SUPERCONDUCTIVITY IN A 2D SEMICONDUCTOR SYSTEM WITH UNCONVENTIONAL PAIRING SYMMETRY: INTER-BAND PAIRING

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Table of Contents

Li	st of I	Figures	v
A	ckno	wledgments	vii
1	Intr	\mathbf{r} oduction	1
2	Sup	erconductivity	6
	2.1	General Background	6
	2.2	Cooper pairs	7
	2.3	BCS theory	10
	2.4	Section Summary	15
3	Sem	niconductors	18
	3.1	General Background: Metal, Semiconductor, Insulator	18
	3.2	Pairing in Semiconductors	22
4	Der	ivation of the gap equation	27
	4.1	This Model	27
	4.2	Detailed Derivation	27
5	S-W	Vave Pairing Symmetry	38
	5.1	Zero Temperature	39
	5.2	Finite Temperature	41

6	D-W	Vave Pairing Symmetry	43
	6.1	Zero Temperature	44
	6.2	Finite Temperature	46
7	Res	ults	49
	7.1	s-wave	50
	7.2	d-wave	57
8	Con	$\operatorname{clusion}$	66
Re	eferen	Ces	69

List of Figures

1	shows the construction of Cooper Pairs above the filled Fermi Surface	10
2	typical BCS data from an experiment showing the temperature depen-	
	dence of the superconducting gap	17
3	energy band model for solids defining the insulator metal crossover at	
	T=0	20
4	a simple band structure with symmetric bands showing possible pairing	
	symmetries	23
5	SIT shown in graph of the superconducting gap versus temperature for	
	d-wave symmetry	25
6	a simple band structure with symmetric bands showing inter-band pair-	
	ing simulated in this model	26
7	graph showing superconducting gap magnitude versus temperature for	
	fixed cutoff with different potential strengths with s-wave symmetry .	51
8	graph showing superconducting gap magnitude versus temperature for	
	critical semiconducting gaps with s-wave symmetry $\ldots \ldots \ldots$	53
9	graph showing superconducting gap magnitude versus temperature for	
	fixed interaction strength with different cutoffs with s-wave symmetry	54
10	graph showing superconducting gap magnitude over critical tempera-	
	ture versus scaled cutoff for s-wave symmetry	56
11	grap showing superconducting gap magnitude versus temperature for	
	fixed cutoff with different potential strengths for d-wave symmetry	58

12	graph showing superconducting gap magnitude versus temperature for	
	critical semiconducting gap with d-wave symmetry, specifically the	
	sharp drop near SIT	60
13	graph showing superconducting gap magnitude versus temperature for	
	fixed interaction strength with different cutoffs for d-wave symmetry .	61
14	graph showing superconducting gap magnitude over critical tempera-	
	ture versus scaled cutoff for d-wave symmetry $\ldots \ldots \ldots \ldots \ldots$	62
15	gap versus temperature with fixed potential and cutoff for both s and	
	d wave symmetry	64

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Chapter 1

Introduction

Ever since the phenomenon of superconductivity was discovered in 1911, physicists have made numerous attempts to explain the observed behavior in various types of systems, and give a full many-body explanation. In this thesis we want to understand some of the basic features of paired fermions, as well as explore possible new physics related to unconventional pairing symmetries in the presence of an inherent gap in two dimensions (2D). This might be for example a constant gap like in semi conductors or a charge density wave or magnetic gap.

The first critical temperatures (T_c) describing the point of transition from the normal to the superconducting state, were fairly small ($\approx 4K$). Bardeen, Cooper and Schrieffer (BCS) [1] were the first to give a complete many body description of the phenomenon for so called conventional superconductors. Through the Cooper instability concept [2] a model was introduced, that allowed the normal state to become unstable against an infinitesimal attractive interaction between electrons near the Fermi surface in 3 dimensions (3D). Later, even higher T_c 's could be observed, demanding further theoretical explanation.

The investigation in this work is motivated by several experimental phenomena; one is the recently discovered superconductivity in solids with a normal state not metallic. This is interesting because usually superconductivity in an insulator is not expected, since Cooper pairs come from electrons at the Fermi Surface. Among other experiments such as Goldman's and Markovic's [3], that are the ones on disordered indium oxide films by M. Steiner and A. Kapitulnik [4] (2005) showing the existence of a field-tuned superconductor-insulator-transition (SIT). There the insulating phase of disordered indium oxide films that undergo a field-tuned SIT is studied. Transport measurements are taken and the strength of the insulating phase is determined. They find that the films do not return to the expected normal state even at high perpendicular magnetic fields where all pairs should be broken and suggest the remaining presence of superconductivity at high fields.

Also, C. Chu, A. Rusakov and S. Huang [5] found large diamagnetic anomalies on cuprous chloride at about 200K, which if interpreted as the occurrence of superconductivity, would show superconductivity out of a semiconducting phase. The long standing interest in a deeper understanding of the high T_c cuprates where the normal state is a strange metal provides evidence for different gap symmetries and coupling mechanisms.

In recent years, there has been a great interest in studying different aspects and possibilities of fermion pairing. Important questions such as 1) What is the general nature of paired states with the absence of the Fermi surface? 2) What possible ways are there to pair in a multi-band model and what differences does that make for the paired states and their properties? 3) Does the pairing gap symmetry play a key role in explaining the observed types of pairing? Of course, there has been previous work in this direction, as discussed later. Remarkably, the concrete nature of the pseudogap is still not quite clear, neither is its true origin nor its specific attributes. What we call pseudogap describes a not perfect gap with reduced density of states with features observed for example in underdoped high T_c cuprates due to correlations. The simple model of a semiconducting gap seems a good choice to simulate the observed gap.

The idea to investigate superconductivity in a semiconductor is not new, it was studied by Kelly and Handke [6], including intra-band interactions in a doped material, giving a possible explanation for the scarcity of carriers. They claimed, that the pairing is dominated by intervalley phonon exchange, whereas at low densities it is essentially due to exchange of electronic (plasmon, electron-hole) excitations. An inter-band pairing (pairing between the bands) was first considered by Kohmoto and Takada [7], who did 3D calculations with s-wave pairing symmetry. They obtained the Meissner effect and infinite dc-conductivity similar to that in the BCS superconductors, but also many unusual properties due to an unconventional gap equation. The next step toward a deeper understanding of the pseudogap between the bands was done by Nozieres and Pistolesi [8], who gave a simple model for the pseudogap with intra-band pairing. Liao and Quader [9] studied the impact of the gap pairing symmetry specifically for the intra-band interaction case (pairing within the bands), using Noziere's and Pistolesi's simple model for the pseudogap. This work also explores the features of the bound fermion states with an inter-band pairing for different gap symmetries such as s- and d-wave. We chose a 2D model with a mean field Hamiltonian allowing only for pairing across the semiconducting gap, due to the experiment by Steiner and Kapitulnik. Using the Matsubara Green's function method, a gap equation is derived and studied for zero and finite temperature. This is the typical equation for BCS to derive the superconducting gap, the main feature of superconductivity (see below). Our interest includes basic features such as the behavior of the superconducting gap with temperature, as well as the comparison of obtained properties such as gap size and transition temperatures to the intra-band case or the regular BCS metal. We also study how the pairing symmetry (s- and dwave) modifies the behavior of the bound states quantitatively and qualitatively and believe the reason for any difference lies within the different strength of interaction for the symmetries.

Before discussing my new results I introduce the composition of the thesis.

The second chapter covers some basics of the well known BCS theory which successfully explains conventional superconductivity in metals. Those are fundamental to understand the background and motivation of this work, as well as the specifically interesting features we would like to explore here.

The third chapter gives some general background in semiconductors, but mainly introduces the basic ideas of possible pairing in semiconductors. It gives specific results of the intra-band case and presents the major difference between that type of pairing and its consequences.

Chapter 4 includes the full derivation of the gap equation used in this work, combining the attained knowledge from chapter two and three.

In Chapters 5 and 6, specific equations in preparation for numerical solutions for s- and d-wave pairing symmetry are derived, both for zero and finite temperature, respectively.

Chapter 7 shows several numerically obtained results along with figures. It treats the findings separately for s- and d-wave symmetry, demonstrating some quite different behavior from the regular BCS limit or the intra-band case. Finally the role of gap symmetry is emphasized in plots with both, s- and d-wave with the same parameters.

The last chapter summarizes all the interesting and newly found results. Concluding the expectations given in this chapter compared to the actual findings, this thesis ends with a small overview of possible improvements in future work.

Chapter 2

Superconductivity

2.1 General Background

There are many good books on superconductivity, explaining background and basic findings. [10], [11], [12] were mainly used to summarize some of it into this over viewing chapter.

Superconductivity was first discovered in 1911 by Heike Kamerlingh Onnes. He studied the resistivity of solid mercury at very low temperature using liquid Helium as a refrigerant, where at the temperature of $T_c = 4.2K$ the DC electrical resistance abruptly disappeared. In 1933 Meissner and Ochsenfeld discovered that metals in the superconducting phase expel applied magnetic fields. London and London showed later on that the Meissner-Ochsenfeld effect was due to the minimization of the free energy carried by the electrical current, advancing a phenomenological theory of the behavior of the superconducting state. Ginzburg and Landau extended this work in 1950, introducing an effective wave function which later on corresponds to the center of mass wave function of the BCS pairs. This phenomenological description of the macroscopic properties was used by Abrikosov to predict a division of superconductors into categories, namely Type I and Type II. In the same year Reynolds and Maxwell independently discovered the so called isotope effect, stating the transition temperature T_c to be a function of the ion mass of the element. This important discovery suggested the electron-phonon interaction to be the microscopic mechanism responsible for superconductivity. The BCS theory in 1957 by Bardeen-Cooper-Schrieffer was the first complete microscopic theory of superconductivity, though Nikolay Bogolyubov also explained the phenomenon independently of the group. Their BCS theory proposes the superconducting state as a result of electron pairing due to an attractive phonon-mediated electron-electron interaction. In the BCS ground state electrons with opposite spin and momentum are coupled into so called Cooper pairs, described in the BCS wave function, which will be discussed in further detail below. The theory also predicted an energy gap in the excitation spectrum, which was first observed with electron tunneling in 1960 by Giaever, verifying BCS theory. In 1962 the first commercial superconducting wire, a niobium-titanium alloy, was developed at Westinghouse Electric Corporation. Brian Josephson made an important theoretical prediction, which is used in superconducting devices such as SQUIDs nowadays. He stated that a supercurrent can flow between two pieces of superconducting material separated by a thin layer of insulator. In 1986 Bednorz and Mller published their discovery of the first so called high- T_c superconductor ($T_c = 35K$), a lanthanum-based cuprate perovskite material. Later on elements with transition temperatures up to $T_c = 133K$ were found. A correct theoretical attempt to explain this phenomenon is yet to be made. Experiments show a missing isotope effect and suggest that phonons are not the main reason. BCS theory does not work here.

2.2 Cooper pairs

The simplest model to describe how an attraction can bind pairs of electrons into a bound state was first derived in 1956 by Cooper. He showed how the Fermi sea of electrons becomes unstable against a bound pair of electrons, for an arbitrary small positive attraction. A so called Cooper pair therefore describes a bound state of two electrons above the filled Fermi surface. In the Cooper problem two fermions (with wave vectors k_1, k_2) interact above the Fermi surface through a two-body spinindependent potential at T=0. All electrons but those two are assumed to be noninteracting. Assuming the lowest energy state to have zero total momentum, the two electrons must have equal and opposite momenta. In the figure at the end of this section one can see a simple sketch of the model.

The orbital wave function of the pair is written as:

$$\Psi_{CP}(r_1, r_2) = \sum_{k>k_F} g_k e^{ikr_1} e^{-ikr_2}$$
(2.1)

with g_k being the weighting coefficients. The Hamiltonian of the pair disregarding Coulomb Interaction is:

$$H_{CP} = H_0 + V_{eff} \tag{2.2}$$

with $H_0 = \frac{(\Delta_k)^2}{2m} = \xi_k$ being the kinetic energy term of the pair. V_{eff} is the phonon mediated electron-electron interaction, for simplicity given by:

$$V_{eff} = \begin{cases} V_0 \text{ for } |\xi_k| > \omega_D \\ 0 \text{ otherwise} \end{cases}$$
(2.3)

where ω_D is the Debye-frequency of the phonons. The solution to the Schrdinger equation

$$H_{CP}|\Psi_{CP}\rangle = E_{CP}|\Psi_{CP}\rangle \tag{2.4}$$

gives the eigen energy

$$E_{CP} = 2\omega_D (e^{\frac{2}{Vd(\epsilon_F)}} - 1)^{-1}$$
(2.5)

with $d(\epsilon_F)$ being the density of states at the Fermi level. In the so called weak coupling limit, where $Vd(\epsilon_F) \ll 1$, the energy gain by forming a Cooper pair will be around:

$$\Delta_{CP} = |E_{CP}| \approx 2\omega_D e^{\frac{-2}{Vd(\epsilon_F)}} \tag{2.6}$$

Thus, there exists a two-electron bound state with energy ≥ 0 . This energy is gained starting from the free electron gas, once an interaction is turned on. The electrons will bind in pairs, therefore making the normal state unstable. Most importantly one can see that no matter how small the interaction is, as long as it is attractive, any pair of electrons will gain energy by forming a pair near the Fermi surface. This is quite distinct from the usual two-body problems, where particles coupled with an attractive potential do not form a bound state with gain in energy, unless the interaction exceeds a certain threshold. Physically one can imagine the electrons propagating through the crystal and attracting positive ions. Those basically cause a positive trace, which is felt by the other electrons as an interaction. Therefore only fermions occupying states with reversed momenta can utilize this trail of each other. Moreover the characteristic energy scale seems not to be the Debye frequency ω_D , rather ω_D suppressed by the exponential factor from above, including interaction. That explains the rather small transition temperatures. In real superconducting systems the pairs are either rather separated in space and/or interacting weakly, which is different from the model considered above.



