occupying state $|\nu_j\rangle$. The occupation number operator has these basis states as eigenstates and n_{ν_j} as its eigenvalue.

Creation operators, $c_{\nu_j}^\dagger$, and annihilation operators, c_{ν_j} , can be introduced. These operators raise and lower the occupation number in a state by one.

The operator algebra for the fermionic creation and annihilation operators can be defined by the following three anti-commutation relations:

$$\{c_{\nu_j}^\dagger, c_{\nu_k}^\dagger\} = 0, \quad \{c_{\nu_j}, c_{\nu_k}\} = 0 \quad \{c_{\nu_j}, c_{\nu_k}^\dagger\} = \delta_{\nu_j\nu_k}. \quad (2.2)$$

3 BCS theory in momentum space

The BCS mean-field Hamiltonian is given by

$$H_{BCS}^{MF} = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} - \sum_{\mathbf{k}} \Delta_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger - \sum_{\mathbf{k}} \Delta_{\mathbf{k}}^* c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \quad (3.1)$$

Where the gap function is given by

$$\Delta_{\mathbf{k}} = - \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \langle c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \rangle \quad (3.2)$$

$V_{\mathbf{k}\mathbf{k}'}$, is the effective phonon-mediated electron-electron attraction, which leads to the formation of Cooper pairs. Although the attraction varies with the momenta of the electrons, the model is simplified by letting it be attractive when half the magnitude of the kinetic energy of the pair is smaller than the Debye frequency, ω_D , of the phonons [6]. Thus $-V < 0$ for all $|\xi_{\mathbf{k}}| < \omega_D$. Throughout the project, a two-dimensional tight binding model has been used, with a dispersion relation of the form

$$\xi(k_x, k_y) = \varepsilon(k_x, k_y) - \mu = (2t[\cos(k_x a) + \cos(k_y a)] + \mu) \quad (3.3)$$

Where μ denotes the Fermi energy. The above Hamiltonian can be diagonalised by a rotation of the c -operators into γ -operators, known as the Bogoliubov transformation [6]. We then have

$$\begin{pmatrix} \gamma_{\mathbf{k}\uparrow} \\ \gamma_{-\mathbf{k}\downarrow}^\dagger \end{pmatrix} = \begin{pmatrix} u_{\mathbf{k}}^* & v_{\mathbf{k}} \\ -v_{\mathbf{k}}^* & u_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c_{-\mathbf{k}\downarrow}^\dagger \end{pmatrix} \quad (3.4)$$

and accordingly, the γ -operators can be rotated to c -operators

$$\begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c_{-\mathbf{k}\downarrow}^\dagger \end{pmatrix} = \begin{pmatrix} u_{\mathbf{k}} & -v_{\mathbf{k}} \\ v_{\mathbf{k}}^* & u_{\mathbf{k}}^* \end{pmatrix} \begin{pmatrix} \gamma_{\mathbf{k}\uparrow} \\ \gamma_{-\mathbf{k}\downarrow}^\dagger \end{pmatrix} = \begin{pmatrix} u_{\mathbf{k}} \gamma_{\mathbf{k}\uparrow} - v_{\mathbf{k}} \gamma_{-\mathbf{k}\downarrow}^\dagger \\ -v_{\mathbf{k}}^* \gamma_{\mathbf{k}\uparrow} + u_{\mathbf{k}}^* \gamma_{-\mathbf{k}\downarrow}^\dagger \end{pmatrix} \quad (3.5)$$

. The gap equation can be rewritten as

$$\begin{aligned} \Delta &= \sum_{\mathbf{k}} V \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle \\ &= \sum_{\mathbf{k}} V \left\langle (u_{\mathbf{k}}^* \gamma_{-\mathbf{k}\downarrow} - v_{\mathbf{k}} \gamma_{\mathbf{k}\uparrow}^\dagger) (u_{\mathbf{k}}^* \gamma_{\mathbf{k}\uparrow} + v_{\mathbf{k}} \gamma_{-\mathbf{k}\downarrow}^\dagger) \right\rangle \\ &= \sum_{\mathbf{k}} V (u_{\mathbf{k}}^* v_{\mathbf{k}} \langle \gamma_{-\mathbf{k}\downarrow} \gamma_{-\mathbf{k}\downarrow}^\dagger \rangle - v_{\mathbf{k}} u_{\mathbf{k}}^* \langle \gamma_{\mathbf{k}\uparrow}^\dagger \gamma_{\mathbf{k}\uparrow} \rangle) \end{aligned} \quad (3.6)$$

The quasi-particles acted on by the γ -operators are nicknamed bogoliubons. They behave as free fermions, and they are distributed according to Fermi-Dirac statistics. This implies that $\langle \gamma_{\mathbf{k}\sigma}^\dagger \gamma_{\mathbf{k}'\sigma'} \rangle = n_F(E_{\mathbf{k}}) \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'}$. In combination with the anticommutation relations for fermion operators, this yields

$$\begin{aligned} \Delta &= \sum_{\mathbf{k}} V \left[u_{\mathbf{k}}^* v_{\mathbf{k}} (1 - n_F(E_{\mathbf{k}})) - v_{\mathbf{k}} u_{\mathbf{k}}^* n_F(E_{\mathbf{k}}) \right] \\ &= \sum_{\mathbf{k}} V u_{\mathbf{k}}^* v_{\mathbf{k}} [1 - 2n_F(E_{\mathbf{k}})] \end{aligned} \quad (3.7)$$

The values of $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ that diagonalise the Hamiltonian are found in appendix A. They are

$$u_{\mathbf{k}} = \pm \sqrt{\frac{E_{\mathbf{k}} + \xi_{\mathbf{k}}}{2E_{\mathbf{k}}}}, \quad v_{\mathbf{k}} = \pm \sqrt{\frac{E_{\mathbf{k}} - \xi_{\mathbf{k}}}{2E_{\mathbf{k}}}} \quad (3.8)$$

By using this result and by rewriting $1 - 2n_F(E_{\mathbf{k}})$ with common denominator, followed by multiplication by $e^{-E_{\mathbf{k}}/2kT}$, the expression in the gap equation reduces to

$$\Delta = \sum_{\mathbf{k}} V \frac{\Delta}{2E_{\mathbf{k}}} \tanh\left(\frac{E_{\mathbf{k}}}{2kT}\right) \quad (3.9)$$

where k and T come from the Fermi-Dirac distribution, and are the Boltzmann constant and the temperature, respectively. This gap equation can be solved self-consistently to give the value of the gap parameter. The momenta of the electrons are quantised as were they particles of a free electron gas:

$$\mathbf{k} = \pm \frac{2\pi n}{N}, \quad n \in \mathbb{Z} \quad (3.10)$$

The sum over \mathbf{k} runs over the momenta of the first Brillouin zone. The numerical treatment of this problem will be handled in section 7.2.

4 BCS theory with Matsubara Green's functions

The review of this topic follows chapter 18 in [6]. The normal Matsubara Green's function $\mathcal{G}_{\uparrow\uparrow}(\mathbf{k}, \tau)$ and the anomalous Matsubara Green's function $\mathcal{F}_{\downarrow\uparrow}(\mathbf{k}, \tau)$ are defined as [6]

$$\mathcal{G}_{\uparrow\uparrow}(\mathbf{k}, \tau) = -\langle T_{\tau} c_{\mathbf{k}\uparrow}(\tau) c_{\mathbf{k}\uparrow}^{\dagger}(0) \rangle = -\theta(\tau) \langle c_{\mathbf{k}\uparrow}(\tau) c_{\mathbf{k}\uparrow}^{\dagger}(0) \rangle \quad (4.1)$$

$$\mathcal{F}_{\downarrow\uparrow}(\mathbf{k}, \tau) = -\langle T_{\tau} c_{-\mathbf{k}\downarrow}^{\dagger}(\tau) c_{\mathbf{k}\uparrow}^{\dagger}(0) \rangle = -\theta(\tau) \langle c_{-\mathbf{k}\downarrow}^{\dagger}(\tau) c_{\mathbf{k}\uparrow}^{\dagger}(0) \rangle \quad (4.2)$$

Where T_{τ} is the time-ordering symbol. It orders operators 'historically', with the later times to the left. To find the equations of motion for $\mathcal{G}_{\uparrow\uparrow}(\mathbf{k}, \tau)$ and $\mathcal{F}_{\downarrow\uparrow}(\mathbf{k}, \tau)$ by using that the time derivative of an operator in imaginary time is given by

$$\partial_{\tau} A(\tau) = [H, A](\tau) \quad (4.3)$$

and that the time derivative of a general Matsubara Green's function of the form

$$\mathcal{C}_{AB}(\tau, \tau') = -\langle T_{\tau} [A(\tau) B(\tau')] \rangle \quad (4.4)$$

is

$$\partial_{\tau} \langle T_{\tau} [A(\tau) B(\tau')] \rangle = \partial_{\tau} [\theta(\tau - \tau') \langle A(\tau) B(\tau') \rangle \pm \theta(\tau' - \tau) \langle B(\tau') A(\tau) \rangle] \quad (4.5)$$

Where fermion operators require the minus sign. The derivatives of the two step-functions will have differing signs, resulting in

$$\partial_{\tau} \langle T_{\tau} [A(\tau) B(\tau')] \rangle = \delta(\tau - \tau') \langle AB - (\pm) BA \rangle + \langle T_{\tau} [H, A](\tau) B(\tau') \rangle \quad (4.6)$$

which for fermion operators becomes

$$\partial_{\tau} \langle T_{\tau} [A(\tau) B(\tau')] \rangle = \delta(\tau - \tau') \langle \{A, B\} \rangle + \langle T_{\tau} [H, A](\tau) B(\tau') \rangle \quad (4.7)$$

We now find the equations of motion for both the normal and anomalous Matsubara Green's functions by use of 4.7

$$\begin{aligned} \partial_\tau \mathcal{G}_{\uparrow\uparrow}(\mathbf{k}, \tau) &= -\delta(\tau) \langle \{c_{\mathbf{k}\uparrow}(\tau) c_{\mathbf{k}\uparrow}^\dagger(0)\} \rangle \\ &\quad - \langle \partial_\tau c_{\mathbf{k}\uparrow}(\tau) c_{\mathbf{k}\uparrow}^\dagger(0) \rangle \end{aligned} \quad (4.8)$$

$$\begin{aligned} \partial_\tau \mathcal{F}_{\downarrow\uparrow}(\mathbf{k}, \tau) &= -\delta(\tau) \langle \{c_{-\mathbf{k}\downarrow}^\dagger(\tau), c_{\mathbf{k}\uparrow}^\dagger(0)\} \rangle \\ &\quad - \langle \partial_\tau c_{-\mathbf{k}\downarrow}^\dagger(\tau) c_{\mathbf{k}\uparrow}^\dagger(0) \rangle \end{aligned} \quad (4.9)$$