Figure 1: shows the construction of Cooper Pairs above the filled Fermi Surface

2.3 BCS theory

When Bardeen, Cooper and Schrieffer tried to give a microscopic theory of the phenomenon mentioned above, they were looking for a many-body wave function acting on the vacuum state which describes the Cooper pairing. It should include the phonon mediated electron-electron interaction for fermions near the Fermi surface as well as the instability of the normal state of the Fermi surface with the formation of such Cooper pairs. They took as their form of the superconducting ground state the following variational wave function:

$$\left|\Psi_{BCS}\right\rangle = \prod_{k} \left(u_{k} + v_{k}c_{k\uparrow}^{+}c_{-k\downarrow}^{+}\right) \left|0\right\rangle$$
(2.7)

with $|u_k|^2 + |v_k|^2 = 1$ and $|0\rangle$ being the Fermi sea. The probability of the pair $(k \uparrow, -k \downarrow)$ to be occupied is given by $|v_k|^2$, whereas the probability to be not occupied is given by $|u_k|^2 = 1 - |v_k|^2$, both being complex expansion coefficients. Since the number of particles involved is huge, no enormous mistake is made by working in a system where the average particle number is fixed. The wave function therefore

contains an undetermined integer number of Cooper pairs, being in contact with an electron reservoir allowing for fluctuations in the particle number. Basically we work in a grand canonical ensemble. The determination of the coefficients $|v_k|^2$, $|u_k|^2$ can be done in different ways, but that shall not be a matter of discussion here. Instead, the BCS mean field approximation shall be introduced. Turning on an electron-electron interaction in any non-interacting electron gas usually causes a low-energy excitation $\frac{\hbar^2 k^2}{2m} - \mu$ to become an excitation of quasi particles with energy ξ_k with same momentum k. The additional phonon mediated interaction between those quasi particles only is considered to be responsible for Cooper pairing. Therefore the BCS Hamiltonian looks as follows:

$$H_{BCS} = \sum_{k\sigma} \xi_k c^+_{k\sigma} c_{k\sigma} + \sum_{kk'} V_{kk'} c^+_{k\uparrow} c^+_{-k\downarrow} c_{-k'\downarrow} c_{k'\uparrow}$$
(2.8)

with $V_{kk'}$ being the attractive interaction. The Cooper pair formation described with this Hamiltonian creates the Bose-Einstein like condensate of bound quasi particle fermions, each with zero momentum and spin. That newly formed state is described with the BCS ground state $|\Psi_{BCS}\rangle$.

The mean field approximation comes in due to the presence of so many Cooper pairs in the BCS ground state. It replaces operators by expectation values. Therefore the ground state expectation value $\langle c_{k\uparrow}^+ c_{-k\downarrow}^+ \rangle \neq 0$ and the fluctuations around it are assumed to be very small. The critical temperature T_C separates the normal state from the superconducting phase in which this expectation value in non-zero. Keeping this in mind, the BCS mean field Hamiltonian can be derived from (eq. 2.8) and has the form:

$$H_{BCS}^{MF} = \sum_{k\sigma} \xi_k c_{k\sigma}^+ c_{k\sigma} - \sum_k \Delta_k c_{k\uparrow}^+ c_{-k\downarrow}^+ - \sum_k \Delta_k^* c_{-k'\downarrow} c_{k'\uparrow}$$

$$\Delta_k = -\sum_{k'} V_{kk'} < c_{-k'\downarrow} c_{k'\uparrow} >$$
(2.9)

There are different ways to solve this Hamiltonian, for example with Bogoliubov transformations, what BCS did or in terms of Matsubara Green's functions, [13]. Considering my calculations are based on the second attempt I will present the Greens Function Method here, the results in both cases being the same, of course.

The normal Green's function $G_{\uparrow\uparrow}(k,\tau)$ and the anomalous Green's function $F_{\downarrow\uparrow}(k,\tau)$ are defined as:

$$G_{\uparrow\uparrow}(k,\tau) = - \langle T_{\tau}c_{k\uparrow}(\tau)c_{k\uparrow}^{+}(0) \rangle$$

$$F_{\downarrow\uparrow}(k,\tau) = - \langle T_{\tau}c_{-k\downarrow}^{+}(\tau)c_{k\uparrow}^{+}(0) \rangle$$
(2.10)

with T_{τ} representing the time ordered product of the following operators with respect to τ . The anomalous Green's function is zero in the normal state, but with the BCS assumption for the ground state expectation value to have non-zero components, there will be non-zero values in the superconducting state. The goal is now to find selfconsistent equations for the correlation functions F and G. The time ordered product will be evaluated first.

$$G_{\uparrow\uparrow}(k,\tau) = -\Theta(\tau)c_{k\uparrow}(\tau)c_{k\uparrow}^+(0) - \Theta(-\tau)c_{k\uparrow}^+(0)c_{k\uparrow}(\tau)$$
(2.11)

Taking the derivative with respect to τ gives:

$$\partial_{\tau}G_{\uparrow\uparrow}(k,\tau) = -\delta(\tau)c_{k\uparrow}(\tau)c_{\uparrow}^{+}(0) - \delta(\tau)c_{k\uparrow}^{+}(0)c_{k\uparrow}(\tau) - \Theta(\tau)\partial_{\tau}c_{k\uparrow}(\tau)c_{k\uparrow}^{+}(0) + \Theta(-\tau)c_{k\uparrow}^{+}(0)\partial_{\tau}c_{k\uparrow}(\tau)$$
$$= -\delta(\tau) - \langle T_{\tau}\partial_{\tau}c_{k\uparrow}(\tau)c_{k\uparrow}^{+}(0) \rangle$$
(2.12)

The equation of motion method is used to express the derivatives of each operator with respect to τ .

$$\frac{d}{d\tau}c_{k\sigma}(\tau) = [H_{BCS}^{MF}, c_{k\sigma}] = -\xi_k c_{k\uparrow}(\tau) - \Delta_k c_{-k\downarrow}^+(\tau)$$
(2.13)

Thus, the first equation can be simplified to:

$$\partial_{\tau}G_{\uparrow\uparrow}(k,\tau) = -\delta(\tau) + \xi_k < Tc_{k\uparrow}(\tau)c_{k\uparrow}^+(0) > -\Delta_k < Tc_{-k\downarrow}^+(\tau)c_{k\uparrow}^+(0) >$$

$$= -\delta(\tau) - \xi_k G_{\uparrow\uparrow}(k,\tau) + \Delta_k F_{\downarrow\uparrow}(k,\tau)$$
(2.14)

Equivalently for the anomalous correlation function one finds:

$$\partial_{\tau} F_{\downarrow\uparrow}(k,\tau) = -\xi_k F_{\downarrow\uparrow}(k,\tau) + \Delta_k^* G_{\uparrow\uparrow}(k,\tau)$$
(2.15)

Using the so called Matsubara Green's function technique, a Fourier transform from τ -space into ω is performed, followed by a Matsubara frequency summation (also see: [14], p.639ff).

$$(-i\omega_n + \xi_k)G_{\uparrow\uparrow}(k, i\omega_n) = -1 + \Delta_k F_{\downarrow\uparrow}(k, i\omega_k)$$

$$(-i\omega_n - \xi_k)F_{\downarrow\uparrow}(k, i\omega_n) = \Delta_k^* G_{\uparrow\uparrow}(k, i\omega_k)$$

$$(2.16)$$

These algebraic equations can be easily solved, the poles of the correlation functions now giving the quasi particle energy excitation spectrum:

$$F_{\downarrow\uparrow}(k, i\omega_k) = \frac{-\Delta_k^*}{(i\omega_n)^2 - (\xi_k^2 + |\Delta_k|^2)}$$

$$G_{\uparrow\uparrow}(k, i\omega_k) = \frac{i\omega_n + \xi_k}{(i\omega_n)^2 - (\xi_k^2 + |\Delta_k|^2)}$$
(2.17)

with the poles: $i\omega_n = \pm E_k = \pm \sqrt{\xi^2 + |\Delta_k|^2}$.

The BCS order parameter was originally defined in eq. 2.9 and can be related to the anomalous correlation function in the following way:

$$\Delta_k = V \sum_{k}^{k < \omega_D} < c_{-k\downarrow} c_{k\uparrow} > = V \sum_{k}^{k < \omega_D} F_{\downarrow\uparrow}^*(k, \tau = 0)$$
(2.18)

with $F_{\downarrow\uparrow}^*(k,\tau=0)$ being the Fourier transformed correlation function from above. If that is put in one gets an expression for the BCS energy gap $\Delta_k(T)$

$$\Delta_{k} = V \sum_{k}^{k < \omega_{D}} \sum_{i\omega_{n}} \frac{-\Delta_{k} e^{-i\omega_{n}0}}{(i\omega_{n})^{2} - (\xi_{k}^{2} + |\Delta_{k}|^{2})}$$

$$= -V \sum_{k}^{k < \omega_{D}} \Delta_{k} \left(\frac{n_{F}(E_{k})}{2E_{k}} + \frac{n_{f}(-E_{k})}{-2E_{k}}\right)$$
(2.19)

Using the frequency summation: $S = \frac{1}{\beta} \sum_{n} f(i\omega_n) = -\sum_{i} r_i n_F(Z_i)$, where r_i stands for the residue of the function $f(i\omega_n)$ one gets:

$$1 = V \sum_{k}^{k < \omega_D} \frac{1 - 2n_F(E_k)}{2E_k} = V d(\epsilon_F) \int_{-\omega_D}^{\omega_D} d\xi_k \frac{tanh(\frac{\beta}{2}\sqrt{\xi^2 + |\Delta_k|^2})}{2\sqrt{\xi^2 + |\Delta_k|^2}}$$
(2.20)

with $d(\epsilon_F)$ being the electronic density of states at the Fermi level. The sum over k was converted into an integral in energy space over ξ_k and tanh(x) coming from the exponential functions of the Fermi-function $n_F(\epsilon)$ explicitly. A concrete expression for the BCS energy gap for finite Temperature can be determined from this equation numerically. In the T=0 limit we can find an analytic expression with:

$$1 = Vd(\epsilon_F) \int_0^{\omega_D} \frac{d\xi}{\sqrt{\xi^2 + |\Delta_k|^2}} = Vd(\epsilon_F)sinh(\frac{\omega_D}{|\Delta_k|})^{-1}$$
(2.21)

which gives for the weak-coupling limit $Vd(\epsilon_F) \ll 1$:

$$|\Delta(T=0)| = 2\omega_D e^{\frac{-1}{Vd(\epsilon_F)}}$$
(2.22)

Finally, the finite T equation can be used to get out an explicit expression of the critical temperature T_c . Therefore the limit of Δ going to zero is taken. Physically the superconducting state breaks down for any value greater than T_c , which gives a

zero value for the order parameter gap.

$$\lim_{T \to 0} 1 = V d(\epsilon_F) \int_{-\omega_D}^{\omega_D} d\xi_k \frac{tanh(\frac{\beta}{2}\sqrt{\xi^2 + |\Delta_k|^2})}{2\sqrt{\xi^2 + |\Delta_k|^2}}$$
(2.23)

$$1 = Vd(\epsilon_F) \int_0^{\omega_D} d\xi \frac{1}{\xi} tanh(\frac{\xi}{2k_B T_c}) = Vd(\epsilon_F) \int_0^{\frac{\omega_D}{2k_B T_c}} dx tanh(x) \quad (2.24)$$

$$k_B T_c \approx 1.13 \omega_D e^{\overline{Vd(\epsilon_F)}}$$
 (2.25)

An important and strong prediction can be obtained by dividing the zero temperature limit gap by the analytic expression for T_c which is found to be without any parameters, valid in the weak coupling limit and for pairing in s-wave with l=0.

$$\frac{\Delta(T=0)}{k_B T_c} = \frac{2\omega_D e^{\frac{-1}{Vd(\epsilon_F)}}}{1.13\omega_D e^{\frac{-1}{Vd(\epsilon_F)}}}$$
(2.26)

$$\frac{\Delta(T=0)}{k_B T_c} = 1.76$$
(2.27)

Note that the universal value for this ratio is different for non-s-wave symmetry.

2.4 Section Summary

Bardeen, Cooper and Schrieffer presented a complete microscopic description of the phenomenon of superconductivity, proving that for any finite attractive potential between fermions, the gain in energy by a bound pair of electrons above the Fermi surface makes the normal state less favorable and unstable. This interaction is supposed to be attractive and phonon mediated. Starting with a mean-field assumption due to the presence of many Cooper pairs of fermions with equal but opposite momenta k, a mean-field Hamiltonian was derived. Thus,

$$\begin{aligned} |\Psi_{BCS}\rangle &= \prod_{k} (u_k + v_k c_{k\uparrow}^+ c_{-k\downarrow}^+) \bigg| 0 > \\ \text{with } |u_k|^2 + |v_k|^2 = 1 \text{ acting on the vacuum state} \\ |v_k|^2 \text{ corresponding to the probability of the pair } (k\uparrow, -k\downarrow) \text{ to be occupied} \end{aligned}$$

$$H_{BCS}^{MF} = \sum_{k\sigma} \xi_k c_{k\sigma}^+ c_{k\sigma} - \sum_k \Delta_k c_{k\uparrow}^+ c_{-k\downarrow}^+ - \sum_k \Delta_k^* c_{-k'\downarrow} c_{k'\uparrow}$$
$$\Delta_k = -\sum_{k'} V_{kk'} < c_{-k'\downarrow} c_{k'\uparrow} >$$

 Δ_k is introduced as an order parameter, corresponding to a physical energy gap which can be actually measured and agrees well with the presented theory. With the Matsubara Green's function method an equation for the finite gap was derived, which can be solved numerically.

$$1 = V d(\epsilon_F) \int_{-\omega_D}^{\omega_D} d\xi_k \frac{tanh(\frac{\beta}{2}\sqrt{\xi^2 + |\Delta_k|^2})}{2\sqrt{\xi^2 + |\Delta_k|^2}}$$

with $d(\epsilon_F)$ being the density of states at the Fermi level
and ω_D being the Debye frequency

The zero temperature limit can be evaluated analytically and leads to a result determining the energy scale typically to ω_D suppressed by an exponential factor causing very low transition temperatures in usual superconductors.

$$|\Delta(T=0)| = 2\omega_D e^{\frac{-1}{Vd(\epsilon_F)}}$$

Finally the important prediction was made, $\frac{\Delta(T=0)}{k_B T_c}$ being a universal function of ≈ 1.76 for the l=0 case. A typical BCS behavior of the superconducting gap with temperature is shown in figure 2, together with experimental data [15].



Figure 2: typical BCS data from an experiment showing the temperature dependence of the superconducting gap

Chapter 3

Semiconductors

In this work we want to understand the pairing of electrons in superconductors with an unconventional gap. In the conventional case of superconductivity this would be a regular metal with s-wave symmetry and a phonon mediated electron-electron interaction. Our case though, will be an unconventional gap with different pairing symmetries such as d-wave or p-wave. The underlying model introduces an electronic gap Δ_0 which is representative for any kind of so called pseudogap (gap in the single particle energy spectrum), created by for example through a magnetic instability or lattice distortion. Therefore all the following considerations stand representative for an arbitrary energy gap distinct from the superconducting gap. For simplicity, we work with a semiconducting model in two dimensions where this gap Δ_0 is constant.

3.1 General Background: Metal, Semiconductor, Insulator

The basic differentiation between metals, semiconductors and insulators is determined through the band theory of solids, [16]. All three of them describe a different type of solid with specific properties regarding the conduction of electrical current. Because of the periodicity of atoms and overlapping of molecular orbitals, discrete atom states evolve into a band structure with electrons in the conduction band and holes in the valence band. A hole is an alternate description of a band with one missing electron. Each have well-defined energy momentum dispersion relations, which we will be using to calculate the density of states at the Fermi level. The Fermi level ϵ_F itself is the maximum energy level up to which all levels below are occupied at zero temperature in a metal. The chemical potential that regulates occupation lies between the energy of the conduction band and the valence band. Since fermions have to obey the Pauli exclusion principle, at zero temperature, all electrons fill up the lowest energy state possible and form the so called Fermi sea of electron energy. As can be see in figure 3 below from [17], the energy states available in a macroscopic solid are in the form of bands instead of discrete energies.



Figure 3: energy band model for solids defining the insulator metal crossover at T=0

The insulator possesses a large energy gap between valence and conduction band. The band gap is the difference in energy between the lowest point of the conduction band and the highest point of the valence band, it is a region of forbidden occupancy. In semiconductors at room temperature, just as in insulators, very few electrons gain enough thermal energy to leap the band gap, which is necessary for conduction. For this reason, pure semiconductors and insulators, in the absence of applied fields, have roughly similar electrical properties. However, the smaller band gaps of semiconductors allow for variation and control of their electrical properties, for example through temperature. Typical values for such a semiconductor energy gap at zero temperature would be for example: Silicon 1.17eV, Germanium 0.74eV or Gallium-Arsenic 1.52eV. Materials with energy gaps larger than 3eV would be considered usually insulators [18]. Metals are the best conductors with their valence and conduction band overlapping each other, the Fermi level lies within the conduction band, such that the band is only partly filled with electrons. In this case it is easier for the electrons to find other unoccupied states to move into, and hence for current to flow. Experimentally the differentiation between metals and semiconductors becomes more difficult because at T=0 where semiconductors should not conduct electrical current, superconductivity can be an impact on the measurement.

Regular semiconductors can be classified into two types, the so called pure or intrinsic semiconductors, and the so called doped or extrinsic semiconductors. An intrinsic semiconductor is a semiconductor which is pure enough that the impurities in it do not greatly affect its electrical behavior. In this case, all carriers are created by thermally or optically excited electrons from the full valence band into the empty conduction band, which causes equal numbers of electrons and holes. The concentration of so called carriers in an intrinsic semiconductor depends on the temperature. At low temperatures, the valence band is completely full, making the material an insulator. Increasing the temperature leads to an increase in the number of carriers and a corresponding increase in conductivity. This is quite different from regular metals, where as the temperature is raised due to increasing resistance the conductivity decreases. An extrinsic semiconductor is a semiconductor that has been doped n-type or p-type with impurities to modify the number and type of free charge carriers present. In the p-type doping the dopant adds more holes or vacancies to the material, increasing the conductivity. In the n-type doping extra electrons are added, causing a similar effect. Both electron and hole can move across the material and therefore contribute to the conduction process. The doped case is very interesting and will be considered in further works, but cannot be taken into further consideration in this paper.

3.2 Pairing in Semiconductors

In order to explore the features of unconventional pairing in a 2D system, I first want to set up the problem. The general idea of an inherent gap in the form of a semiconductor gap suggests a model with valence and conduction band, as mentioned above. In order for electrons to form pairs and thus, superconductivity to occur, an attraction of some kind between the fermions has to be present. This attraction can be either within the bands, i.e. called intra-band interaction, or in between the bands, i.e. inter-band interaction. In general, it could be a combination of both, but for simplicity I will only go into details on either one of the cases. Previous work on the intra-band case were done by Nozieres and Pistolesi [8] in 3D for s-wave symmetry, as well as Liao and Quader [9] in 2 dimensions with s- and d-wave pairing symmetry. For inter-band pairing, the s-wave 3D case was studied by Kohmoto and Takada [7]. All share the general idea of an existing attraction in the bands of some kind, causing the gain in energy for a formed pair to be bigger than the energy cost for an electron-hole pair across the semiconducting gap, first stated by W. Kohn [19]. Otherwise exciton pairs (electron-hole bound pairs) would just form and move across the material and no superconductivity could be seen. The idea suggests that free pairs occur spontaneously even in undoped systems. In the figure 4 one can see two possible pairings, where each of two particles with wave vector k and -k form a Cooper pair. In green one can see the intra-band case, in which within the valence and conduction band pairs are formed. The inter-band case can be seen in blue, where a particle in each case from valence and conduction band form the pair.



Figure 4: a simple band structure with symmetric bands showing possible pairing symmetries

In between both bands one can see the semiconducting gap Δ_0 . The Fermi level μ lies in between both bands at $\epsilon(k) = 0$. The valence band below is filled, the conduction band empty. For simplicity we consider symmetric bands, which is an idealization of the real system. One would have to take an effective mass into account since both bands contribute differently in reality. However, this simplified picture captures a lot of the key physics that we explore.

Nozieres-Pistolesi as well as Kohmoto-Takada have analyzed the s-wave case with spherical symmetry. Liao-Quader also looked into the d- and p-wave case, with different gap symmetries for the intra-band case, as well as for finite doping. Their findings are: qualitatively for both s-wave and d-wave, the gap behaves BCS like and shows the typical exponential decrease; also some interesting features such as the existence of a critical gap Δ_0^* where the superconducting gap Δ drops sharply to zero, indicating a superconductor-insulator-transition (SIT). In figure 5 one can see the scaled superconducting gap over scaled temperature for different critical gap sizes, [9]. For d-wave gap pairing symmetry there appears to be an elongated low plateau when it gets closer to SIT. The physical origin of this behavior is explained by the following: the quasi-particle excitations are less efficient in destroying the superconducting order than they would be in the BCS case. Moreover they studied the behavior of the superconducting gap as a function of semiconducting gap and found that the gap size Δ decreases as the semiconducting gap size increases. Further the size of the gap with s-wave symmetry is larger than in the d-wave case for zero and finite temperature. Also, the transition temperatures were found to be less in the d-wave case, so pairing seems more difficult with non-s-wave symmetry. Suhl, Mathias and Walker [20] discussed a model with two bands such as in transition elements, considering s-d-wave scattering.



Figure 5: SIT shown in graph of the superconducting gap versus temperature for d-wave symmetry

In this work the inter-band case is considered and both s- and d-wave symmetry studied. Concretely our model looks as follows with ω_c being the cutoff frequency. Eventually, in comparison with physical systems, the cutoff frequency should correspond to a collective mode frequency such as the Debye frequency in conventional superconductors. If the cutoff frequency is larger than the semiconducting gap Δ_0 the superconducting state is stable against the normal states. The semiconducting gap is independent of k and ω . Spin degrees of freedom are neglected for reasons of simplicity also. In the limit of Δ_0 going to zero one should see the regular metal case with no band separating energy gap and be able to compare to regular BCS results. However with the chosen pairing Hamiltonian this is not possible, which will be discussed in further detail later.



Figure 6: a simple band structure with symmetric bands showing inter-band pairing simulated in this model

Chapter 4

Derivation of the gap equation

4.1 This Model

As in figure 5, consider a normal 2D Fermi liquid, which consists of a valence band and a conduction band, separated by a semiconducting gap Δ_0 . The Fermi level μ lies in between the two bands. The Fermion creation and annihilation orators will be denoted with a + or without, respectively. The upper band is called band a with operators $a_{k\sigma}^+$, $a_{k\sigma}$, the lower band is b with $b_{k\sigma}^+$, $b_{k\sigma}$. The density of states in a 2D system is a constant, denoted by ρ . The positive attraction between the fermions leading to superconductivity will be introduced through the coupling constant V, which is at first considered to be existing, but possibly infinitesimal, as regular BCS proposes. Spin degrees of freedom are neglected, only momentum dependency for the pairing is taken into account (k and -k).

4.2 Detailed Derivation

For the actual derivation of the gap equation we choose the Mastubara Green's functions method since it allows for an elegant treatment at finite temperatures. First the Hamiltonian is introduced, expressing the effective inter-band pairing interaction that allows pairs to form across the gap. This is distinct from the inter-band superconductivity model of Suhl, Mathias and Walker [20], where the mean field decomposition is different. There inter-band interaction is assumed to form pairs in each of the bands.

$$H = \sum_{k\sigma} \epsilon^a(k) a^+_{k\sigma} a_{k\sigma} + \sum_{k\sigma} \epsilon^b(k) b^+_{k\sigma} b_{k\sigma} - V_k \sum_{k \neq k} a^+_k b^+_{-k} b_{-k} a_k \tag{4.1}$$

Using the usual BCS mean-field approximation, where the labels a and b denote the upper (conduction) and lower (valence) band, respectively:

$$\Delta_k = V_k \sum_k \langle b_{-k} a_k \rangle \tag{4.2}$$

$$\Delta_k^* = V_k \sum_k \langle a_k^+ b_{-k}^+ \rangle$$
(4.3)

This leaves the Hamiltonian to be:

$$H = \sum_{k} \epsilon^{a}(k)a_{k}^{+}a_{k} + \sum_{k} \epsilon^{b}(k)b_{k}^{+}b_{k} - \sum_{k} \Delta_{k}a_{k}^{+}b_{-k}^{+} - \sum_{k} \Delta_{k}^{*}b_{-k}a_{k}$$
(4.4)

The <u>normal Green's function</u> is defined as:

$$G^{a}(k,\tau) = -\langle Ta_{k}(\tau)a_{k}^{+}(0) \rangle$$
 (4.5)

$$G^{b}(k,\tau) = -\langle Tb_{-k}(\tau)b^{+}_{-k}(0) \rangle$$
 (4.6)

whereas we only use the Greens function for the a-band. Under the assumption of $\epsilon^a(k) = \epsilon^b(k)$ using the b-band normal Green's function will give the equivalent result and lead to the same final gap equation.