We look at the time derivative of $c_{\mathbf{k}\uparrow}(\tau)$ when using the BCS mean field-Hamiltonian

$$\begin{aligned} \partial_\tau c_{\mathbf{k}\uparrow}(\tau) &= [H_{BCS}^{MF}, c_{\mathbf{k}\uparrow}] = \left[\sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} - \sum_{\mathbf{k}} \Delta_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger - \sum_{\mathbf{k}} \Delta_{\mathbf{k}}^* c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}, c_{\mathbf{k}\uparrow} \right] \\ &= \sum_{\mathbf{k}} \left(\xi_{\mathbf{k}} \left[c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\uparrow}, c_{\mathbf{k}\uparrow} \right] + \xi_{\mathbf{k}} \left[c_{-\mathbf{k}\downarrow}^\dagger c_{-\mathbf{k}\downarrow}, c_{\mathbf{k}\uparrow} \right] - \Delta_{\mathbf{k}} \left[c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger, c_{\mathbf{k}\uparrow} \right] - \Delta_{\mathbf{k}}^* \left[c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}, c_{\mathbf{k}\uparrow} \right] \right) \end{aligned} \quad (4.10)$$

$\partial_\tau c_{-\mathbf{k}\downarrow}^\dagger(\tau)$ is treated similarly. By evaluation of the commutators using B.2, one obtains

$$\partial_\tau c_{\mathbf{k}\uparrow}(\tau) = -\xi_{\mathbf{k}} c_{\mathbf{k}\uparrow}(\tau) + \Delta_{\mathbf{k}} c_{-\mathbf{k}\downarrow}^\dagger(\tau). \quad (4.11)$$

$$\partial_\tau c_{-\mathbf{k}\downarrow}^\dagger(\tau) = \xi_{\mathbf{k}} c_{-\mathbf{k}\downarrow}^\dagger(\tau) + \Delta_{\mathbf{k}}^* c_{\mathbf{k}\uparrow}(\tau). \quad (4.12)$$

By inserting these results into 4.8 and 4.9 we get the equations of motion. These equations of motion will later be used to obtain an analytic expression for the Nambu Green's function.

$$\partial_\tau \mathcal{G}_{\uparrow\uparrow}(\mathbf{k}, \tau) = -\delta(\tau) - \xi_{\mathbf{k}} \mathcal{G}_{\uparrow\uparrow}(\mathbf{k}, \tau) + \Delta_{\mathbf{k}} \mathcal{F}_{\downarrow\uparrow}(\mathbf{k}, \tau) \quad (4.13)$$

$$\partial_\tau \mathcal{F}_{\downarrow\uparrow}(\mathbf{k}, \tau) = +\xi_{\mathbf{k}} \mathcal{F}_{\downarrow\uparrow}(\mathbf{k}, \tau) + \Delta_{\mathbf{k}}^* \mathcal{G}_{\uparrow\uparrow}(\mathbf{k}, \tau) \quad (4.14)$$

$\partial_\tau \mathcal{F}_{\downarrow\uparrow}(\mathbf{k}, \tau)$ lacks has no delta-term because the anticommutator in 4.9 is zero. The Nambu formalism of BCS theory can be introduced through the following spinors:

$$\alpha_{\mathbf{k}}(\tau) = \begin{pmatrix} c_{\mathbf{k}\uparrow}(\tau) \\ c_{-\mathbf{k}\downarrow}^\dagger(\tau) \end{pmatrix}, \quad \alpha_{\mathbf{k}}^\dagger(\tau) = \begin{pmatrix} c_{\mathbf{k}\uparrow}^\dagger(\tau) & c_{-\mathbf{k}\downarrow}(\tau) \end{pmatrix} \quad (4.15)$$

The Nambu Green's function, $\bar{\bar{\mathcal{G}}}(\mathbf{k}, \tau)$, is defined by

$$\bar{\bar{\mathcal{G}}}(\mathbf{k}, \tau) = -\langle T_\tau \alpha_{\mathbf{k}}(\tau) \alpha_{\mathbf{k}}^\dagger(0) \rangle = \begin{pmatrix} \mathcal{G}_{\uparrow\uparrow}(\mathbf{k}, \tau) & \mathcal{F}_{\downarrow\uparrow}^*(\mathbf{k}, \tau) \\ \mathcal{F}_{\downarrow\uparrow}(\mathbf{k}, \tau) & \mathcal{G}_{\downarrow\downarrow}^*(\mathbf{k}, \tau) \end{pmatrix} \quad (4.16)$$

The equation of motion for the Nambu Green's function is obtained by writing the equations of motions for its elements on matrix form. Two of these have been calculated explicitly in 4.13 and 4.14. Thus we find that

$$\partial_\tau \bar{\bar{\mathcal{G}}}(\mathbf{k}, \tau) = -\delta(\tau) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} \xi_{\mathbf{k}} & -\Delta_{\mathbf{k}} \\ -\Delta_{\mathbf{k}}^* & -\xi_{\mathbf{k}} \end{pmatrix} \bar{\bar{\mathcal{G}}}(\mathbf{k}, \tau) \quad (4.17)$$

If the Hamiltonian does not explicitly depend on time, the Green's functions only depend on the imaginary time argument, and one can rewrite the above equation in the

Matsubara frequency domain by use of a Fourier transform. Fourier transformation of the differential operator gives $\partial_t \rightarrow -i\omega$ and for the delta function one has $\delta(t) \rightarrow 1$. 4.17 becomes

$$\begin{pmatrix} i\omega_k - \xi_{\mathbf{k}} & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}}^* & i\omega_k + \xi_{\mathbf{k}} \end{pmatrix} \bar{\bar{\mathcal{G}}}(\mathbf{k}, i\omega_k) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (4.18)$$

where the leftmost matrix in the above equation is the inverse of the Nambu Green's function, $\bar{\bar{\mathcal{G}}}^{-1}(\mathbf{k}, i\omega_k)$. The Nambu Green's function is found to be

$$\bar{\bar{\mathcal{G}}}(\mathbf{k}, i\omega_k) = \frac{1}{(i\omega_k)^2 - E_{\mathbf{k}}^2} \begin{pmatrix} i\omega_k + \xi_{\mathbf{k}} & -\Delta_{\mathbf{k}} \\ -\Delta_{\mathbf{k}}^* & i\omega_k - \xi_{\mathbf{k}} \end{pmatrix} \quad (4.19)$$

5 Abrikosov Gor'kov theory

To account for scattering effects, we introduce an impurity Hamiltonian, \hat{H}_{imp} , which can be added to 3.1.

$$\hat{H}_{imp} = V_1 \sum_{\mathbf{k}\mathbf{k}'\sigma} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}'\sigma} + \sum_{\mathbf{k}\mathbf{k}'\sigma} V_\sigma c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}'\sigma} \quad \begin{cases} V_\sigma = V_2 & \text{if } \sigma = \uparrow \\ V_\sigma = -V_2 & \text{if } \sigma = \downarrow \end{cases} \quad (5.1)$$

The first term is for scattering off non-magnetic impurities. The attractive or repulsive potential V_1 is the same, independent of the electron spin. The second term describes scattering off magnetic impurities. This simple model takes the spin of the impurity atom and the spin of the electron to both have only a z -component. The magnetic dipole interaction can then be either stabilising or destabilising, with the same absolute magnitude in both cases.

From 3.2 we have

$$\Delta_{\mathbf{k}} = V \sum_{\mathbf{k}}^{|\xi_{\mathbf{k}}| < \omega_D} \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle \quad (5.2)$$

Consider now the complex conjugate of \mathcal{F} from 4.2.

$$\mathcal{F}_{\downarrow\uparrow}(\mathbf{k}, \tau) = -\langle T_\tau c_{-\mathbf{k}\downarrow}^\dagger(\tau) c_{\mathbf{k}\uparrow}^\dagger(0) \rangle \quad (5.3)$$

Using that $(AB)^\dagger = B^\dagger A^\dagger$ its complex conjugate becomes

$$\mathcal{F}_{\downarrow\uparrow}^*(\mathbf{k}, \tau) = -\langle T_\tau c_{\mathbf{k}\uparrow}(0) c_{-\mathbf{k}\downarrow}(\tau) \rangle = \langle T_\tau c_{-\mathbf{k}\downarrow}(\tau) c_{\mathbf{k}\uparrow}(0) \rangle \quad (5.4)$$

where the rightmost equality is due to the fact that $\{c_{\mathbf{k}\uparrow}, c_{-\mathbf{k}\downarrow}\} = 0$, which gives $c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} = -c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}$. The operators should be considered for the same imaginary time τ , and this is achieved by letting τ approach 0 from above. Thus

$$\mathcal{F}_{\downarrow\uparrow}(\mathbf{k}, \tau = 0^+) = \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle \quad (5.5)$$

hence we have

$$\Delta = V \sum_{\mathbf{k}}^{|\xi_{\mathbf{k}}| < \omega_D} \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle = V \sum_{\mathbf{k}}^{|\xi_{\mathbf{k}}| < \omega_D} \mathcal{F}_{\downarrow\uparrow}^*(\mathbf{k}, \tau = 0^+) \quad (5.6)$$

\mathcal{F}^* is Fourier transformed to Matsubara frequency space, so that it can be found from the Nambu Green's function. With the Matsubara summation we get

$$\Delta = V \sum_{\mathbf{k}} \sum_{i\omega_k}^{|k_{\mathbf{k}}| < \omega_D} \frac{1}{\beta} \mathcal{F}_{\downarrow\uparrow}^*(\mathbf{k}, i\omega_k) e^{i\omega_k 0^+} \quad (5.7)$$

where β is $1/kT$, and the exponential function of 0^+ is 1. The Matsubara frequency for fermions is given by

$$\omega_n = \frac{(2n+1)\pi}{\beta} \quad (5.8)$$

and we can therefore take the sum to be over the integer n . [6] Evidently, the spacing between Matsubara frequencies scales with temperature, so for small temperatures, the frequencies lie very close. The Nambu Green's function which describes the electron in the presence of impurities is a renormalised function that is determined by the equation [1]

$$\bar{\mathcal{G}}^{-1}(\mathbf{k}, i\omega_k) = [\bar{\mathcal{G}}^0(\mathbf{k}, i\omega_k)]^{-1} - \Sigma(\mathbf{k}, \omega_k) \quad (5.9)$$