Writing the time-expectation value out explicitly one gets:

$$G^{a}(k,\tau) = -\Theta(\tau)a_{k}(\tau)a_{k}^{+}(0) - \Theta(-\tau)a_{k}^{+}(0)a_{k}(\tau)$$
(4.7)

Taking the derivative with $\partial_{\tau}\Theta(\tau) \Rightarrow \delta(\tau)$

$$\partial_{\tau} G^{a}(k,\tau) = -\delta(\tau) a_{k}(\tau) a^{+}(0) - \delta(\tau) a_{k}^{+}(0) a_{k}(\tau) - \Theta(\tau) \partial_{\tau} a_{k}(\tau) a_{k}^{+}(0) + \Theta(-\tau) a_{k}^{+}(0) \Theta a_{k}(\tau)$$
(4.8)

$$\partial_{\tau} G^{a}(k,\tau) = -\delta(\tau) \left[a_{k}(\tau) a_{k}^{+}(0) + a_{k}^{+}(0) a_{k}(\tau) \right] - \Theta(\tau) \partial_{\tau} a_{k}(\tau) a_{k}^{+}(0) +$$

$$\Theta(-\tau) a_{k}^{+}(0) \Theta a_{k}(\tau)$$
(4.9)

Using fermion commutation rules:

$$a_k(\tau)a_k^+(0) + a_k^+(0)a_k(\tau) = \left[a_k(\tau)a_k^+(0)\right] = 1$$
(4.10)

gives:

$$\partial_{\tau}G^{a}(k,\tau) = -\delta(\tau) - \langle T_{\tau}\partial_{\tau}a_{k}(\tau)a_{k}^{+}(0) \rangle$$
(4.11)

 $\partial_\tau a_k(\tau)$ is evaluated with the equation of motion method:

$$\partial_{\tau} a_k(\tau) = \left[H, a_k(\tau)\right]_+ \tag{4.12}$$

with

$$H = \sum_{k} \epsilon^{a}(k) a_{k}^{+} a_{k} - \sum_{k} \Delta_{k} a_{k}^{+} b_{-k}^{+} - \sum_{k} \Delta_{k}^{*} b_{-k} a_{k}$$
(4.13)

$$\partial_{\tau} a_k(\tau) = \left[(\epsilon^a(k) a_k^+ a_k - \Delta_k a_k^+ b_{-k}^+ - \Delta_k^* b_{-k} a_k), a_k(\tau) \right]_+$$
(4.14)

$$\partial_{\tau}a_{k}(\tau) = \left[\epsilon^{a}(k)a_{k}^{+}a_{k}, a_{k}(\tau)\right]_{+} - \left[\Delta_{k}a_{k}^{+}b_{-k}^{+}, a_{k}(\tau)\right]_{+} - \left[\Delta_{k}^{*}b_{-k}a_{k}, a_{k}(\tau)\right]_{+} (4.15)$$

with

$$[AB,C]_{+} = A [B,C]_{+} - [A,C]_{+} B$$
(4.16)

Using the fermion commutation relations

$$[a_k, a_k]_+ = a_k a_k + a_k a_k = 0 (4.17)$$

$$\left[a_{k}^{+}, a_{k}\right]_{+} = a_{k}^{+}a_{k} + a_{k}a_{k}^{+} = 1$$
(4.18)

$$\left[b_{-k}^{+}, a_{k}\right]_{+} = b_{-k}^{+} a_{k} + a_{k} b_{-k}^{+} = 0 \qquad (4.19)$$

$$[b_{-k}, a_k]_+ = b_{-k}a_k + a_kb_{-k} = 0 (4.20)$$
Evaluating the three terms explicitly:

$$\left[\epsilon^{a}(k)a_{k}^{+}a_{k},a_{k}(\tau)\right]_{+} = \epsilon^{a}(k)a_{k}^{+}\underbrace{\left[a_{k},a_{k}\right]_{+}}_{0} - \underbrace{\left[\epsilon^{a}(k)a_{k}^{+},a_{k}\right]_{+}}_{\epsilon^{a}(k)*1}a_{k} \qquad (4.21)$$

$$\left[\epsilon^{a}(k)a_{k}^{+}a_{k},a_{k}(\tau)\right]_{+} = -\epsilon^{a}(k)a_{k} \qquad (4.22)$$

$$\left[\Delta_{k}a_{k}^{+}b_{-k}^{+}, a_{k}(\tau)\right]_{+} = \Delta_{k}a_{k}^{+}\underbrace{\left[b_{-k}^{+}, a_{k}\right]_{+}}_{0} - \underbrace{\left[\Delta_{k}a_{k}^{+}, a_{k}\right]_{+}}_{\Delta_{k}*1}b_{-k}^{+}$$
(4.23)

$$\left[\Delta_k a_k^+ b_{-k}^+, a_k(\tau)\right]_+ = -\Delta_k b_{-k}^+ \tag{4.24}$$

$$[\Delta_k^* b_{-k} a_k, a_k(\tau)]_+ = \Delta_k^* b_{-k} \underbrace{[a_k, a_k]_+}_0 - \underbrace{[\Delta_k^* b_{-k}, a_k]_+}_0 a_k \tag{4.25}$$

$$[\Delta_k^* b_{-k} a_k, a_k(\tau)]_+ = 0 (4.26)$$

$$\Longrightarrow \partial_{\tau} a_k(\tau) = -\epsilon^a(k) a_k(\tau) - \Delta_k b^+_{-k}(\tau)$$
(4.27)

Going back to the normal Green's function:

$$\partial_{\tau} G^{a}(k,\tau) = -\delta(\tau) - \langle T_{\tau} \partial_{\tau} a_{k}(\tau) a_{k}^{+}(0) \rangle$$

$$(4.28)$$

$$\partial_{\tau}G^{a}(k,\tau) = -\delta(\tau) - \Theta(\tau)\partial_{\tau}a_{k}(\tau)a_{k}^{+}(0) + \Theta(-\tau)a_{k}^{+}(0)\partial_{\tau}a_{k}(\tau)$$
(4.29)

$$\partial_{\tau}G^{a}(k,\tau) = -\delta(\tau) - \Theta(\tau) \left[-\epsilon^{a}(k)a_{k}(\tau) - \Delta_{k}b^{+}_{-k}(\tau) \right] a^{+}_{k}(0) +$$

$$\Theta(-\tau)a^{+}_{k}(0) \left[-\epsilon^{a}(k)a_{k}(\tau) - \Delta_{k}b^{+}_{-k}(\tau) \right]$$

$$\partial_{\tau}G^{a}(k,\tau) = -\delta(\tau) + \Theta(\tau)\epsilon^{a}(k)a_{k}(\tau)a^{+}_{k}(0) - \Theta(\tau)\Delta_{k}b^{+}_{-k}(\tau)a^{+}_{k}(0) - \Theta(-\tau)a^{+}_{k}(0)\epsilon^{a}(k)a_{k}(\tau) + \Theta(-\tau)a^{+}_{k}(0)\Delta_{k}b^{+}_{-k}(\tau)$$

$$(4.31)$$

$$-\Theta(-\tau)a^{+}_{k}(0)\epsilon^{a}(k)a_{k}(\tau) + \Theta(-\tau)a^{+}_{k}(0)\Delta_{k}b^{+}_{-k}(\tau)$$

$$(4.31)$$

$$\partial_{\tau} G^{a}(k,\tau) = -\delta(\tau) + \epsilon^{a}(k) \underbrace{\left[\Theta(\tau)a_{k}(\tau)a_{k}^{+}(0) - \Theta(-\tau)a_{k}^{+}(0)a_{k}(\tau)\right]}_{} - \Delta_{k} \underbrace{\left[\Theta(\tau)b_{-k}^{+}(\tau)a_{k}^{+}(0) + \Theta(-\tau)a_{k}^{+}(0)b_{-k}^{+}(\tau)\right]}_{}$$

$$(4.32)$$

with the definition of the normal Green's function: $G^a(k,\tau) = -\langle Ta_k(\tau)a_k^+(0) \rangle$ and defining the <u>anomalous Green's function</u> as follows: $F(k,\tau) = -\langle Tb_{-k}^+(\tau)a_k^+(0) \rangle$ one gets:

$$\partial_{\tau}G^{a}(k,\tau) = -\delta(\tau) - \epsilon^{a}(k)G^{a}(k,\tau) + \Delta_{k}F(k,\tau)$$
(4.33)

A second equation is needed to solve self consistently for the order parameter Δ_k . Thus, the same procedure as above is applied on the anomalous Green's Function.

$$F(k,\tau) = -\langle Tb^{+}_{-k}(\tau)a^{+}_{k}(0) \rangle$$
(4.34)

$$F(k,\tau) = -\Theta(\tau)b^{+}_{-k}(\tau)a^{+}_{k}(0) + \Theta(-\tau)a^{+}_{k}(0)b^{+}_{-k}(\tau)$$
(4.35)

Taking the derivative with $\partial_{\tau}\Theta(\tau) \Rightarrow \delta(\tau)$

$$\partial_{\tau}F(k,\tau) = -\delta(\tau)b^{+}_{-k}(\tau)a^{+}_{k}(0) - \delta(\tau)a^{+}_{k}(0)b^{+}_{-k}(\tau) - \Theta(\tau)\partial_{\tau}b^{+}_{-k}(\tau)a^{+}_{k}(0) + \Theta(-\tau)a^{+}_{k}(0)\partial_{\tau}b^{+}_{-k}(\tau)$$

$$(4.36)$$

$$\partial_{\tau} F(k,\tau) = -\delta(\tau) \underbrace{\left[b^{+}_{-k}(\tau) a^{+}_{k}(0) + a^{+}_{k}(0) b^{+}_{-k}(\tau) \right]_{+}}_{\left[b^{+}_{-k}(\tau), a^{+}_{k}(0) \right]_{+}} (4.37)$$
$$-\Theta(\tau) \partial_{\tau} b^{+}_{-k}(\tau) a^{+}_{k}(0) + \Theta(-\tau) a^{+}_{k}(0) \partial_{\tau} b^{+}_{-k}(\tau)$$

Using fermion commutation relations, the first term vanishes because:

$$\left[b_{-k}^{+}(\tau), a_{k}^{+}(0)\right]_{+} = 0 \tag{4.38}$$

$$\partial_{\tau} F(k,\tau) = -\Theta(\tau) \partial_{\tau} b^{+}_{-k}(\tau) a^{+}_{k}(0) + \Theta(-\tau) a^{+}_{k}(0) \partial_{\tau} b^{+}_{-k}(\tau)$$
(4.39)

The partial derivative $\partial_{\tau} b^+_{-k}(\tau)$ is evaluated with the equation of motion method again

$$\partial_{\tau} b^{+}_{-k}(\tau) = \left[H, b^{+}_{-k}(\tau) \right]_{+}$$
(4.40)

with

$$H = \sum_{k} \epsilon^{b}(k) b_{k}^{+} b_{k} - \sum_{k} \Delta_{k} a_{k}^{+} b_{-k}^{+} - \sum_{k} \Delta_{k}^{*} b_{-k} a_{k}$$
(4.41)

$$\partial_{\tau}b^{+}_{-k}(\tau) = \left[(\epsilon^{b}(k)b^{+}_{k}b_{k} - \Delta_{k}a^{+}_{k}b^{+}_{-k} - \Delta^{*}_{k}b_{-k}a_{k}), b^{+}_{-k}(\tau) \right]_{+}$$
(4.42)

$$\partial_{\tau}b^{+}_{-k}(\tau) = \left[\epsilon^{b}(k)b^{+}_{k}b_{k}, b^{+}_{-k}(\tau)\right]_{+} - \left[\Delta_{k}a^{+}_{k}b^{+}_{-k}, b^{+}_{-k}(\tau)\right]_{+} - \left[\Delta^{*}_{k}b_{-k}a_{k}, b^{+}_{-k}(\tau)\right]_{+}$$

$$(4.43)$$

with

$$[AB, C]_{+} = A [B, C]_{+} - [A, C]_{+} B$$
(4.44)

and using the fermion commutation relations

$$\left[b_{k}^{+}, b_{k}^{+}\right]_{+} = b_{k}^{+}b_{k}^{+} + b_{k}^{+}b_{k}^{+} = 0$$

$$(4.45)$$

$$\left[b_k, b_k^+\right]_+ = b_k b_k^+ + b_k^+ b_k^+ = 1 \tag{4.46}$$

$$\left[a_{k}^{+}, b_{-k}^{+}\right]_{+} = a_{k}^{+}b_{-k}^{+} + b_{-k}^{+}a_{k}^{+} = 0$$

$$(4.47)$$

$$\left[a_{k}, b_{-k}^{+}\right]_{+} = a_{k}b_{-k}^{+} + b_{-k}^{+}a_{k} = 0$$
(4.48)

The terms are evaluated explicitly and lead to:

$$\left[\epsilon^{b}(k)b_{k}^{+}b_{k},b_{-k}^{+}(\tau)\right]_{+} = \epsilon^{b}(k)b_{k}^{+}\left[b_{k},b_{k}^{+}\right]_{+} - \left[\epsilon^{b}(k)b_{k}^{+},b_{k}^{+}\right]_{+}b_{k} = \epsilon^{b}(k)b_{k}^{+}$$
(4.49)

$$\left[\Delta_{k}a_{k}^{+}b_{-k}^{+},b_{-k}^{+}(\tau)\right]_{+} = \Delta_{k}a_{k}^{+}\left[b_{k}^{+},b_{k}^{+}\right]_{+} - \left[\Delta_{k}a_{k}^{+},b_{k}^{+}\right]_{+}b_{k}^{+} = 0$$
(4.50)

$$\left[\Delta_{k}^{*}b_{-k}a_{k},b_{-k}^{+}(\tau)\right]_{+} = \Delta_{k}^{*}b_{-k}\left[a_{k},b_{k}^{+}\right]_{+} - \left[\Delta_{k}^{*}b_{-k},b_{k}^{+}\right]_{+} = \Delta_{k}^{*}a_{k}$$
(4.51)

$$\Longrightarrow \partial_{\tau} b^+_{-k}(\tau) = \epsilon^b(k) b^+_{-k}(\tau) + \Delta^*_k a_k(\tau)$$
(4.52)

The derivative is plugged back into the anomalous Green's function and gives:

$$\partial_{\tau} F(k,\tau) = -\Theta(\tau) \partial_{\tau} b^{+}_{-k}(\tau) a^{+}_{k}(0) + \Theta(-\tau) a^{+}_{k}(0) \partial_{\tau} b^{+}_{-k}(\tau)$$
(4.53)

$$\partial_{\tau}F(k,\tau) = -\Theta(\tau) \left[\epsilon^{b}(k)b^{+}_{-k}(\tau) + \Delta^{*}_{k}a_{k}(\tau)\right] a^{+}_{k}(0) + \Theta(-\tau)a^{+}_{k}(0) \left[\epsilon^{b}(k)b^{+}_{-k}(\tau) + \Delta^{*}_{k}a_{k}(\tau)\right]$$

$$\partial_{\tau}F(k,\tau) = \epsilon^{b}(k)b^{+}_{-k} \underbrace{\left[-\Theta(\tau)b^{+}_{-k}(\tau)a^{+}_{k}(0) + \Theta(-\tau)a^{+}_{k}(0)b^{+}_{-k}(\tau)\right]}_{-\langle Tb^{+}_{-k}(\tau)a^{+}_{k}(0) \rangle}$$

$$+ \Delta^{*}_{k} \underbrace{\left[-\Theta(\tau)a_{k}(\tau)a^{+}_{k}(0) + \Theta(-\tau)a^{+}_{k}(0)a_{k}(\tau)\right]}_{-\langle Ta_{k}(\tau)a^{+}_{k}(0) \rangle}$$

$$(4.54)$$

$$(4.55)$$

With the definition of both Green's functions in mind, one can substitute:

$$G^{a}(k,\tau) = - \langle Ta_{k}(\tau)a_{k}^{+}(0) \rangle$$

$$F(k,\tau) = - \langle Tb_{-k}^{+}(\tau)a_{k}^{+}(0) \rangle$$

$$\partial_{\tau}F(k,\tau) = \epsilon^{b}(k)F(k,\tau) + \Delta_{k}^{*}G^{a}(k,\tau)$$
(4.57)

Finally there is a self consistent expression for the order parameter Δ_k , which is given by a set of two equations.

$$\partial_{\tau}G^{a}(k,\tau) = -\delta(\tau) - \epsilon^{a}(k)G^{a}(k,\tau) + \Delta_{k}F(k,\tau)$$
(4.58)

and equ.4.57. In order to solve these - a Fourier transform into frequency space is performed with: $\partial_{\tau} \rightarrow -i\omega_n$ and $\delta(\tau) \rightarrow 1$

$$-i\omega_n G^a(k,\tau) = 1 - \epsilon^a(k)G^a(k,\tau) + \Delta_k F(k,\tau)$$

$$-i\omega_n F(k,\tau) = \epsilon^b(k)F(k,\tau) + \Delta_k^* G^a(k,\tau)$$

(4.59)

Thus,

$$(-i\omega_n + \epsilon^a(k))G^a(k,\tau) = -1 + \Delta_k F(k,\tau)$$

$$(-i\omega_n - \epsilon^b(k))F(k,\tau) = \Delta_k^* G^a(k,\tau)$$
(4.60)

These algebraic equations are solved easily for each of the Matsubara Green's functions.

$$F(k,\tau) = \frac{\Delta_k^* G^a(k,\tau)}{-i\omega_n - \epsilon^b(k)}$$
(4.61)

$$(-i\omega_n + \epsilon^a(k))G^a(k,\tau) = -1 + G^a(k,\tau)\frac{\Delta_k \Delta_k^*}{-i\omega_n - \epsilon^b(k)}$$

$$(4.62)$$

$$-1 = (-i\omega_n + \epsilon^a(k) - \frac{\Delta_k \Delta_k^*}{-i\omega_n - \epsilon^b(k)})G^a(k,\tau) \quad (4.63)$$

$$G^{a}(k,\tau) = \frac{-1}{-i\omega_{n} + \epsilon^{a}(k) - \frac{\Delta_{k}\Delta_{k}^{*}}{-i\omega_{n} - \epsilon^{b}(k)}}$$
(4.64)

$$G^{a}(k,\tau) = \frac{-1(-i\omega_{n} - \epsilon^{b}(k))}{(-i\omega_{n} - \epsilon^{b}(k))(-i\omega_{n} + \epsilon^{a}(k)) - \Delta_{k}\Delta_{k}^{*}} \quad (4.65)$$

with

$$\Delta_k \Delta_k^* = |\Delta_k|^2 \tag{4.66}$$

The final equations are:

$$G^{a}(k,\tau) = \frac{i\omega_{n} + \epsilon^{b}(k)}{(-i\omega_{n} - \epsilon^{b}(k))(-i\omega_{n} + \epsilon^{a}(k)) - |\Delta_{k}|^{2}}$$

$$F(k,\tau) = \frac{-\Delta_{k}^{*}}{(-i\omega_{n} - \epsilon^{b}(k))(-i\omega_{n} + \epsilon^{a}(k)) - |\Delta_{k}|^{2}}$$
(4.67)

The poles of these functions give the quasi particle excitation energy spectrum:

$$i\omega_{n1/2} = \frac{\epsilon_a - \epsilon_b}{2} \pm \sqrt{\left(\frac{\epsilon_a + \epsilon_b}{2}\right)^2 + \left|\Delta_k\right|^2}$$
(4.68)

In order to determine the BCS order parameter Δ_k the interaction model from before is used:

$$\Delta_k = V_k \sum_k \langle b_{-k} a_k \rangle \tag{4.69}$$

$$F(k,\tau = 0^{+}) = -\langle Tb^{+}_{-k}(0)a^{+}_{k}(0) \rangle = \langle a^{+}_{k}b^{+}_{-k} \rangle$$
(4.70)

$$F^*(k, \tau = 0^+) = \langle a_k^+ b_{-k}^+ \rangle^* = \langle b_{-k} a_k \rangle$$
(4.71)

Therefore:

$$\Delta_k = V_k \sum_k F^*(k, \tau = 0^+)$$
(4.72)

$$F^*(k,\tau=0^+) = \sum_{i\omega_n} \frac{1}{\beta} \frac{\Delta_k e^{-i\omega_n \tau}}{(-i\omega_n - \epsilon^b(k))(-i\omega_n + \epsilon^a(k)) - |\Delta_k|^2}$$

$$\tau \to 0^+$$
(4.73)

It may be noted that for fermions we have the following frequency summation:

$$S = \frac{1}{\beta} \sum_{n} f(i\omega_n) = -\sum_{i} R_i$$
(4.74)

$$R_i = r_i n_F(Z_i) \tag{4.75}$$

with Z_i being the pole of the arbitrary function $f(i\omega_n)$, n_F being the Fermi function $n_F(\epsilon) = \frac{1}{e^{\beta\epsilon} - 1}$

and r_i being the residue of the function $f(i\omega_n)$

$$\Delta_k = V_k \sum_k \sum_{i\omega_n} \frac{1}{\beta} \frac{\Delta_k}{(-i\omega_n - \epsilon^b(k))(-i\omega_n + \epsilon^a(k)) - |\Delta_k|^2}$$
(4.76)

$$\Delta_{k} = V_{k} \sum_{k} (-\Delta_{k}) \left[r_{1} n_{F}(i\omega_{n1}) + r_{2} n_{F}(i\omega_{n2}) \right]$$
(4.77)

The residues r_1, r_2 are calculated for a pole of the nth order in case of n=1.

$$Resf(z)|_{z=a} = \frac{1}{(m-1)!} \frac{d^{m-1}}{dz^{m-1}} \left[f(z)(z-a)^m \right] \Big|_{z=a}$$
(4.78)

$$Resf(z)|_{z=a} = f(z)(z-a)|_{z=a} for \qquad m=1$$
(4.79)

$$f(z) = \frac{1}{(-i\omega_n - \epsilon^b(k))(-i\omega_n + \epsilon^a(k)) - |\Delta_k|^2}$$

$$(4.80)$$

$$f(z) = \frac{1}{(z - i\omega_{n1})(z - i\omega_{n2})} = \frac{1}{(i\omega_n - i\omega_{n1})(i\omega_n - i\omega_{n2})}$$
(4.81)

with $i\omega_{n1/2}$ being the poles from above.

For r_1 that means:

$$r_1 = Resf(i\omega_{n1}) = f(z)(z-a)|_{z=a}$$
 (4.82)

$$z = i\omega_{n1} \tag{4.83}$$

$$r_{1} = \frac{1}{(i\omega_{n1} - i\omega_{n1})(i\omega_{n1} - i\omega_{n2})}(i\omega_{n1} - i\omega_{n1})$$
(4.84)

$$r_1 = \frac{1}{i\omega_{n1} - i\omega_{n2}} \tag{4.85}$$

For r_2 that means:

$$r_2 = Resf(i\omega_{n2}) = f(z)(z-a)|_{z=a}$$
(4.86)

$$z = i\omega_{n2} \tag{4.87}$$

$$r_2 = \frac{1}{(i\omega_{n2} - i\omega_{n1})(i\omega_{n2} - i\omega_{n2})}(i\omega_{n2} - i\omega_{n2})$$
(4.88)

$$r_2 = \frac{1}{i\omega_{n2} - i\omega_{n1}}$$

$$(4.89)$$

The residues are put in explicitly now and lead to the final gap equation with the given Hamiltonian and pairing symmetry:

$$\Delta_k = V_k \sum_k (-\Delta_k) \left[r_1 n_F(i\omega_{n1}) + r_2 n_F(i\omega_{n2}) \right]$$
(4.90)

$$\Delta_k = -V_k \sum_k \Delta_k \left[\frac{n_F(i\omega_{n1})}{i\omega_{n1} - i\omega_{n2}} + \frac{n_F(i\omega_{n2})}{i\omega_{n2} - i\omega_{n1}} \right]$$
(4.91)

$$\Delta_k = -V_k \sum_k \Delta_k \left[\frac{n_F(i\omega_{n1}) - n_F(i\omega_{n2})}{i\omega_{n1} - i\omega_{n2}} \right]$$
(4.92)

$$i\omega_{n1} - i\omega_{n2} = \frac{\epsilon_a - \epsilon_b}{2} + \sqrt{\left(\frac{\epsilon_a + \epsilon_b}{2}\right)^2 + \left|\Delta_k\right|^2} - \frac{\epsilon_a - \epsilon_b}{2} + \sqrt{\left(\frac{\epsilon_a + \epsilon_b}{2}\right)^2 + \left|\Delta_k\right|^2}$$
(4.93)

$$i\omega_{n1} - i\omega_{n2} = 2\sqrt{\left(\frac{\epsilon_a + \epsilon_b}{2}\right)^2 + \left|\Delta_k\right|^2} = 2E_k$$
(4.94)

$$i\omega_{n1} = \frac{\epsilon_a - \epsilon_b}{2} + \sqrt{\left(\frac{\epsilon_a + \epsilon_b}{2}\right)^2 + |\Delta_k|^2} = \frac{\epsilon_a - \epsilon_b}{2} + E_k = E_k^+ \quad (4.95)$$

$$i\omega_{n2} = \frac{\epsilon_a - \epsilon_b}{2} - \sqrt{(\frac{\epsilon_a + \epsilon_b}{2})^2 + |\Delta_k|^2} = \frac{\epsilon_a - \epsilon_b}{2} - E_k = E_k^-$$
 (4.96)

Therefore the final gap equation for the two-band BCS model with inter-band interaction for this specific Hamiltonian is:

$$\Delta_k = -\sum_{kk'} V_{kk'} \Delta_{k'} \frac{1}{2E_{k'}} \left[n_F(E_{k'}^+) - n_F(E_{k'}^-) \right]$$
(4.97)

with the expressions from above.