Where $\Sigma(\mathbf{k}, \omega_k)$ is the self energy. Up until now, we have considered the electrons as free particles. Electrons in a crystal are not free, but subject to crystal field effects. These effects are contained in the self-energy. In the Born approximation, scattering events are approximated to events where the electrons scatter off of one impurity without further scattering off of others and without scattering doubly off of a single impurity. In the Born approximation the self-energy is given by

$$\Sigma(\mathbf{k}, \omega_k) = n \int \frac{d^3\mathbf{k}'}{(2\pi)^3} [\hat{U}(\mathbf{k} - \mathbf{k}') \bar{\mathcal{G}}(\mathbf{k}', i\omega_k) \hat{U}(\mathbf{k} - \mathbf{k}')] \quad (5.10)$$

From insertion of 5.9 into 5.10 we obtain an equation that can be used to self-consistently determine the self-energy:

$$\Sigma(\mathbf{k}, \omega_k) = n \int \frac{d^3\mathbf{k}'}{(2\pi)^3} [\hat{U}(\mathbf{k} - \mathbf{k}') [\bar{\mathcal{G}}^0(\mathbf{k}', i\omega_k)]^{-1} - \Sigma(\mathbf{k}', \omega_k)]^{-1} \hat{U}(\mathbf{k} - \mathbf{k}')] \quad (5.11)$$

$\hat{U}(\mathbf{k} - \mathbf{k}')$ is the impurity scattering Hamiltonian in the Nambu basis. It depends only on the the difference $\mathbf{k} - \mathbf{k}'$ due to the translational symmetry of the lattice. n is the concentration of impurities. We will rewrite the Hamiltonian in 5.1 in the Nambu basis of 4.15. Starting with the term for non-magnetic impurities we have

$$V_1 \sum_{\mathbf{k}\mathbf{k}'} c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}'\uparrow} + c_{-\mathbf{k}'\downarrow}^\dagger c_{-\mathbf{k}\downarrow} = V_1 \sum_{\mathbf{k}\mathbf{k}'} c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}'\uparrow} - c_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow}^\dagger + 1 = \sum_{\mathbf{k}\mathbf{k}'} \alpha_{\mathbf{k}}^\dagger \begin{pmatrix} V_1 & 0 \\ 0 & -V_1 \end{pmatrix} \alpha_{\mathbf{k}} + V_1 \quad (5.12)$$

for the magnetic impurity scattering term we have

$$\sum_{\mathbf{k}\mathbf{k}'} V_2 c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}'\uparrow} - V_2 c_{-\mathbf{k}'\downarrow}^\dagger c_{-\mathbf{k}\downarrow} = V_2 \sum_{\mathbf{k}\mathbf{k}'} c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}'\uparrow} + c_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow}^\dagger - 1 = \sum_{\mathbf{k}\mathbf{k}'} \alpha_{\mathbf{k}}^\dagger \begin{pmatrix} V_2 & 0 \\ 0 & V_2 \end{pmatrix} \alpha_{\mathbf{k}} - V_2 \quad (5.13)$$

The constant terms in the Hamiltonian do not affect the energy spectra except for lowering or raising them by a constant value, and are therefore left out in the following. In the case of a finite lattice of N sites, we replace the integral in 5.10 by a sum over

the discrete values of the momentum, previously mentioned. Going from integral to sum we will also lose the factor $1/(2\pi)^3$. We separate the sum over momentum into a sum over k_x and k_y , and end up with

$$\Sigma(\mathbf{k}, \omega_k) = n \sum_{k_x k_y} \hat{U} \bar{\bar{\mathcal{G}}}(\mathbf{k}', i\omega_k) \hat{U} \quad (5.14)$$

$$= n \sum_{k_x k_y} (V_1 \boldsymbol{\rho}_3 + V_2 \mathbf{I}_2) \bar{\bar{\mathcal{G}}}(\mathbf{k}', i\omega_k) (V_1 \boldsymbol{\rho}_3 + V_2 \mathbf{I}_2) \quad (5.15)$$

where $\boldsymbol{\rho}_3$ is the third Pauli matrix and \mathbf{I}_2 is the 2×2 identity matrix.

6 BCS theory in real space

We will now consider a square lattice with N^2 positions, numbered as follows:

$$\begin{pmatrix} 1 & 2 & \dots & N \\ N+1 & N+2 & \dots & 2N \\ \vdots & \vdots & \ddots & \vdots \\ N^2 - (N-1) & N^2 - (N-2) & \dots & N^2 \end{pmatrix} \quad (6.1)$$

The Hamiltonian governing the system is found by Fourier transforming the BCS mean-field Hamiltonian given by 3.1 from momentum space to real space. Starting with the first term, we use that

$$a_{\mathbf{q}}^\dagger = \frac{1}{\sqrt{\mathcal{V}}} \int d\mathbf{r} e^{i\mathbf{q}\cdot\mathbf{r}} \Psi^\dagger(\mathbf{r}), \quad a_{\mathbf{q}} = \frac{1}{\sqrt{\mathcal{V}}} \int d\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} \Psi(\mathbf{r}) \quad (6.2)$$

$$\sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} = \frac{1}{\mathcal{V}} \sum_{\mathbf{k}} \int_{\mathcal{V}} d\mathbf{r} \int_{\mathcal{V}} d\mathbf{r}' \int_{\mathcal{V}} d\mathbf{r}'' \xi(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} \Psi_\sigma^\dagger(\mathbf{r}') e^{i\mathbf{k}\cdot\mathbf{r}'} \Psi_\sigma(\mathbf{r}'') e^{-i\mathbf{k}\cdot\mathbf{r}''} \quad (6.3)$$

Using that

$$\frac{1}{\mathcal{V}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}} = \delta(\mathbf{r}) \quad (6.4)$$

this reduces to

$$\begin{aligned} \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} &= \int_{\mathcal{V}} d\mathbf{r} \int_{\mathcal{V}} d\mathbf{r}' \int_{\mathcal{V}} d\mathbf{r}'' \xi(\mathbf{r}) \Psi_\sigma^\dagger(\mathbf{r}') \Psi_\sigma(\mathbf{r}'') \delta(-\mathbf{r} + \mathbf{r}' - \mathbf{r}'') \\ &= \int_{\mathcal{V}} d\mathbf{r}' \int_{\mathcal{V}} d\mathbf{r}'' \Psi_\sigma^\dagger(\mathbf{r}') \xi(\mathbf{r}' - \mathbf{r}'') \Psi_\sigma(\mathbf{r}'') \end{aligned} \quad (6.5)$$

$\xi(\mathbf{r})$ is found from

$$\xi(\mathbf{r}) = \frac{1}{\mathcal{V}} \sum_{\mathbf{k}} \xi(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}} \quad (6.6)$$

In two dimensions this becomes

$$\begin{aligned}
\xi(x, y) &= \frac{1}{\mathcal{V}} \sum_{k_x k_y} \xi(k_x, k_y) e^{ik_x x} e^{ik_y y} = \frac{1}{\mathcal{V}} \sum_{k_x k_y} -(2t[\cos(k_x a) + \cos(k_y a)] + \mu) e^{ik_x x} e^{ik_y y} \\
&= -\frac{1}{\mathcal{V}} \sum_{k_x k_y} -(t[e^{ik_x a} + e^{-ik_x a} + e^{ik_y a} + e^{-ik_y a}] + \mu) e^{ik_x x} e^{ik_y y} \\
&= -\frac{1}{\mathcal{V}} \sum_{k_x k_y} (t[e^{ik_x(x+a)} + e^{ik_x(x-a)}] e^{ik_y y} + [e^{ik_y(y+a)} + e^{ik_y(y-a)}] e^{ik_x x} + \mu e^{ik_x x} e^{ik_y y}) \\
&= - (t[\delta(x+a) + \delta(x-a)]\delta(y) + t[\delta(y+a) + \delta(y-a)]\delta(x) + \mu\delta(x)\delta(y))
\end{aligned} \tag{6.7}$$

Thus \mathbf{r} can either be in the x - or y -direction, and the Fourier transformed dispersion relation becomes

$$\xi(\mathbf{r}) = -(t[\delta(\mathbf{r}+a) + \delta(\mathbf{r}-a)] + \mu\delta(\mathbf{r})) \tag{6.8}$$

6.5 becomes

$$\begin{aligned}
&\int d\mathbf{r}' \int d\mathbf{r}'' \Psi_\sigma^\dagger(\mathbf{r}') \left[-t(\delta(\mathbf{r}' - \mathbf{r}'' + a) + \delta(\mathbf{r}' - \mathbf{r}'' - a)) - \mu\delta(\mathbf{r}' - \mathbf{r}'') \right] \Psi_\sigma(\mathbf{r}'') \\
&= -t \int d\mathbf{r}' \Psi_\sigma^\dagger(\mathbf{r}') \Psi_\sigma(\mathbf{r}' - a) - t \int d\mathbf{r}' \Psi_\sigma^\dagger(\mathbf{r}') \Psi_\sigma(\mathbf{r}' + a) - \mu \int d\mathbf{r}' \Psi_\sigma^\dagger(\mathbf{r}') \Psi_\sigma(\mathbf{r}')
\end{aligned} \tag{6.9}$$

The first and second term describe how an electron can tunnel from a site, to any of the closest neighbouring sites, changing the energy of the system by $-t$. As the lattice in 6.1 has N^2 discrete positions the integral is replaced by a sum over these.

$$-t \sum_{\langle ij \rangle \sigma}^{N^2} c_{i\sigma}^\dagger c_{j\sigma} - \mu \sum_{i\sigma}^{N^2} c_{i\sigma}^\dagger c_{i\sigma} \tag{6.10}$$

To restrict tunneling to between neighbouring sites, we sum over nearest neighbours, here written as $\langle ij \rangle$. The remaining two terms of the \mathbf{k} -space Hamiltonian are handled similarly (see appendix B) and their Fourier transform is

$$-\sum_i^{N^2} \left(\Delta_i c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger + \Delta_i^* c_{i\uparrow} c_{i\downarrow} \right) \tag{6.11}$$

Where Δ_i is given by

$$\Delta_i = V \langle c_{i\downarrow} c_{i\uparrow} \rangle \tag{6.12}$$

The important difference between this equation and the other equations for the gap parameter previously considered is that 6.12 gives the value for the gap at a specific lattice point. Depending on how impurities are distributed throughout the system, the gap will take different values at different sites. The spin-generalised Bogoliubov transformation is defined as [7]

$$\begin{aligned}
c_{i\uparrow} &= \sum_n \left[u_{n,i\uparrow} \gamma_{n\uparrow} + v_{n,i\uparrow}^* \gamma_{n\downarrow}^\dagger \right] \\
c_{i\downarrow} &= \sum_n \left[u_{n,i\downarrow} \gamma_{n\downarrow} + v_{n,i\downarrow}^* \gamma_{n\uparrow}^\dagger \right]
\end{aligned} \tag{6.13}$$

where the sum only runs over n corresponding to positive eigenvalues. The superconducting gap becomes

$$\Delta_i = V \langle c_{i\downarrow} c_{i\uparrow} \rangle = V \sum_n \langle (u_{n,i\downarrow} \gamma_{n\downarrow} + v_{n,i\downarrow}^* \gamma_{n\uparrow}^\dagger) (u_{n,i\uparrow} \gamma_{n\uparrow} + v_{n,i\uparrow}^* \gamma_{n\downarrow}^\dagger) \rangle \quad (6.14)$$