Chapter 5

S-Wave Pairing Symmetry

For the regular s-wave with spherical symmetry we start off with the derived gap equation, eq.4.97. The zero temperature and finite temperature cases will be studied separately, where the finite T equation should lead back to the zero temperature result in the limit of $T \rightarrow 0$. To obtain a gap with s-wave pairing symmetry the pairing interaction $V_{kk'}$ as in BCS has to be a constant V. Then equation 4.97 for the gap magnitude is $(\Delta_k = \Delta)$:

$$|\Delta_k| = \sum_{k'} -V_{kk'} \frac{|\Delta_k|}{2E_{k'}[n_F(E_{k'}^+) - n_F(E_{k'}^-)]}$$
(5.1)

with

$$E_k = \sqrt{\left(\frac{\epsilon_a + \epsilon_b}{2}\right)^2 + \left(|\Delta_k|\right)^2} \tag{5.2}$$

$$E_k^{\pm} = \frac{\epsilon_a - \epsilon_b}{2} \pm E_k \tag{5.3}$$

The following simplifications and assumptions are made: a) symmetric bands

$$\epsilon_a = \frac{\hbar^2 k^2}{2m} + \Delta_0 - \mu \tag{5.4}$$

$$\epsilon_b = \frac{-\hbar^2 k^2}{2m} - \Delta_0 - \mu \tag{5.5}$$

and b) no doping:

$$\mu = 0 \tag{5.6}$$

Thus, we have

$$\epsilon_a = -\epsilon_b \tag{5.7}$$

$$E_k = |\Delta| \tag{5.8}$$

$$E_k^{\pm} = \epsilon_a \pm |\Delta| \tag{5.9}$$

The gap equation for the magnitude of the gap is given as follows:

$$|\Delta| = -\frac{V}{2} \sum_{k} \left[n_F \left(\frac{\hbar^2 k^2}{2m} + \Delta_0 + |\Delta_k| \right) - n_F \left(\frac{\hbar^2 k^2}{2m} + \Delta_0 - |\Delta_k| \right) \right]$$
(5.10)

Note one striking feature is the absence of the energy denominator, different from the BCS gap equation. Hence, the attractive potential V can work in its full strength on the entire sum over k, causing even a very small V to produce a solution.

5.1 Zero Temperature

For zero temperature the Fermi functions n_F become step functions with values of zero or one.

$$\Theta(\epsilon) = \frac{1}{e^{\beta\epsilon} + 1} = \begin{cases} 0 \text{ for } \epsilon > 0\\ 1 \text{ for } \epsilon < 0 \end{cases}$$
(5.11)

with $\beta = k_B T$. Looking at the two terms in the Fermi functions, one can see that the first term is always bigger than zero, therefore it becomes zero in the zero temperature limit.

$$\frac{\hbar^2 k^2}{2m} + \Delta_0 + |\Delta_k| > 0 \tag{5.12}$$

The second term becomes one under the following condition, which has to be imposed on all further calculations:

$$\frac{\hbar^2 k^2}{2m} + \Delta_0 - |\Delta_k| < 0 \tag{5.13}$$

for
$$|\Delta_k| > \frac{\hbar^2 k^2}{2m} + \Delta_0$$
 (5.14)

The final gap equation for s-wave in the zero temperature limit looks as follows:

$$|\Delta_k| = \frac{V}{2} \sum_k 1$$
for $|\Delta_k| > \frac{\hbar^2 k^2}{2m} + \Delta_0$

$$(5.15)$$

Converting the sum over k into an integral in energy space, integrating from zero to the Debye-cutoff frequency ω_c an equation results, that is independent of the semiconducting gap Δ_0 and goes linear with the interaction strength $V\rho$, ρ being the constant 2D density of states.

$$\sum_{k} \to \int_{0}^{\omega_{c}} d\xi \to \boxed{|\Delta| = \frac{V\rho}{2}\omega_{c}}$$
(5.16)

Imposing the condition for $|\Delta_k|$ on the last equation we find a validity condition for the interaction strength, depending on the semiconducting gap Δ_0 :

$$\frac{V\rho}{2}\omega_c > \omega_c + \Delta_0 \tag{5.17}$$

$$\frac{V\rho}{2} > 1 + \frac{\Delta_0}{\omega_c} \tag{5.18}$$

$$V\rho > 2 + \frac{2\Delta_0}{\omega_c} \tag{5.19}$$

This result represents a very important difference from the usual BCS case in which an arbitrarily small interaction is sufficient to stabilize the superconducting state over the normal state, whereas here a finite V is necessary! This is understandable since the inter-band pairing interaction $V\rho$ has to overcome he semiconducting gap Δ_0 . The dependence on the cutoff frequency should also be noted.

5.2 Finite Temperature

Starting with the same gap equation after all simplifications (eq. 5.10) and writing out the Fermi functions explicitly, we arrive at the following equation that has to be solved:

$$|\Delta| = -\frac{V\rho}{2} \int_0^{\omega_c} d\xi \frac{1}{e^{\beta(\xi + \Delta_0 + |\Delta|)} + 1} + \frac{V\rho}{2} \int_0^{\omega_c} d\xi \frac{1}{e^{\beta(\xi + \Delta_0 - |\Delta|)} + 1}$$
(5.20)

with $\xi = \frac{\hbar^2 k^2}{2m}$ and ρ being the constant density of states in 2 dimensions and $\beta = \frac{1}{k_B T}$.

$$|\Delta| = \frac{V\rho}{2} \left(\int_0^{\omega_c} d\xi \frac{1}{e^{\beta(\xi + \Delta_0 - |\Delta|)} + 1} + \frac{1}{e^{\beta(-\xi - \Delta_0 - |\Delta|)} + 1} - 1 \right)$$
(5.21)

It may be noted that:

$$\frac{1}{e^{\beta(\xi+a)}+1} = 1 - \frac{e^{\beta(\xi+a)}}{e^{\beta(\xi+a)}+1}$$
(5.22)

$$|\Delta| = \frac{V\rho}{2} \int_0^{\omega_c} d\xi \left[+1 - \frac{e^{\beta(\xi+a)}}{e^{\beta(\xi+a)} + 1} + 1 - \frac{e^{\beta(-\xi+b)}}{e^{\beta(-\xi+b)} + 1} - 1 \right]$$
(5.23)

with $a = \Delta_0 - |\Delta|$ and $b = -\Delta_0 - |\Delta|$

$$|\Delta| = \frac{V\rho}{2} \int_0^{\omega_c} d\xi \left[-\frac{e^{\beta(\xi+a)}}{e^{\beta(\xi+a)}+1} - \frac{e^{\beta(-\xi+b)}}{e^{\beta(-\xi+b)}+1} + 1 \right]$$
(5.24)

$$|\Delta| = \frac{V\rho}{2\beta} \left[-\ln(e^{\beta(\xi+a)} + 1) + \ln(e^{\beta(-\xi+b)} + 1) + \beta\xi \right]_0^{\omega_c}$$
(5.25)

$$|\Delta| = \frac{V\rho}{2\beta} \left(ln \left(\frac{e^{\beta(-\xi+b)} + 1}{e^{\beta(\xi+a)} + 1} \right) + \beta\xi \right) |_{0}^{\omega_{c}}$$
(5.26)

Aside:

$$\ln\left(\frac{e^{\beta(-\xi+b)}+1}{e^{\beta(\xi+a)}+1}\right)|_{0}^{\omega_{c}} = \ln\left(\frac{e^{\beta(-\omega_{c}+b)}+1}{e^{\beta(\omega_{c}+a)}+1}\right) - \ln\left(\frac{e^{\beta b}+1}{e^{\beta a}+1}\right)$$
(5.27)

Therefore the final gap equation is:

$$|\Delta| = \frac{V\rho}{2\beta} \left(ln(\frac{e^{\beta(-\omega_c - \Delta_0 - |\Delta|)} + 1}{e^{\beta(\omega_c + \Delta_0 - |\Delta|)} + 1}) - ln(\frac{e^{\beta(-\Delta_0 - |\Delta|)} + 1}{e^{\beta(\Delta_0 - |\Delta|)} + 1}) + \beta\omega_c \right)$$
(5.28)

This equation has to be solved for the gap parameter Δ numerically, in different contexts .

Chapter 6

D-Wave Pairing Symmetry

The d-wave pairing symmetry will be an example of unconventional pairing symmetry in systems with an inherent gap. Therefore a couple specifications have to be made which take the orbital symmetry into account. As before the zero and finite temperature cases will be studied separately, overlapping for the limit $T \rightarrow 0$. We start with the derived gap equation above, eq.4.97.

$$\Delta_k = \sum_{k'} -V_{kk'} \frac{\Delta_k}{2E_{k'} [n_F(E_{k'}^+) - n_F(E_{k'}^-)]}$$
(6.1)

with

$$E_{k'} = \sqrt{\left(\frac{\epsilon_a + \epsilon_b}{2}\right)^2 + \left(|\Delta_{k'}|\right)^2}$$
(6.2)

$$E_{k'}^{\pm} = \frac{\epsilon_a - \epsilon_b}{2} \pm E_{k'} \tag{6.3}$$

The specific orbital symmetry properties are realized with an additional degree of freedom, an angular dependence of Φ . This gives the following form for the gap function and the pairing interaction:

$$\Delta_{k} = \Delta cos(2\Phi)$$

$$V_{kk'} = V cos(2\Phi) cos(2\Phi')$$
(6.4)

The assumption of a) symmetric bands and b) no doping leads to:

$$\mu = 0 \tag{6.5}$$

$$\epsilon_a = -\epsilon_b = \frac{\hbar^2 k^2}{2m} + \Delta_0 \tag{6.6}$$

$$E_{k'} = \sqrt{|\Delta_{k'}|^2} = \left|\Delta \cos(2\Phi')\right| \tag{6.7}$$

$$E_{k'}^{\pm} = \epsilon_a \pm E_{k'} = \epsilon_a \pm \left| \Delta \cos(2\Phi') \right|$$
(6.8)

(6.9)

$$\Delta \cos(2\Phi) = -V \sum_{kk'} \cos(2\Phi) \cos(2\Phi') \frac{\Delta \cos(2\Phi')}{2 \left| \Delta \cos(2\Phi') \right|} \left[n_F(\epsilon_a + \left| \Delta \cos(2\Phi') \right|) \right]$$
(6.10)

$$-n_{F}(\epsilon_{a} - \left|\Delta \cos(2\Phi')\right|)]$$

$$-\frac{V}{2}\sum \frac{\cos(2\Phi')^{2}}{\left[n_{F}(\epsilon_{a} + \Delta \left|\cos(2\Phi')\right|\right) - n_{F}(\epsilon_{a} - \Delta \left|\cos(2\Phi')\right|)\right]}$$
(6.11)

$$\Delta = -\frac{V}{2} \sum_{k'} \frac{\cos(2\Phi')^2}{|\cos(2\Phi')|} [n_F(\epsilon_a + \Delta \left|\cos(2\Phi')\right|) - n_F(\epsilon_a - \Delta \left|\cos(2\Phi')\right|)]$$
(6.11)

Thus,

$$\Delta = -\frac{V}{2} \sum_{k'} \left| \cos(2\Phi') \right| \left[n_F(\epsilon_a + \Delta \left| \cos(2\Phi') \right|) - n_F(\epsilon_a - \Delta \left| \cos(2\Phi') \right|) \right]$$
(6.12)

will be the final gap equation for d-wave pairing symmetry.

6.1 Zero Temperature

In the zero temperature limit the Fermi functions $n_F(x)$ become step functions $\Theta(x)$ with values of either 0 or 1 as shown in the s-wave case.

The first Fermi function has arguments always bigger than zero, which leaves only the second term.

$$\frac{\hbar^2 k^2}{2m} + \Delta_0 + \Delta \left| \cos(2\Phi') \right| > 0 \tag{6.13}$$

The second term only can become 1 and therefore creates a condition which has to be imposed in all further calculations:

$$\frac{\hbar^2 k^2}{2m} + \Delta_0 - \Delta \left| \cos(2\Phi') \right| < 0 \tag{6.14}$$

$$\Delta \left| \cos(2\Phi') \right| > \frac{\hbar^2 k^2}{2m} + \Delta_0 \tag{6.15}$$

$$\Delta = \frac{V}{2} \sum_{k'} \left| \cos(2\Phi') \right| 1$$
for $\Delta \left| \cos(2\Phi') \right| > \frac{\hbar^2 k^2}{2m} + \Delta_0$
(6.16)

The sum over all k' is converted into an integral over energy space ξ and angle Φ' , integrating from zero to some cutoff frequency ω_c and angle Φ_c .

$$\sum_{k'} \longrightarrow \int_0^{\omega_c} d\xi \int_0^{\Phi_c} \frac{d\Phi'}{2\pi}$$
(6.17)

$$\Delta = \frac{V}{2} \int_0^{\omega_c} d\xi \int_0^{\Phi_c} \frac{d\Phi'}{2\pi} \left| \cos(2\Phi') \right| \tag{6.18}$$

The cutoff angle Φ_c is set to be 2π . The choice of a different cutoff will affect the result to some extent, but not qualitatively. The final result is independent of the semiconducting gap Δ_0 and goes linear with interaction strength $V\rho$.

$$\Delta = \frac{V\rho}{\pi}\omega_c \tag{6.19}$$

This result is qualitatively very similar to the s-wave case (eq. 5.16).