As before, the quasi-article bogoliubons are free fermions distributed according to Fermi-Dirac statistics, meaning that $\langle \gamma_{i\sigma}^\dagger \gamma_{i'\sigma'} \rangle = f(E_i) \delta_{ii'} \delta_{\sigma\sigma'}$, where E_i is the i 'th energy level of the system. Two of the products in 6.14 will be zero, and this leaves

$$\Delta_i = V \sum_n \left[u_{n,i\downarrow} v_{n,i\uparrow}^* \langle \gamma_{n\downarrow} \gamma_{n\downarrow}^\dagger \rangle + v_{n,i\downarrow}^* u_{n,i\uparrow} \langle \gamma_{n\uparrow}^\dagger \gamma_{n\uparrow} \rangle \right] \quad (6.15)$$

We use that $u_{n,i\downarrow} v_{n,i\uparrow}^* = -v_{n,i\downarrow}^* u_{n,i\uparrow}$, as shown in appendix C, and

$$\Delta_i = V \sum_n u_{n,i\downarrow} v_{n,i\uparrow}^* (\langle \gamma_{n\downarrow} \gamma_{n\downarrow}^\dagger \rangle - \langle \gamma_{n\uparrow}^\dagger \gamma_{n\uparrow} \rangle) = V \sum_n u_{n,i\downarrow} v_{n,i\uparrow}^* (1 - 2f(E_n)) \quad (6.16)$$

Similarly to the expression for the gap in momentum-space, this can be simplified to

$$\Delta_i = V \sum_n u_{n,i\downarrow} v_{n,i\uparrow}^* \tanh \left(\frac{E_n}{2kT} \right) \quad (6.17)$$

The full Hamiltonian is the sum of 6.10 and 6.11. This Hamiltonian can be written compactly by use of the following spinors:

$$\psi^\dagger \equiv (c_{1\uparrow}^\dagger, \dots, c_{N\uparrow}^\dagger, c_{1\downarrow}, \dots, c_{N\downarrow}), \quad \psi \equiv \begin{pmatrix} c_{1\uparrow} \\ \vdots \\ c_{N\uparrow} \\ c_{1\downarrow}^\dagger \\ \vdots \\ c_{N\downarrow}^\dagger \end{pmatrix} \quad (6.18)$$

The real space Hamiltonian can now, by use of an appropriate matrix, be written as

$$\hat{H} = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} - \mu \sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma} - \sum_i \left(\Delta_i c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger + \Delta_i^* c_{i\uparrow} c_{i\downarrow} \right) = \psi^\dagger \mathbf{M} \psi \quad (6.19)$$

The matrix \mathbf{M} consists of four sections of equal size, where the top left quadrant contains the coefficients of terms where both operators have \uparrow indices. The element $M_{m,n}$ is the coefficient of the term $c_{m\uparrow}^\dagger c_{n\uparrow}$. The bottom right quadrant contains the coefficients of terms where both operators have \downarrow indices. The element $M_{(N^2+m, N^2+n)}$ is the coefficient of the term $c_{m\downarrow} c_{n\downarrow}^\dagger$. In order for these terms to match those of the Hamiltonian in 6.10, we use the anticommutation relations given by 2.2 to obtain $c_{m\downarrow} c_{n\downarrow}^\dagger = 1 - c_{m\downarrow}^\dagger c_{n\downarrow}$. The elements of the bottom right quadrant are as a consequence the same as those of the top left quadrant, but multiplied by negative 1 to counter the sign due to the anticommutation. The many terms arising from the term 1 from the

anticommutation relation do not affect the energies, except for raising or lowering the entire spectrum by a constant value.

The coefficients for the terms with different spin indices are contained in the upper right and lower left quadrants of \mathbf{M} . The element $M_{(N^2+m,n)}$ is the coefficient of the term $c_{m\downarrow}c_{n\uparrow}$, while $M_{(m,N^2+n)}$ is the coefficient of the term $c_{m\uparrow}^\dagger c_{n\downarrow}^\dagger$.

We introduce periodic boundary conditions for the lattice. Thus an electron tunnelling to the right from the right edge of the lattice enters through the left edge. In order to construct \mathbf{M} , we must know to which lattice sites an electron can tunnel from a lattice site a . An electron on site a , not on the edges of the lattice in 6.1, can tunnel to sites $a+1$, $a-1$, $a+N$ and $a-N$, corresponding to tunnelling to neighbouring sites in the x - and y -direction.

Accommodation of the periodic boundary conditions is achieved by the implementation of the four following rules for the cases where a lies along the upper, lower, left and right edge of the lattice, respectively:

$$\begin{aligned}
&\text{lattice sites along the upper edge, where } a - N \leq 0 \quad \text{couple to } a - N + N^2 \\
&\text{lattice sites along the lower edge, where } a + N > N^2 \quad \text{couple to } a + N - N^2 \\
&\text{lattice sites along the left edge, where } \frac{a-1}{N} \in \mathbb{Z} \quad \text{couple to } a + N - 1 \\
&\text{lattice sites along the right edge, where } \frac{a}{N} \in \mathbb{Z} \quad \text{couple to } a - N + 1
\end{aligned} \tag{6.20}$$

In appendix E the matrix \mathbf{M} is shown for a lattice with sides of length $N = 3$. 6.17 provides an equation for the gap parameter that can be solved self consistently. The gap parameter does not enter directly on the right hand side of 6.17, but the energy states of the system are given by the eigenvalues of \mathbf{M} . Associated with each eigenvalue E_n , there is an eigenvector which has $2N^2$ elements. This vector consists of two halves, with the upper half containing N^2 elements. The i 'th element of the upper half is $u_{n,i\downarrow}$, while the i 'th element of the bottom half (and thus the $(i+N^2)$ 'th element of the entire vector) is $v_{n,i\uparrow}^*$. \mathbf{M} depends on the gap, and thus one can find a self-consistent value for the gap. This is done in section 7.4.

In the real space representation, localised impurities can be introduced. Consider an impurity scattering Hamiltonian that can be added to the Hamiltonian in 6.19.

$$\hat{H}_{imp} = V_1 \sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma} + \sum_{i\sigma} V_\sigma c_{i\sigma}^\dagger c_{i\sigma} \quad \begin{cases} V_\sigma = V_2 & \text{if } \sigma = \uparrow \\ V_\sigma = -V_2 & \text{if } \sigma = \downarrow \end{cases} \tag{6.21}$$

Similarly to the Hamiltonian in 6.19, this can be rewritten on matrix form in the basis given by the spinors in 6.18. In 5.12 and 5.13 the same scattering Hamiltonian in \mathbf{k} -space was rewritten in the Nambu basis. By the same logic, we see that the matrix elements that are the coefficients of terms with only spin down indices take different signs, depending on whether the impurity is magnetic or non-magnetic. We will only consider magnetic impurities. All sites on which an impurity is placed will thus have an added Hamiltonian term governing it. Placing an impurity on site i will change element $M_{i,i}$ from μ to $\mu + V_2$ and element M_{N^2+i,N^2+i} from $-\mu$ to $-\mu + V_2$ in the \mathbf{M} -matrix. Impurities can thus be placed at random in the two-dimensional model, and the resulting gap on each site i can be found.

7 Numerical calculations

7.1 Note on parameters

The numerical simulations have all been programmed in python. As mentioned in connection with 3.10, we consider values of \mathbf{k} that are in the first Brillouin zone. Thus we have

$$k_x = \left\{ -\pi, -\pi + \frac{2\pi}{N}, -\pi + \frac{4\pi}{N}, \dots, \pi - \frac{2\pi}{N} \right\} \quad (7.1)$$

and similarly for k_y , when we let the lattice constant be unity. The Debye frequency is set to 1, μ is set to -1, and the Boltzmann constant is set to 1. Furthermore, in the code, we use $H = N^2$ and $L = 2N^2$.

7.2 Gap equation in momentum space

Equation 3.9 can be used to self-consistently determine the BCS gap parameter. We use the tight binding model of 3.3. The procedure is as follows

1. Guess at a value, Δ_A , for the gap parameter.
2. Compute the sum of the usual gap equation 3.9 using Δ_A as the gap to obtain a new value, Δ_B , for the gap. This is achieved with the following code:

```

1 def ksi(a, b):
2     ksi = -2.0*(np.cos(a) + np.cos(b)) - mu
3     return ksi
4
5 def selfconusualksi(T, N):
6     gapnew = 0.0
7     for i in np.nditer(k_x):
8         for j in np.nditer(k_y):
9             if abs(ksi(i, j)) < debye:
10                 gapnew = gapnew - ((V_sc*gap*np.tanh(np.sqrt
11                     (ksi(i, j)**2+gap**2)/(2.0*T)))/(2.0*np.
12                     sqrt(ksi(i, j)**2+gap**2)))/(N**2)
13     return gapnew

```

3. Iterate over step 2, always using the previously obtained value for the gap to compute the sum. This is done until Δ converges.

The sum over \mathbf{k} is handled by splitting it up into a sum over k_x and k_y , with appropriate normalisation of the sum. Throughout the numerical treatment, we let $k=1$ for simplicity. Below is shown a plot of the dependence of the gap parameter on the temperature.

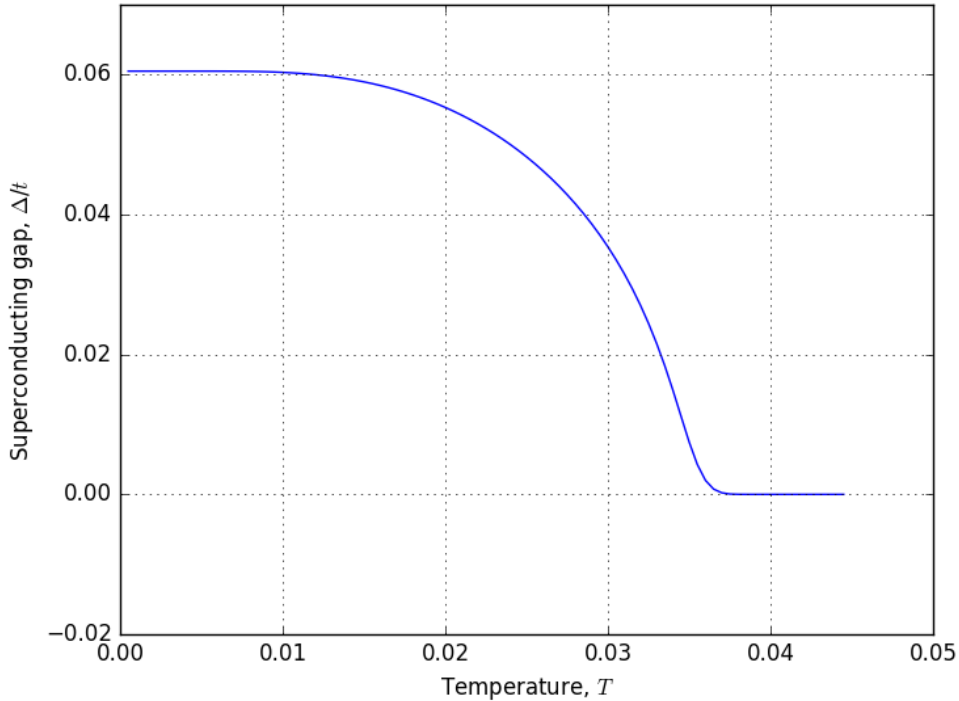


Figure 1: Gap parameter vs. temperature

7.3 Gap equation with Matsubara Green's functions

The standard gap equation does not take impurities into account. Impurities can be handled by use of 5.7, where \mathcal{F}^* is an element in the Nambu Green's matrix, which can be found from 5.9.

In the following, we consider the cases of either magnetic or non-magnetic impurities in a superconductor. A combination of both impurities is not considered. If the impurity scattering potential is uniform (the impurities are evenly smeared out, and nowhere localised) the scattering Hamiltonian takes the following forms in Nambu space:

$$\hat{U} = \begin{cases} V_1 \boldsymbol{\rho}_3 & \text{for non-magnetic impurities} \\ V_2 \mathbf{I}_2 & \text{for magnetic impurities} \end{cases}$$

In the numerical simulation the same scattering potential was used for magnetic and non-magnetic impurities i.e. $V_1 = V_2 = V$. In both cases above, the scattering potentials can be taken outside the sum and merged with the impurity concentration to become one parameter, nV^2 . Now two methods present themselves. One can use $\bar{\mathcal{G}}^0$, in place of $\bar{\mathcal{G}}$ in 5.14, reducing the equation to

$$\Sigma(\mathbf{k}, \omega_k) = n \sum_{k_x k_y} \hat{U} \bar{\mathcal{G}}^0(\mathbf{k}', i\omega_k) \hat{U} \quad (7.2)$$

to find the self-energy, a method we will refer to as a self-consistent computation of the gap using $\bar{\mathcal{G}}^0$. This method has not been used to obtain data in this thesis. One can also use the full Nambu Green's function to find the self-energy, i. e. by use of

5.9, a method we will refer to as a self-consistent computation of the gap using $\bar{\mathcal{G}}$. In order to find the gap parameter, the following is done.

1. Guess at a value, Δ_A , for the gap parameter.
2. Compute $\bar{\mathcal{G}}^0(\mathbf{k}, i\omega_k)$ from 4.19 with the gap being Δ_A . A function to do this is defined:

```

1 def selfenzero (x, y, gap, omega, nimpVsq):
2     selfenzero = nimpVsq/((omega*1.0j)**2-(ksi(x, y)**2 +
3         gap**2))*(np.matrix([[omega*1.0j+ksi(x, y), gap],
4             [gap, omega*1.0j-ksi(x, y)]]))
5     return selfenzero

```

3. Compute $\Sigma(\mathbf{k}, \omega_k)$ from 7.2 with the gap being Δ_A . This can be done with the following:

```

1 def selflistzero(T, N, N_mat, nimpVsq):
2     a_list = []
3     for i in range(-N_mat, N_mat+1):
4         selfen = np.matrix([[0.0, 0.0],[0.0, 0.0]])
5         for k in np.nditer(k_x):
6             for l in np.nditer(k_y):
7                 selfen = selfen + selfenzero(k, l, gap, (2*i
8                     +1)*np.pi*T, nimpVsq)/(N**2)
9         a_list.append(selfen)
10    return a_list

```

4. Now that both $\bar{\mathcal{G}}^0$ and $\Sigma(\mathbf{k}, \omega_k)$ are known, solve 5.9 to find $\bar{\mathcal{G}}$.
5. Select element $\bar{\mathcal{G}}_{1,2} = \mathcal{F}_{\downarrow\uparrow}^*(\mathbf{k}, i\omega_k)$ and solve 5.7 to find a new value, Δ_B , for the gap parameter. A function that combines step 4 and 5 is

```

1 def selfconfull(T, N, N_mat, nimpVsq):
2     gapnew = 0.0
3     for n in range(-N_mat, N_mat+1):
4         for i in np.nditer(k_x):
5             for k in np.nditer(k_y):
6                 if abs(ksi(i,k))<debye:
7                     gapnew = gapnew + V_sc*T*np.linalg.inv(np
8                         .matrix([[ (2*n+1)*np.pi*T*1.0j-ksi(i,k)
9                             ], [-gap], [-gap, (2*n+1)*np.pi*T*1.0j+
10                                ksi(i,k)]])- selfen_list[n + N_mat]).
11                         item((0,1))/(N**2)
12    return gapnew

```

6. Assign the value Δ_B to the variable Δ_A and go back to step 2.

Step 3 is carried out during the first iteration in both methods. This step uses 7.2 to obtain the self-energy matrix. This matrix is needed as input when solving 5.11 self-consistently. Without some initial self-energy matrix, the self-consistency loop cannot be started. The difference between the methods is that the self-consistent

computation of the gap using $\bar{\mathcal{G}}^0$ keeps using 7.2 to find the self-energy matrix for subsequent iterations. This is the method outlined in the steps above.

After one iteration, 5.14 can be used to find the self-energy matrix, and the self-consistent computation of the gap using $\bar{\mathcal{G}}$, therefore, after one iteration, changes step 3 to be 'computation of $\Sigma(\mathbf{k}, \omega_k)$ from 5.14 with the gap being Δ_A '. A function to do this is defined:

```

1 def selflistfull(T, N, N_mat, nimpVsq):
2     a_list = []
3     for i in range(-N_mat, N_mat+1):
4         selfen = np.matrix([[0.0, 0.0],[0.0, 0.0]])
5         for k in np.nditer(k_x):
6             for l in np.nditer(k_y):
7                 selfen = selfen + nimpVsq*np.matrix
                    ([[1.0,0.0],[0.0, 1.0]])*(np.linalg.inv(np.
                    matrix([[ (2*i+1)*np.pi*T*1.0j-ksi(k,l), -gap
                    ],[-gap, (2*i+1)*np.pi*T*1.0j+ksi(k,l)]])) -
                    selfen_list[i + N_mat]))*np.matrix
                    ([[1.0,0.0],[0.0, 1.0]])/(N**2)
8         a_list.append(selfen)
9     return a_list

```

For the case of non-magnetic impurities the identity matrices would be replaced by the third Pauli matrix. The gap parameter can thus be found self-consistently by starting with a guessed value for the gap and repeating the prescribed procedure until the gap reaches a convergence value:

```

1 selfen_list = []
2 selfen_list = selflistzero(T, N, N_mat, nimpVsq)
3     for a in range(iterations):
4         temp = selfconfull(T, N, N_mat, nimpVsq)
5         gap = np.real(temp)
6         selfen_list = selflistfull(T, N, N_mat, nimpVsq)

```

The above procedure gives the gap for a specific temperature and impurity concentration. In order to find the dependence of the critical temperature on nV^2 one can set up a conditional loop, starting at a temperature greater than the critical one, which is made to terminate once the value of the gap exceeds some very small value. Employing this method for a range of values for the impurity concentration, the dependence of the critical temperature on nV^2 can be found. Below graphs are seen of the gap as a function of temperatures for various values of nV^2 , for both magnetic and non-magnetic impurities. The graphs are for systems where $N = 40$ and the number of iterations is 60.

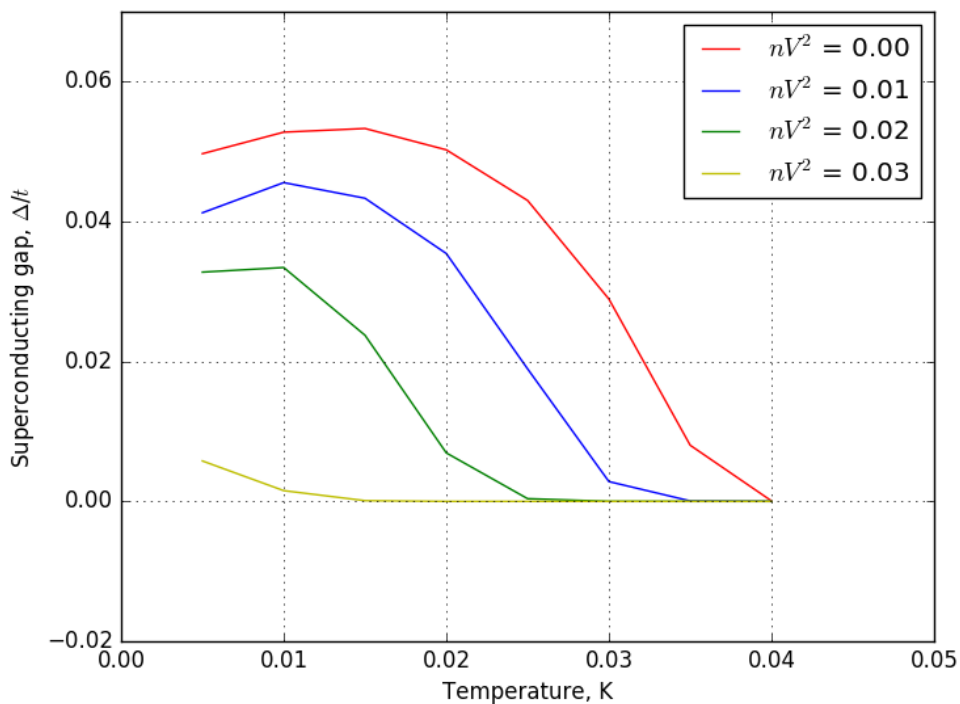


Figure 2: Gap parameter vs. temperature for various values of nV^2 , where the impurities are magnetic.