Imposing the condition for Δ on the equation we get a validity condition for the interaction strength.

$$\frac{V\rho}{\pi}\omega_c \left|\cos(2\Phi')\right| > \omega_c + \Delta_0 \tag{6.20}$$

$$\frac{V\rho}{\pi} > (1 + \frac{\Delta_0}{\omega_c}) \frac{1}{|\cos(2\Phi')|} \tag{6.21}$$

$$V\rho > (\pi + \frac{\pi\Delta_0}{\omega_c})\frac{1}{|\cos(2\Phi')|} \tag{6.22}$$

The angular integration will only contribute to the integral for argument values near 1, therefore the condition can be simplified to:

$$V\rho > \pi + \frac{\pi\Delta_0}{\omega_c} \tag{6.23}$$

This result is again quite different from the regular BCS calculation where even an infinitesimal attractive potential is sufficient to create superconductivity. Here a definite finite interaction is needed to stabilize the BCS state against the normal state!

6.2 Finite Temperature

For the finite Temperature case with d-wave pairing symmetry the simplified gap equation from above, eq.6.12 will be the starting point. The Fermi functions are written out explicitly.

$$\Delta = -\frac{V}{2} \sum_{k'} \left| \cos(2\Phi') \right| \left[n_F(\epsilon_a + \Delta \left| \cos(2\Phi') \right|) - n_F(\epsilon_a - \Delta \left| \cos(2\Phi') \right|) \right]$$
(6.24)

with $\xi = \frac{\hbar^2 k^2}{2m}$ and $\beta = \frac{1}{k_B T}$. The sum over all k' is converted into an integral over energy space ξ and angle Φ' , integrating from zero to some cutoff frequency ω_c and angle wise to 2π .

$$\Delta = -\frac{V\rho}{2} \int_{0}^{\omega_{c}} d\xi \int_{0}^{2\pi} \frac{d\Phi'}{2\pi} \left| \cos(2\Phi') \right| \left[n_{F}(\xi + \Delta_{0} + \Delta \left| \cos(2\Phi') \right|) - n_{F}(\xi + \Delta_{0} - \Delta \left| \cos(2\Phi') \right|) \right]$$

$$(6.25)$$

$$\Delta = \frac{V\rho}{2} \int_0^{\omega_c} d\xi \int_0^{2\pi} \frac{d\Phi'}{2\pi} \left| \cos(2\Phi') \right| \left[n_F(\xi + \Delta_0 - \Delta \left| \cos(2\Phi') \right| \right)$$
(6.26)

$$+ n_{F}(-\xi - \Delta_{0} - \Delta \left| \cos(2\Phi') \right|) - 1]$$

$$\Delta = \frac{V\rho}{2} \int_{0}^{\omega_{c}} d\xi \int_{0}^{2\pi} \frac{d\Phi'}{2\pi} \left| \cos(2\Phi') \right| \left[\frac{1}{e^{\beta(\xi + \Delta_{0} + \Delta \left| \cos(2\Phi') \right|)} + 1} \right]$$
(2.27)

$$+\frac{1}{e^{\beta(-\xi-\Delta_0-\Delta|\cos(2\Phi')|)}+1}-1]$$
(6.27)

It may be noted, that: $\frac{1}{e^{\beta(\xi+a)}} = 1 - \frac{e^{\beta(\xi+a)}}{e^{\beta(\xi+a)}+1}$

$$\Delta = \frac{V\rho}{2} \int_{0}^{\omega_{c}} d\xi \int_{0}^{2\pi} \frac{d\Phi'}{2\pi} \left| \cos(2\Phi') \right| \left[1 - \frac{e^{\beta(\xi+a)}}{e^{\beta(\xi+a)} + 1} + 1 - \frac{e^{\beta(-\xi+b)}}{e^{\beta(-\xi+b)} + 1} - 1 \right] \quad (6.28)$$

with $a = \Delta_{0} - \Delta \left| \cos(2\Phi') \right|$ and $b = -\Delta_{0} - \Delta \left| \cos(2\Phi') \right|$

The energy integral can be evaluated analytically.

$$\Delta = \frac{V\rho}{2} \int_{0}^{\omega_{c}} d\xi \int_{0}^{2\pi} \frac{d\Phi'}{2\pi} \left| \cos(2\Phi') \right| \left[1 - \frac{e^{\beta(\xi+a)}}{e^{\beta(\xi+a)} + 1} - \frac{e^{\beta(-\xi+b)}}{e^{\beta(-\xi+b)} + 1} \right]$$
(6.29)
$$\Delta = \frac{V\rho}{4\pi\beta} \int_{0}^{2\pi} d\Phi' \left| \cos(2\Phi') \right| \left[\beta\xi - \ln(e^{\beta(\xi+a)} + 1) + \ln(e^{\beta(-\xi+b)} + 1) \right] \Big|_{0}^{\omega_{c}}$$
(6.30)

$$\Delta = \frac{V\rho}{4\pi\beta} \int_0^{2\pi} d\Phi' \left| \cos(2\Phi') \right| \left[\beta\xi + \ln(\frac{e^{\beta(-\xi+b)} + 1}{e^{\beta(\xi+a)} + 1}) \right] \Big|_0^{\omega_c}$$
(6.31)

Aside: $ln(\frac{e^{\beta(-\xi+b)}+1)}{e^{\beta(\xi+a)}+1})\Big|_{0}^{\omega_{c}} = ln(\frac{e^{\beta(-\omega_{c}+b)}+1)}{e^{\beta(\omega_{c}+a)}+1}) - ln(\frac{e^{\beta(b)}+1)}{e^{\beta(a)}+1})$

$$\Delta = \frac{V\rho}{4\pi\beta} \int_0^{2\pi} d\Phi' \left| \cos(2\Phi') \right| \left[\beta\omega_c + \ln(\frac{e^{\beta(-\omega_c+b)} + 1}{e^{\beta(\omega_c+a)} + 1}) - \ln(\frac{e^{\beta(b)} + 1}{e^{\beta(a)} + 1}) \right]$$
(6.32)

The following simplification are made to reduce the angular integral as much as possible:

$$\int_{0}^{2\pi} d\Phi' \left| \cos(2\Phi') \right| \longrightarrow 4 \int_{0}^{\frac{\pi}{2}} d\Theta \cos(\Theta) \tag{6.33}$$

$$\Delta = \frac{V\rho}{\pi\beta} \int_0^{\frac{\pi}{2}} d\Theta \cos(\Theta) [\beta\omega_c + ln(\frac{e^{\beta(-\omega_c - \Delta_0 - \Delta\cos(\Theta))} + 1)}{e^{\beta(\omega_c + \Delta_0 - \Delta\cos(\Theta))} + 1}) - ln(\frac{e^{\beta(-\Delta_0 - \Delta\cos(\Theta))} + 1}{e^{\beta(\Delta_0 - \Delta\cos(\Theta))} + 1})]$$
(6.34)

with: $\int_0^{\frac{\pi}{2}} d\Theta \cos(\Theta) = 1.$

Hence, the final gap equation for d-wave pairing symmetry in the finite temperature case looks as follows. It has to be solved numerically in different contexts discussed later.

$$\Delta = \frac{V\rho}{\pi}\omega_c + \frac{V\rho}{\pi\beta}\int_0^{\frac{\pi}{2}} d\Theta\cos(\Theta)\left[ln\left(\frac{e^{\beta(-\omega_c-\Delta_0-\Delta\cos(\Theta))}+1\right)}{e^{\beta(\omega_c+\Delta_0-\Delta\cos(\Theta))}+1}\right) - ln\left(\frac{e^{\beta(-\Delta_0-\Delta\cos(\Theta))}+1}{e^{\beta(\Delta_0-\Delta\cos(\Theta))}+1}\right)\right]$$
(6.35)

Chapter 7

Results

We would like to point out first the remarkable results of this model as a function of the semiconducting gap. Taking the limit of the semiconducting gap Δ_0 going to zero in order to get out the regular BCS metal case is not possible. If we go further back to the chosen pairing Hamiltonian in the beginning, (eq. 4.4)

$$H = \sum_{k} \epsilon^{a}(k) a_{k}^{+} a_{k} + \sum_{k} \epsilon^{b}(-k) b_{k}^{+} b_{k} - \Delta_{k} \sum_{k} a_{k}^{+} b_{-k}^{+} - \Delta_{k}^{*} \sum_{k} b_{-k} a_{k}$$
(7.1)

one can see that pairing is only allowed for fermions of opposite bands. Apparently in the limit of Δ_0 going to zero both bands physically overlap, simulating the metal solid. There inter-band pairing cannot occur within the description of this Hamiltonian because basically there are no longer two bands. Therefore with any kind of pairing symmetry the chosen Hamiltonian does not allow for simple comparison with the metal case. This is different from the intra-band case studied by Liao-Quader, where this limit was taken to compare with and the results scaled to the regular superconducting gap in metals Δ_m , or that of the inter-band model of Suhl, Mathias, Walker [20]

Also noteworthy is the need for a finite interaction strength $V\rho$ in order to create pairs with all pairing symmetries, quite different from the regular BCS model, as discussed above.

All numerical calculations were done with the Newton approximation method, using Maple and C. The plots were evaluated with Origin.

7.1 s-wave

If we recall the two key equations for the s-wave pairing symmetry, eq.5.16, 5.28 one can first check the form of both equations in the limiting case of T going to zero. One can do that analytically or extrapolate from the finite temperature case and compare. Therefore I solved the finite T equation for $\frac{\Delta}{\Delta_0}$ versus $\frac{k_b T}{\Delta_0}$. The cutoff frequency $\frac{\omega_c}{\Delta_0}$ was kept constant to be 6 and the interaction strength $V\rho$ was varied to be 3, 6 and 10. First the usual BCS trend of an exponential behavior of $\Delta(T)$ is visible. Also, as the interaction strength is increased, the gap size is increased. The qualitative behavior seems in good agreement with regular BCS: The gap drops as temperature is raised. As can be seen from the equation, the magnitude of the gap however goes linear with the attractive potential, which is different from BCS, where the dependency is exponential. With a graphic extrapolation the scaled transition temperatures seem to be at $k_BT_c = 2.8$ for $V\rho = 3$, $k_BT_c = 8.5$ for $V\rho = 6$ and $k_BT_c = 14.7$ for $V\rho = 10$. Moreover, comparing with the T = 0 case, the superconducting gap scaled to semiconducting gap should have values satisfying $\frac{\Delta}{\Delta_0} = \frac{V\rho}{2} \frac{\omega_c}{\Delta_0}$. Plugging the given parameters (see above) in the equation and comparing with the graphic result reading off at $\frac{k_B T}{\Delta_0} = 0$, we see a very good agreement.

Obviously the zero temperature equation is semi-independent of the semiconducting gap. A condition on the gap depending on the semiconducting gap comes in with the restriction on the attractive pairing potential $V\rho$. If the potential is fixed to some number, one can get out a $\frac{\Delta_0}{\omega_c max}$, above which it is not possible to create a superconducting state. Physically that makes sense since the pairing happens across the semiconducting gap. If the cutoff frequency is less than the semiconducting gap



Figure 7: graph showing superconducting gap magnitude versus temperature for fixed cutoff with different potential strengths with s-wave symmetry

there will be no pairing allowed because no fermions in the other band are available. The exact condition is:

$$V\rho > 2 + \frac{2\Delta_0}{\omega_c} \tag{7.2}$$

In the following graph one can see that for a fixed interaction strength (chosen to be $V\rho=10$ here) the superconductivity breaks down above the $\frac{\Delta_0}{\omega_c max} = 4$. In the intra-band case Liao-Quader found a somewhat elongated plateau for the critical semiconducting gap. In this case, getting closer to critical semiconducting gap, one can see a very sharp drop of the superconducting gap, indicating an SIT. The physical origin of this behavior is explained quite similar to the intra-band case, namely, the quasi-particle excitations are less efficient in destroying the superconducting order than they would be in the BCS case.

Furthermore, the zero temperature gap goes linear with cutoff frequency (see eq. 5.16). As in the finite temperature case, the cutoff frequency is increased, the gap increases also. Physically more and more fermions are available for pairing if the cutoff frequency is increased, leading to more pairs and thus, a larger gap (see below).