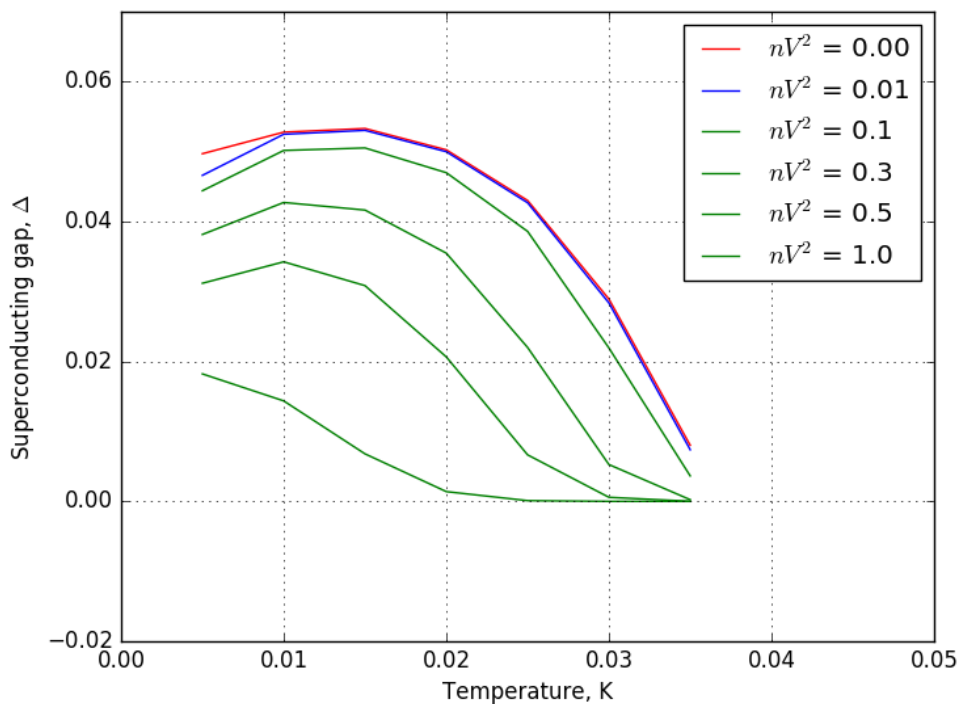


Figure 3: Gap parameter vs. temperature for various values of nV^2 , where the impurities are non-magnetic.

7.4 Gap equation in real space

The AG theory approach previously described takes impurities into account, but they are smeared out and not localised. The real space gap equation of 6.17 allows us to place impurities at certain lattice points and find the value for the gap parameter at each discrete point.

This computation uses the matrix from 6.19. The procedure is the following:

1. The matrix \mathbf{M} is constructed, by use of the rules outlined in 6.20.
2. Impurities are randomly distributed. Generate a set of random values of i and let elements $M_{i,i} = \mu \rightarrow \mu + V_2$ and $M_{N^2+i,N^2+i} = -\mu \rightarrow -\mu + V_2$.
3. Guess at a value, Δ_A , for the gap parameter, and assign this value to all matrix elements of the form $M_{(N^2+i,i)}$ and $M_{(i,N^2+i)}$.
4. Diagonalise the matrix, i.e. find its set of eigenvalues and -vectors.
5. Select elements i and $i + N^2$ from all eigenvectors in the set and use them to solve 6.17 to get the gap Δ_i on site i . Do this for all lattice sites. To achieve this, we use

```

1 def i_gap(vectors, eigenvals, T, i):
2     gap = 0.0
3     for a in range(H):
4         gap = gap + V_sc*vectors[i, a]*np.conjugate(vectors[
5             i+H, a])*np.tanh(np.real(eigenvals[a])/(2*T))
6     return gap

```

6. Redefine the matrix \mathbf{M} by assigning the value Δ_i to element $M_{(i,N^2+i)}$ and the value Δ_i^* to element $M_{(N^2+i,i)}$. Return to step 2.

This procedure can be repeated until the gap at every site reaches its convergence value. Instead of checking every site, which would be laborious for large systems, one can simply check for the convergence of the sum of the gaps on each site. This iteration procedure is written as follows:

```

1 for b in range(iterations):
2     total = 0.0
3     vals, vecs = np.linalg.eigh(lattice)
4     idx = vals.argsort()[::-1]
5     vals = vals[idx]
6     vecs = vecs[:,idx]
7     for i in range(H):
8         lattice[i][H+i]=i_gap(vecs, vals, a, i)
9         lattice[H+i][i]=np.conjugate(i_gap(vecs, vals, a, i)
10            )
11         total = total + i_gap(vecs, vals, a, i)
12     print("total: ", abs(total))

```

This routine uses the fact that \mathbf{M} is hermitian to reduce the time for the computation.

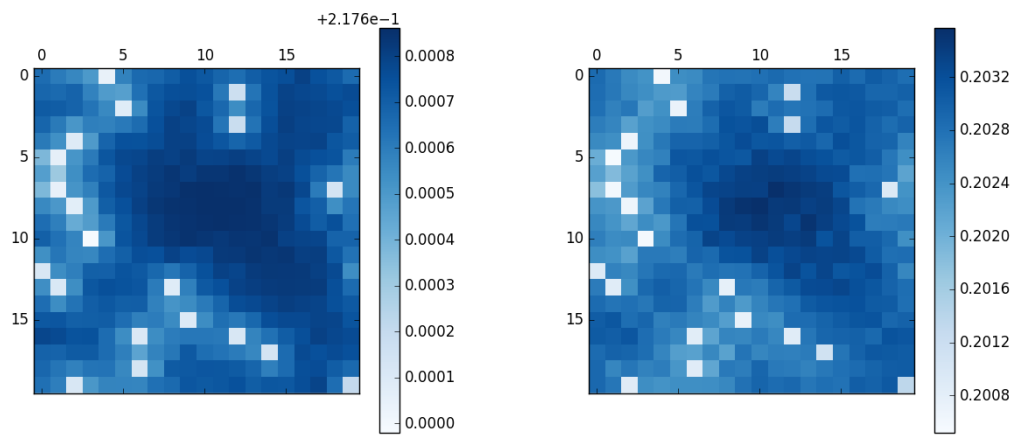
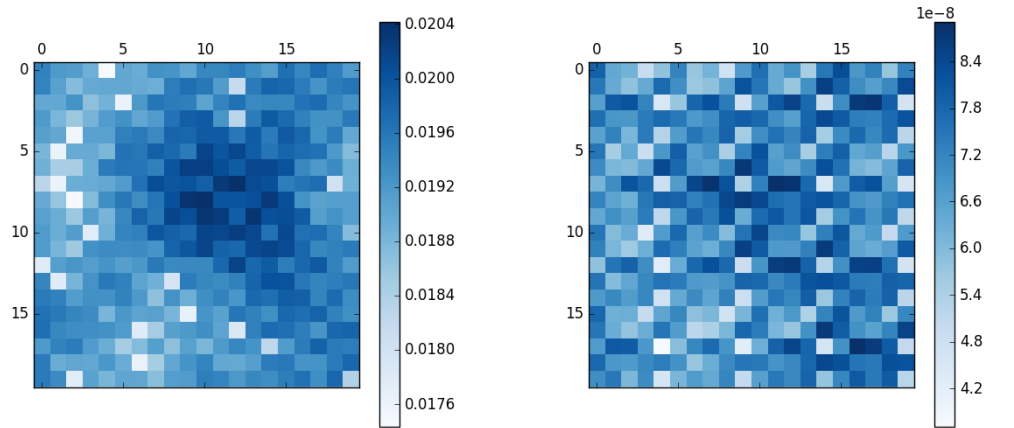
(a) $T=0.01$ K(b) $T=0.07$ K(c) $T=0.13$ K(d) $T=0.19$ K

Figure 4: The gap parameter on the sites of a lattice with $N=20$ and 20 impurity sites for various temperatures. $V_2 = 0.1t$.

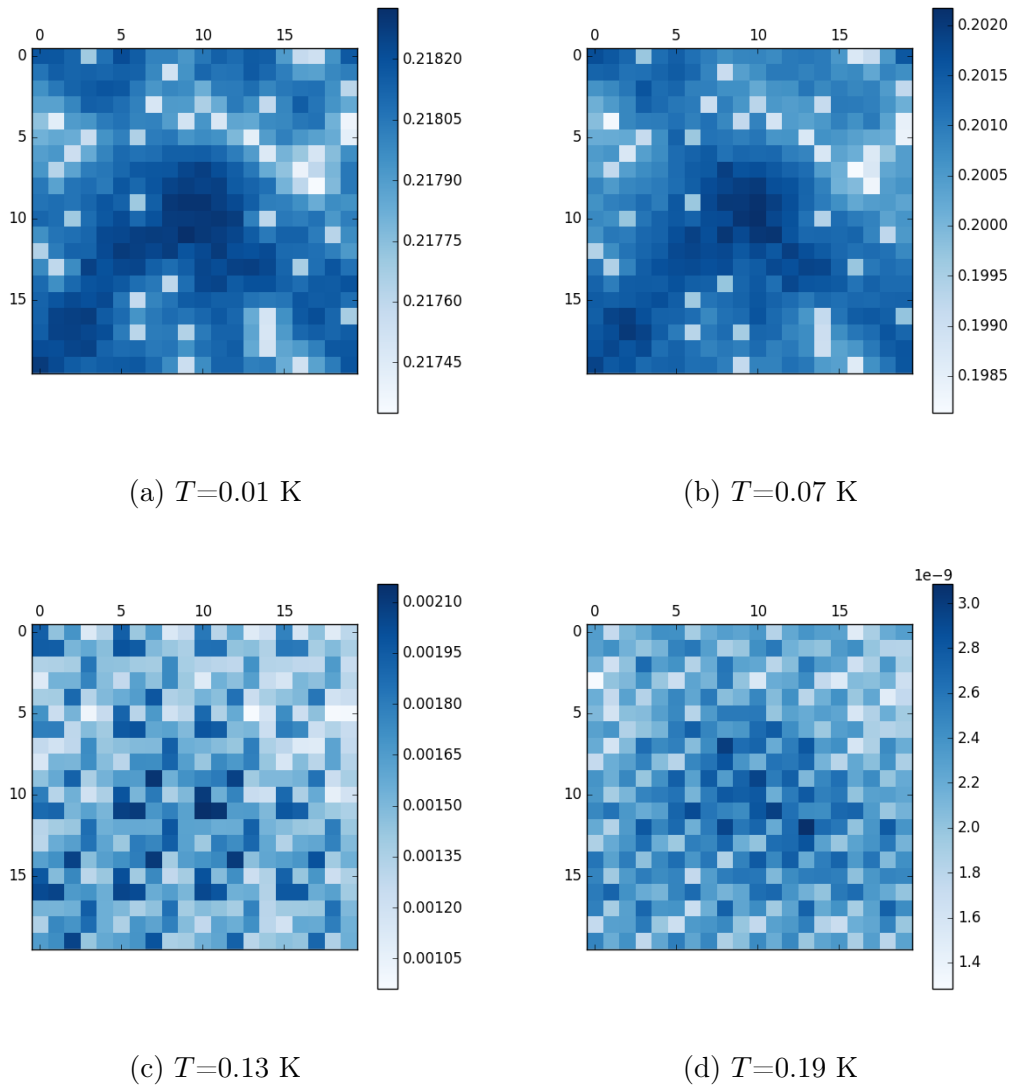


Figure 5: The gap parameter on the sites of a lattice with $N=20$ and 40 impurity sites for various temperatures. $V_2 = 0.1t$.

8 Discussion

The critical temperature, in the presence of a perturbation in the form of magnetic impurities, can be expressed in terms of a function of a Cooper-pair breaking parameter α [1]:

$$\ln\left(\frac{T_c}{T_{c0}}\right) + \psi\left(\frac{1}{2} + \frac{\alpha}{2\pi T_c}\right) - \psi\left(\frac{1}{2}\right) = 0 \quad (8.1)$$

T_{c0} is the critical temperature in the absence of impurities and $\psi(z)$ is the digamma function. Below is shown the relation between α and T_c . Superimposed are data points showing values of T_c for certain impurity concentrations.

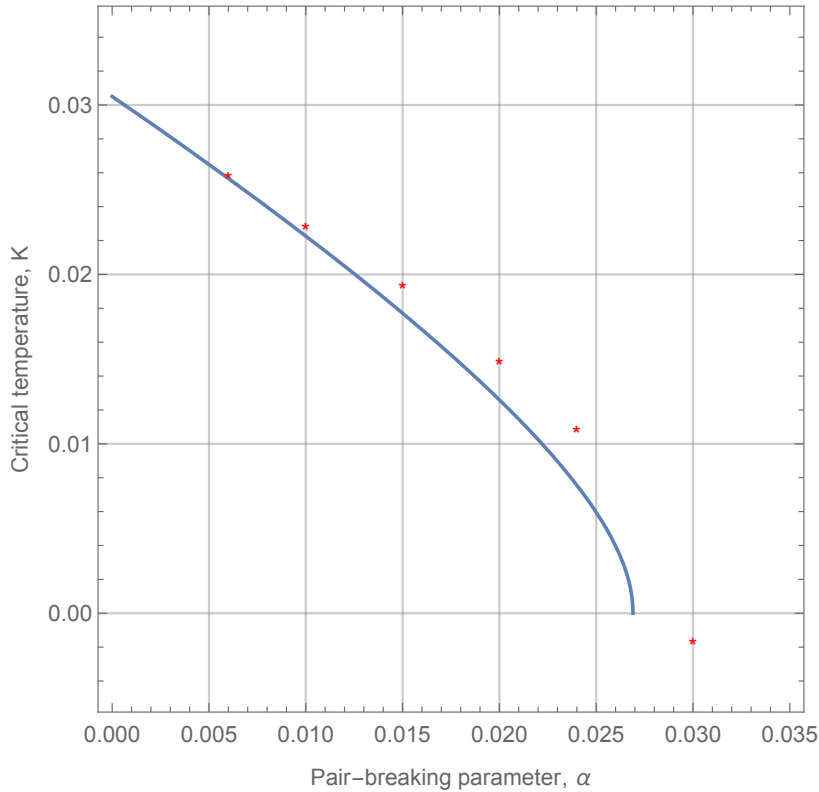


Figure 6: Critical temperature vs. the pair breaking parameter α .

For the plot in figure 6, the value of α is the same as that of nV^2 . The disagreement between the values found from simulation and those of 8.1 could be due to the lattice size, which in principle should be infinitely great to reproduce the expected dependence. However it is more likely that the range of n used for the Matsubara summation, as discussed in relation to 5.7 and 5.8, is too small. As the difference between successive frequencies scales with the temperature, this can be particularly problematic for small values of T , where the sum will not include a wide enough range of frequencies. An example of this is how the graphs in figures 2 and 3 show peaks in the gap parameter. The gap decreases with increasing temperature, as it should, but it also shows the gap decreasing for temperatures lower than that where the peak lies. This should not happen - the graphs should show the same behaviour as figure 1, where the gap is approximately unchanged up to the point where it starts to decrease. For the numerical simulation for AG theory, $n = 80$. A continuation of the work in this thesis could be to run simulations for successively greater n to see the effect on the data points in figure 6 and the low-temperature region of the graphs in figure 2 and 3.

The theoretical prediction of 8.1 follows directly from AG theory. Therefore, with a numerical simulation sophisticated enough, one would expect to reproduce it. The more interesting case is that of the real space formulation. AG theory considers a random distribution of impurity atoms and it would therefore have been very interesting to find the critical temperatures from the real space simulation with randomly distributed, localised impurities, and compare this to 8.1.

The dependence of the gap parameter on the temperature for various values of nV^2 as shown in figures 2 and 3 are partly in accordance with the expectations outlined in the introduction. The introduction of magnetic impurities into the superconductor

suppresses T_c , and as figure 2 clearly shows, the gap parameter quickly decreases in value as nV^2 is increased, and by $nV^2 = 0.03$ it is almost completely gone. For non-magnetic impurities the critical temperature is suppressed, but only for much greater values of nV^2 , contrary to the assumption that non-magnetic impurities would not affect the transition temperature.

Furthermore, the subfigures of both figure 2 and 3 show that as the temperature increases, the gap parameter throughout the lattice is suppressed, but in particular it is suppressed around the impurities.

9 Conclusion

It has been shown how magnetic and non-magnetic impurities suppress the critical temperature in a two-dimensional superconductor by use of AG theory. The spatially dependent suppression of T_c around impurities in the real space formulation of BCS theory has also been shown.

Were the timeframe for the project longer, an extension could be to find the critical temperature for many more values of nV^2 and compare them to the theoretical prediction of 8.1. A more interesting extension would be to find the critical temperatures for various impurity concentrations in the real space formulation to see how well these values agree with the theoretical expectations of AG theory.

10 References

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Appendix

A Calculation of $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$

The BCS mean-field Hamiltonian in 3.1 can, using the Nambu spinors, be rewritten in matrix form as

$$\alpha^\dagger \mathbf{A} \alpha = \begin{pmatrix} c_{\mathbf{k}\uparrow}^\dagger & c_{-\mathbf{k}\downarrow} \end{pmatrix} \begin{pmatrix} \xi_{\mathbf{k}} & -\Delta \\ -\Delta^* & -\xi_{-\mathbf{k}} \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c_{-\mathbf{k}\downarrow}^\dagger \end{pmatrix} \quad (\text{A.1})$$

Introduce the unitary matrix

$$\mathbf{U} = \begin{pmatrix} u_{\mathbf{k}} & -v_{\mathbf{k}} \\ v_{\mathbf{k}}^* & u_{\mathbf{k}}^* \end{pmatrix} \quad (\text{A.2})$$

\mathbf{U} diagonalises the matrix \mathbf{A} and thus

$$\mathbf{U}^\dagger \begin{pmatrix} \xi_{\mathbf{k}} & -\Delta \\ -\Delta^* & -\xi_{-\mathbf{k}} \end{pmatrix} \mathbf{U} = \begin{pmatrix} E_{\mathbf{k}} & 0 \\ 0 & -E_{\mathbf{k}} \end{pmatrix} \quad (\text{A.3})$$

where the diagonal contains the eigenvalues for the Hamiltonian. These eigenvalues are found in the usual way:

$$\det(\mathbf{A} - \lambda \mathbf{I}) = (\xi_{\mathbf{k}} - \lambda)(-\xi_{-\mathbf{k}} - \lambda) - |\Delta|^2 = 0 \quad (\text{A.4})$$

For a crystal symmetric under inversion $\xi_{\mathbf{k}} = \xi_{-\mathbf{k}}$ and the equation reduces to

$$\lambda = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta|^2} = E_{\mathbf{k}} \quad (\text{A.5})$$

By explicitly multiplying through equation A.3

$$\begin{pmatrix} E_{\mathbf{k}} & 0 \\ 0 & -E_{\mathbf{k}} \end{pmatrix} = \begin{pmatrix} u_{\mathbf{k}}(u_{\mathbf{k}}^* \xi_{\mathbf{k}} + v_{\mathbf{k}}^* \Delta^*) + v_{\mathbf{k}}^*(u_{\mathbf{k}}^* \Delta - v_{\mathbf{k}} \xi_{-\mathbf{k}}) & u_{\mathbf{k}}^*(u_{\mathbf{k}}^* \Delta - v_{\mathbf{k}} \xi_{-\mathbf{k}}) - v_{\mathbf{k}}(u_{\mathbf{k}}^* \xi_{\mathbf{k}} + v_{\mathbf{k}} \Delta^*) \\ u_{\mathbf{k}}(u_{\mathbf{k}} \Delta^* - v_{\mathbf{k}}^* \xi_{\mathbf{k}}) + v_{\mathbf{k}}^*(-v_{\mathbf{k}}^* \Delta - u_{\mathbf{k}} \xi_{-\mathbf{k}}) & u_{\mathbf{k}}^*(-v_{\mathbf{k}}^* \Delta - u_{\mathbf{k}} \xi_{-\mathbf{k}}) - v_{\mathbf{k}}(u_{\mathbf{k}} \Delta^* - v_{\mathbf{k}}^* \xi_{\mathbf{k}}) \end{pmatrix} \quad (\text{A.6})$$

If we let $u_{\mathbf{k}}$, $v_{\mathbf{k}}$ og Δ be real numbers for simplicity, while employing $\xi_{\mathbf{k}} = \xi_{-\mathbf{k}}$ we obtain

$$\begin{pmatrix} E_{\mathbf{k}} & 0 \\ 0 & -E_{\mathbf{k}} \end{pmatrix} = \begin{pmatrix} \xi_{\mathbf{k}}(u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2) + 2u_{\mathbf{k}}v_{\mathbf{k}}\Delta & \Delta(u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2) - 2u_{\mathbf{k}}v_{\mathbf{k}}\xi_{\mathbf{k}} \\ \Delta(u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2) - 2u_{\mathbf{k}}v_{\mathbf{k}}\xi_{\mathbf{k}} & \xi_{\mathbf{k}}(v_{\mathbf{k}}^2 - u_{\mathbf{k}}^2) - 2u_{\mathbf{k}}v_{\mathbf{k}}\Delta \end{pmatrix} \quad (\text{A.7})$$

thus we arrive at

$$E_{\mathbf{k}} = \xi_{\mathbf{k}}(u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2) + 2u_{\mathbf{k}}v_{\mathbf{k}}\Delta \quad (\text{A.8})$$