Figure 8: graph showing superconducting gap magnitude versus temperature for critical semiconducting gaps with s-wave symmetry



Figure 9: graph showing superconducting gap magnitude versus temperature for fixed interaction strength with different cutoffs with s-wave symmetry

Moreover, we can calculate the ratio of the superconducting gap at zero temperature scaled to the transition temperature for different cutoff frequencies. For s-wave pairing, regular BCS predicts this to be a universal constant with the magnitude of 1.76 as shown above. An important difference here is that this value is typically bigger, for example in our model calculations, the values for three different interaction strengths $V\rho = 3, 6, 10$ are always at least bigger than 2. As can be seen, the ratio here depends on the cutoff frequency as well as the magnitude of the attractive potential. Takada-Kohmoto found a similar difference in 3D as well. So this result is most probably independent of dimension. Generally, one can see that for increasing interaction strength, one gets closer and closer to the BCS prediction. Physically that could mean that at some point the attractive potential is so strong, that the semiconducting gap separating the two bands really does not affect the pairing behavior any more.



Figure 10: graph showing superconducting gap magnitude over critical temperature versus scaled cutoff for s-wave symmetry

7.2 d-wave

Recalling the zero temperature and finite temperature equation with d-wave symmetry (eq. 6.19, 6.35), one finds very similar dependencies and behavior. First, checking the self-consistency of the two equations one can see good agreement in the extrapolated values for the zero temperature limit compared to what the equation predicts. One can read off zero temperature gaps to have values of: $\frac{\Delta}{\Delta_0} = 10$ for $V\rho = 6$ or $\frac{\Delta}{\Delta_0} = 32.5$ for $V\rho = 17$. Comparing this to the zero temperature equation $\frac{\Delta}{\Delta_0} = \frac{V\rho}{\pi} \frac{\omega_c}{\Delta_0}$, and plugging in value for each the different interaction strength and the constant cutoff $\frac{\omega_c}{\Delta_c} = 6$ one can confirm these values and equations. Generally, the regular BCS trend is visible, an exponential function, where the gap collapses as the temperature reaches the critical temperature T_c . Again as can be seen from the equation, the magnitude of the gap goes linear with the attractive potential, which is different from BCS, with exponential dependence. With graphic extrapolation the scaled transition temperatures seem to be at $k_BT_c = 2.8$ for $V\rho = 6$, $k_BT_c = 6.8$ for $V\rho = 10$, $k_BT_c = 12.4$ for $V\rho = 17$ and $k_BT_c = 18.5$ for $V\rho = 25$.

As in the s-wave case, for the d-wave one can find a $\frac{\Delta_0}{\omega_c \max}$ from the condition on the attractive pairing potential. This was shown earlier to be

$$V\rho > \pi + \frac{\pi\Delta_0}{\omega_c} \tag{7.3}$$

For a fixed interaction strength there has exists a critical gap - cutoff frequency relation, above which superconductivity breaks down. In figure 12, one can see the behavior of the gap for different values of the semiconducting gap scaled to cutoff. As one can see for values above ≈ 1 there is no pairing gap. We determined the $\frac{\Delta_0}{\omega_c \max}$ to be between 0.6 and 2.18 for the given parameters. Also, the curves for different



Figure 11: grap showing superconducting gap magnitude versus temperature for fixed cutoff with different potential strengths for d-wave symmetry

 $\frac{\Delta_0}{\omega_c}$ do not start at the same zero temperature gap (see s-wave case and eq.6.19). For $\frac{\Delta_0}{\omega_c} = 0.1$ the graph starts with the correct zero temperature gap and drops off with temperature in a BCS manner. Anything higher than that does not start at the T=0 gap; this is different from the s-wave case. We believe this difference may have origin in the angular dependence in the d-wave case. Also, for the derivation of the zero temperature equation we gave the argument that only values near 1 contribute. That lead to the relationship above (eq. 7.3). However if one approximates the mean of $|\cos(2\Phi')|$ with 0.5, another factor of two comes in, reducing the derived $\frac{\Delta_0}{\omega_c max}$ significantly. In any case, the behavior is non-BCS like, as observed with s-wave pairing symmetry.

Also, one can look further into the behavior with cutoff itself. In the zero temperature limit the gap behaves linearly (eq. 6.19). In the finite temperature case, solving eq.6.35 numerically for $\frac{\Delta}{\Delta_0}$ versus $\frac{k_BT}{\Delta_0}$ for different cutoff frequencies one sees that if the cutoff is increased, the gap also increases. The interaction strength is kept constant with $V\rho = 10$, see figure 13.



Figure 12: graph showing superconducting gap magnitude versus temperature for critical semiconducting gap with d-wave symmetry, specifically the sharp drop near SIT



Figure 13: graph showing superconducting gap magnitude versus temperature for fixed interaction strength with different cutoffs for d-wave symmetry



Figure 14: graph showing superconducting gap magnitude over critical temperature versus scaled cutoff for d-wave symmetry

With figure 14, we compare our results with the BCS universal value for $\frac{\Delta(T=0)}{T_c} \approx$ 2.2 for d-wave. We see that in contrast to the s-wave case, the taily decreasing start (upturn) is lost at the beginning. This might be due to a higher starting interaction strength due to the different condition for d-wave. As can be seen in the s-wave case also, this behavior fades for higher interaction strengths. Generally though, the universal value is not fulfilled in our model. All values are higher than the predicted value. The trend to approach the BCS predicted value with increasing interaction potential is observable. Overall, compared to the s-wave values, the d-wave behavior might qualitatively be very similar. Quantitatively though, the values are less than with s-wave pairing symmetry. This trend is valid for all calculations.

In order to further undermine this last statement, one can look at the zero temperature equations as well as look at one example finite temperature plot for comparison. In the zero temperature limit we had for s-wave:

$$\Delta = \frac{V\rho}{2}\omega_c \tag{7.4}$$

For the d-wave we had

$$\Delta = \frac{V\rho}{\pi}\omega_c \tag{7.5}$$

Qualitatively these two behave very similar: linear with interaction strength as well as cutoff frequency, but the factor is different, making the d-wave gap smaller than with s-wave pairing symmetry.

In the finite temperature case we would like to compare the plot $\frac{\Delta}{\Delta_0}$ versus $\frac{k_B T}{\Delta_0}$ for the scaled cutoff frequency fixed to $\frac{\omega_c}{\Delta_0} = 6$ as well as the interaction strength $V\rho = 10$. There you can see how, again, the s-wave is significantly larger in value then the d-wave, the qualitative trend of both to drop with temperature being the same, though.

Lastly we would like to take one example transition temperature and calculate back to a real physical system. Since everything in our calculations is either scaled to the semiconducting gap or the cutoff frequency, we would like to know in what real temperature range this model works. For the s wave e.g. with $V\rho = 6$ and $\frac{\omega_c}{\Delta_0} = 6$ we read off a value of $\frac{k_B T_c}{\Delta_0} \approx 8.6$. Taking for example the zero temperature value for the semiconducting gap of Silicon with $\Delta_0 = 1.17 eV$ and dividing by the Boltzman Constant, we get out an actual transition temperature of 110,000K, which is definitely a high T_c superconductor! Other quantities such as the coherence length or interaction strength can also be calculated. In any case the result does not seem very realistic. The very basic model of a constant semiconductor gap with symmetric



Figure 15: gap versus temperature with fixed potential and cutoff for both s and d wave symmetry

bands was meant to represent one possibility for the pseudogap. However, it simulates the physical behavior of a superconductor correctly.
Chapter 8

Conclusion

The intent of this thesis was to explore superconductivity in a 2D system with unconventional pairing symmetry in the presence of semiconducting-like constant inherent gap. With this in mind we have studied some background of BCS theory and semiconductors and set up a two band model which allows only for fermion pairing across the semiconducting gap. With the Matsubara Green's function method a gap equation was derived, and later on modified for two interesting pairing gap symmetries, s- and d-wave. We studied these cases and solve the gap equation each for the limiting case of zero temperature as well as for finite temperature. Most unusual in these equations is the absence of the energy denominator. Focusing on properties of the superconducting gap Δ and its behavior with different parameters, we have shown graphs of the gap versus temperature, for different cutoffs and interaction strengths. In each case, s- and d-wave, the qualitative behavior of the gap versus temperature was very BCS like. The correlation with interaction strength was found to be specifically non-BCS like. For example, for the studied case with inter-band interaction, one needs a finite attractive potential to stabilize the superconducting state against the normal state. Also the dependence is linear and not exponential. We discovered that the universal relation in BCS $\frac{\Delta(T=0)}{T_c}$ does not hold in this model, for either pairing symmetry. It depends rather on cutoff frequency, interaction strength and size of the semiconducting gap. Furthermore we found a relation $\frac{\Delta_0}{\omega_{c max}}$, determined

by the interaction strength, which defines a critical gap for given parameters. In the intra-band case Liao-Quader found a somewhat elongated plateau close to this critical gap. The sharp drop off of the superconducting gap found in our case can be interpreted as a SIT also. Showing the behavior for the limiting case near the critical gap with d wave pairing symmetry has proven to be not as easy. This is probably due to the angular dependence in the symmetry. We see great potential in pursuing further toward finding an exact solution.

Referring back to the questions motivating this work, one can summarize that the general nature of paired states with the absence of the Fermi surface is quite BCS like in features such as behavior with temperature, but more complex in specific functional correlations, possibly due to more parameters. The way of pairing in this simple 2D model with a pseudo gap separating two bands seems to play a key role as very little of the features in the intra-band case match with the results here. We would like to point out, that the pairing gap symmetry does make a difference in general behavior, though it seems qualitatively quite similar. However quantitatively it seems harder to pair with non-s-wave symmetry, as can be seen in lower transition temperatures or gap magnitudes in general for the same given parameters.

Lastly a few remarks regarding future work. We would like to exploit the outstanding property of a semiconductor and study the system in a doped state! That was done for the intra-band case also, hence interesting features are to be expected here. Moreover, this model worked with the simple assumption of symmetric bands. We can imagine it would be very interesting, for example to introduce an effective mass, or somehow modify the equations to realize a more realistic constitution of the bands. Also it would be interesting to study other possible pairing gap symmetries. Some of the questions yet to be answered are, for example, the actual origin of the attractive potential which we just assumed to exist. The controversial issue of source and concrete character of the pseudo gap has not been resolved yet. Lastly, even more possibilities for fermion pairing can be created, such as a combination of both intraand inter-band pairing. Perhaps, one will find a model that includes both intra- and inter-band interaction in a system with inherent gap, and thus may explain a large variety of superconducting phenomena.

References

- J. Bardeen, L. N. Cooper, J. R. Schrieffer, *Theory of Superconductivity*, Phys. Rev. 108, 11751204 (1957)
- [2] M. Tinkham, Introducion to Superconductivity, McGraw-Hill Inc., 1996, ch. 1,3,9
- [3] A. Goldman, N. Markovic, Superconductor-insulator transitions in the twodimensional limit, PHYSICS TODAY 51 (11): 39-44 NOV 1998
- [4] M. Steiner, A. Kapitulnik, Superconductivity in the insulating phase above the field-tuned superconductor insulator transition in disordered indium oxide films, Physica C, Volume 422, Issue 1-2, p. 16-26. 05/2005
- [5] C. W. Chu, A. P. Rusakov, S. Huang, Anomalies in cuprous chloride, Phys. Rev. B 18, 2116-2123 1978
- [6] W. Hanke, M. J. Kelly, Surface Superconductivity and the Metal-Oxide-Semiconductor System, Phys. Rev. Lett. 45, 12031206 (1980)
- [7] Y. Kohmoto, Y. Takada, Superconductivity from an Insulator, J. of Ph. Society Japan, Vol. 59, No. 5 1990
- [8] P. Nozieres, F. Pistolesi, From Semiconductors to superconductors: a simple model for pseudogaps, The European Physical Journal B, Issue Volume 10, Number 4 / August, 1999
- [9] R. Liao, K. Quader, Superconductivity with unconventional pairing symmetry in a 2D system with inherent gap, personal communication
- [10] J.R.Schrieffer, *Theory of Superconductivity*, Perseus Books, 1999, ch. 1,2,5
- [11] A. Fetter, J. Walecka, Quantum Theory of Many-Particle Systems, Dover Publications Inc., 2003, ch.3, 7
- [12] P.G. de Gennes, Superconductivity of Metals and Alloys, Perseus Books, 1999, ch. 4
- [13] H. Bruus, K. Flensberg, Many-body Quantum Theory in Condensed Matter Physics, Oxford University Press (2004), ch. 9, 11, 18
- [14] G. Mahan, *Many-Particle-Physics*, KA/PP, 2000, ch. 3.2., 10

- [15] Department of Physics at University of Strathclyde Glasgow, http://superdevices.phys.strath.ac.uk/12484/ - last viewed June,23th 2006
- [16] K. Seeger, Semiconductor Physics, Springer, 2004, ch.1
- [17] Ch. Kittel, Introduction to Solid State Physics, John Wiley and Sons, 1996, ch.7
- [18] S. Nene, Purification, Growth and Characterization of organic semiconductors, KSU thesis 2004
- [19] D. Jrome*, T. M. Rice, and W. Kohn, *Excitonic Insulator*, Phys. Rev. 158, 462475 (1967)
- [20] H. Suhl, B. Mathias, L. Walker, BCS Theory of Superconductivity in the case of overlapping bands, Phys. Rev. Vol.3, number 12, Dec. 1959