From A.5 we have that $\Delta = \sqrt{E_{\mathbf{k}}^2 - \xi_{\mathbf{k}}^2}$ and as \mathbf{U} is unitary, it follows that $u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1$. With this information, A.8 can be written as

$$E_{\mathbf{k}} = \xi_{\mathbf{k}}(2u_{\mathbf{k}}^2 - 1) + 2u_{\mathbf{k}}\sqrt{1 - u_{\mathbf{k}}^2}\sqrt{E_{\mathbf{k}}^2 - \xi_{\mathbf{k}}^2} \quad (\text{A.9})$$

and

$$E_{\mathbf{k}} = \xi_{\mathbf{k}}(1 - 2v_{\mathbf{k}}^2) + 2v_{\mathbf{k}}\sqrt{1 - v_{\mathbf{k}}^2}\sqrt{E_{\mathbf{k}}^2 - \xi_{\mathbf{k}}^2} \quad (\text{A.10})$$

whence we deduce that

$$|u_{\mathbf{k}}|^2 = \frac{1}{2} \left(1 + \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \right), \quad |v_{\mathbf{k}}|^2 = \frac{1}{2} \left(1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \right) \quad (\text{A.11})$$

B Proof of commutator identities

$$\begin{aligned}
[AB, C] &= ABC - CAB \\
&= ABC + (ACB - ACB) - CAB \\
&= A(BC - CB) + (AC - CA)B \\
&= A[B, C] + [A, C]B
\end{aligned} \tag{B.1}$$

$$\begin{aligned}
[AB, C] &= ABC - CAB \\
&= ABC + (ACB - ACB) - CAB \\
&= A(BC + CB) - (AC + CA)B \\
&= A\{B, C\} - \{A, C\}B
\end{aligned} \tag{B.2}$$

C Fourier transformation of the BCS mean-field Hamiltonian

$$\begin{aligned}
-\sum_{\mathbf{k}} \Delta c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger - \sum_{\mathbf{k}} \Delta^* c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} &= -\frac{1}{\mathcal{V}} \sum_{\mathbf{k}} \int_{\mathcal{V}} d\mathbf{r} \int d\mathbf{r}' \int d\mathbf{r}'' \Delta e^{-i\mathbf{k}\cdot\mathbf{r}} \Psi_{\uparrow}^\dagger(\mathbf{r}') e^{i\mathbf{k}\cdot\mathbf{r}'} \Psi_{\downarrow}^\dagger(\mathbf{r}'') e^{-i\mathbf{k}\cdot\mathbf{r}''} \\
&\quad - \frac{1}{\mathcal{V}} \sum_{\mathbf{k}} \int_{\mathcal{V}} d\mathbf{r} \int d\mathbf{r}' \int d\mathbf{r}'' \Delta e^{-i\mathbf{k}\cdot\mathbf{r}} \Psi_{\downarrow}(\mathbf{r}') e^{i\mathbf{k}\cdot\mathbf{r}'} \Psi_{\uparrow}(\mathbf{r}'') e^{-i\mathbf{k}\cdot\mathbf{r}''} \\
&= -\int_{\mathcal{V}} d\mathbf{r} \int d\mathbf{r}' \int d\mathbf{r}'' \Delta \Psi_{\uparrow}^\dagger(\mathbf{r}') \Psi_{\downarrow}^\dagger(\mathbf{r}'') \delta(-\mathbf{r} + \mathbf{r}' - \mathbf{r}'') \\
&\quad - \int_{\mathcal{V}} d\mathbf{r} \int d\mathbf{r}' \int d\mathbf{r}'' \Delta \Psi_{\downarrow}(\mathbf{r}') \Psi_{\uparrow}(\mathbf{r}'') \delta(-\mathbf{r} + \mathbf{r}' - \mathbf{r}'') \\
&= -\int_{\mathcal{V}} d\mathbf{r} \int d\mathbf{r}' \Delta \Psi_{\uparrow}^\dagger(\mathbf{r}') \Psi_{\downarrow}^\dagger(\mathbf{r}' - \mathbf{r}) \\
&\quad - \int_{\mathcal{V}} d\mathbf{r} \int d\mathbf{r}' \Delta \Psi_{\downarrow}(\mathbf{r}') \Psi_{\uparrow}(\mathbf{r}' - \mathbf{r})
\end{aligned} \tag{C.1}$$

$$\Delta = \frac{1}{\mathcal{V}} \sum_{\mathbf{k}} \Delta e^{i\mathbf{k}\cdot\mathbf{r}} = \Delta \delta(\mathbf{r}) \tag{C.2}$$

$$\begin{aligned}
&-\int_{\mathcal{V}} d\mathbf{r} \int d\mathbf{r}' \Delta \Psi_{\uparrow}^\dagger(\mathbf{r}') \Psi_{\downarrow}^\dagger(\mathbf{r}' - \mathbf{r}) \delta(\mathbf{r}) - \int_{\mathcal{V}} d\mathbf{r} \int d\mathbf{r}' \Delta \Psi_{\downarrow}(\mathbf{r}') \Psi_{\uparrow}(\mathbf{r}' - \mathbf{r}) \delta(\mathbf{r}) \\
&= -\int_{\mathcal{V}} d\mathbf{r}' \Delta \Psi_{\uparrow}^\dagger(\mathbf{r}') \Psi_{\downarrow}^\dagger(\mathbf{r}') - \int_{\mathcal{V}} d\mathbf{r}' \Delta \Psi_{\downarrow}(\mathbf{r}') \Psi_{\uparrow}(\mathbf{r}')
\end{aligned} \tag{C.3}$$

We are looking at a quadratic lattice with sides of length N and discrete lattice sites. The integral is changed to a sum over the positions:

$$\sum_i^N -\Delta_i c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger - \Delta_i^* c_{i\downarrow} c_{i\uparrow} \tag{C.4}$$

D Anticommutation of Bogoliubov-transformed operators

The Bogoliubov transformation cannot violate the canonical anti-commutation relation for fermion operators given by 2.2. For the c -operators in the form defined by the spin-generalised Bogoliubov transformation of 6.13, we have that

$$\begin{aligned}
0 = \{c_{i\uparrow}, c_{i\downarrow}\} &= \sum_n \left[(u_{n,i\uparrow}\gamma_{n\uparrow} + v_{n,i\uparrow}^*\gamma_{n\downarrow}^\dagger)(u_{n,i\downarrow}\gamma_{n\downarrow} + v_{n,i\downarrow}^*\gamma_{n\uparrow}^\dagger) \right. \\
&\quad \left. + (u_{n,i\downarrow}\gamma_{n\downarrow} + v_{n,i\downarrow}^*\gamma_{n\uparrow}^\dagger)(u_{n,i\uparrow}\gamma_{n\uparrow} + v_{n,i\uparrow}^*\gamma_{n\downarrow}^\dagger) \right] \\
&= \sum_n \left[v_{n,i\downarrow}^* v_{n,i\uparrow}^* \underbrace{\{\gamma_{n\uparrow}^\dagger, \gamma_{n\downarrow}^\dagger\}}_0 + u_{n,i\uparrow} u_{n,i\downarrow} \underbrace{\{\gamma_{n\uparrow}, \gamma_{n\downarrow}\}}_0 \right. \\
&\quad \left. + u_{n,i\uparrow} v_{n,i\downarrow}^* \underbrace{\{\gamma_{n\uparrow}, \gamma_{n\uparrow}^\dagger\}}_1 + v_{n,i\uparrow}^* u_{n,i\downarrow} \underbrace{\{\gamma_{n\downarrow}^\dagger, \gamma_{n\downarrow}\}}_1 \right] \\
&= \sum_n u_{n,i\uparrow} v_{n,i\downarrow}^* + \sum_n v_{n,i\uparrow}^* u_{n,i\downarrow} \\
-\sum_n u_{n,i\uparrow} v_{n,i\downarrow}^* &= \sum_n v_{n,i\uparrow}^* u_{n,i\downarrow}
\end{aligned} \tag{D.1}$$

E An example of the M-matrix

Below is shown the matrix M for a lattice with sides of length 3.

$$\psi^\dagger \left(\begin{array}{cccccccc|cccccccc}
-\mu & -t & -t & -t & 0 & 0 & -t & 0 & 0 & \Delta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-t & -\mu & -t & 0 & -t & 0 & 0 & -t & 0 & 0 & \Delta & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-t & -t & -\mu & 0 & 0 & -t & 0 & 0 & -t & 0 & 0 & \Delta & 0 & 0 & 0 & 0 & 0 & 0 \\
-t & 0 & 0 & -\mu & -t & -t & -t & 0 & 0 & 0 & 0 & 0 & \Delta & 0 & 0 & 0 & 0 & 0 \\
0 & -t & 0 & -t & -\mu & -t & 0 & -t & 0 & 0 & 0 & 0 & 0 & \Delta & 0 & 0 & 0 & 0 \\
0 & 0 & -t & -t & -t & -\mu & 0 & 0 & -t & 0 & 0 & 0 & 0 & 0 & \Delta & 0 & 0 & 0 \\
-t & 0 & 0 & -t & 0 & 0 & -\mu & -t & -t & 0 & 0 & 0 & 0 & 0 & 0 & \Delta & 0 & 0 \\
0 & -t & 0 & 0 & -t & 0 & -t & -\mu & -t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta & 0 \\
0 & 0 & -t & 0 & 0 & -t & -t & -t & \mu & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta \\
\hline
\Delta^* & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mu & t & t & t & 0 & 0 & t & 0 & 0 \\
0 & \Delta^* & 0 & 0 & 0 & 0 & 0 & 0 & 0 & t & \mu & t & 0 & t & 0 & 0 & t & 0 \\
0 & 0 & \Delta^* & 0 & 0 & 0 & 0 & 0 & 0 & t & t & \mu & 0 & 0 & t & 0 & 0 & t \\
0 & 0 & 0 & \Delta^* & 0 & 0 & 0 & 0 & 0 & t & 0 & 0 & \mu & t & t & t & 0 & 0 \\
0 & 0 & 0 & 0 & \Delta^* & 0 & 0 & 0 & 0 & 0 & t & 0 & t & \mu & t & 0 & t & 0 \\
0 & 0 & 0 & 0 & 0 & \Delta^* & 0 & 0 & 0 & 0 & 0 & t & t & t & \mu & 0 & 0 & t \\
0 & 0 & 0 & 0 & 0 & 0 & \Delta^* & 0 & 0 & t & 0 & 0 & t & 0 & 0 & \mu & t & t \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta^* & 0 & 0 & t & 0 & 0 & t & 0 & t & \mu & t \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta^* & 0 & 0 & t & 0 & 0 & t & t & t & \mu
\end{array} \right) \psi \tag{E.1}$$