

Disorder and spin imbalance induced exotic phases in weakly coupled s-wave superconductors

by

Poulumi Dey

A Thesis

submitted for the degree of

Doctor of Philosophy

Thesis Supervisor

Dr. Saurabh Basu



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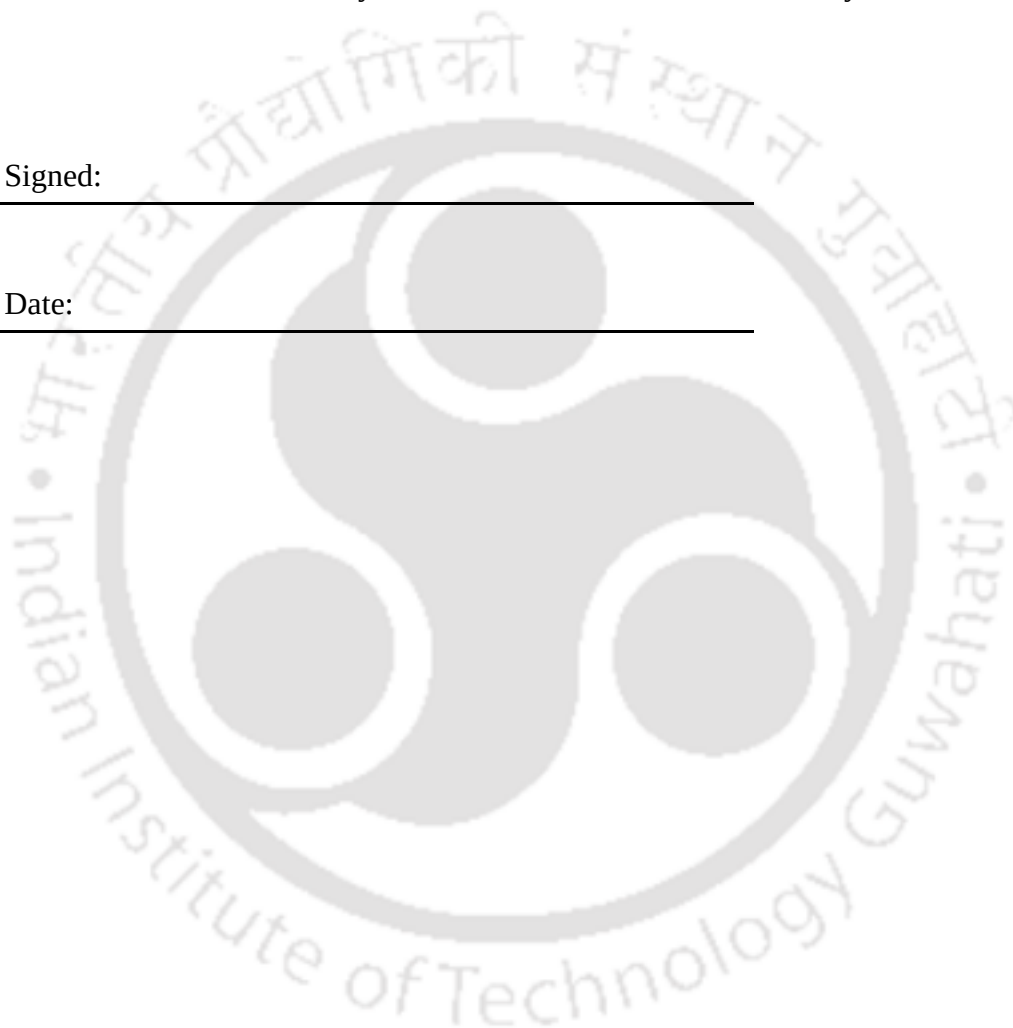


Declaration

The work in this thesis is based on research carried out at the Department of Physics, Indian Institute of Technology Guwahati, India under the supervision of Dr. Saurabh Basu. No part of this thesis has been submitted elsewhere for any other degree or qualification. Works presented in the thesis are all my own unless referenced to the contrary in the text.

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Certificate

It is certified that the work contained in the thesis entitled “*Disorder and spin imbalance induced exotic phases in weakly coupled s-wave superconductors*” by Ms. Poulumi Dey, a student of the Department of Physics, IIT Guwahati was carried out under my supervision and has not been submitted elsewhere for award of any degree.

Saurabh Basu







Dedicated to my family



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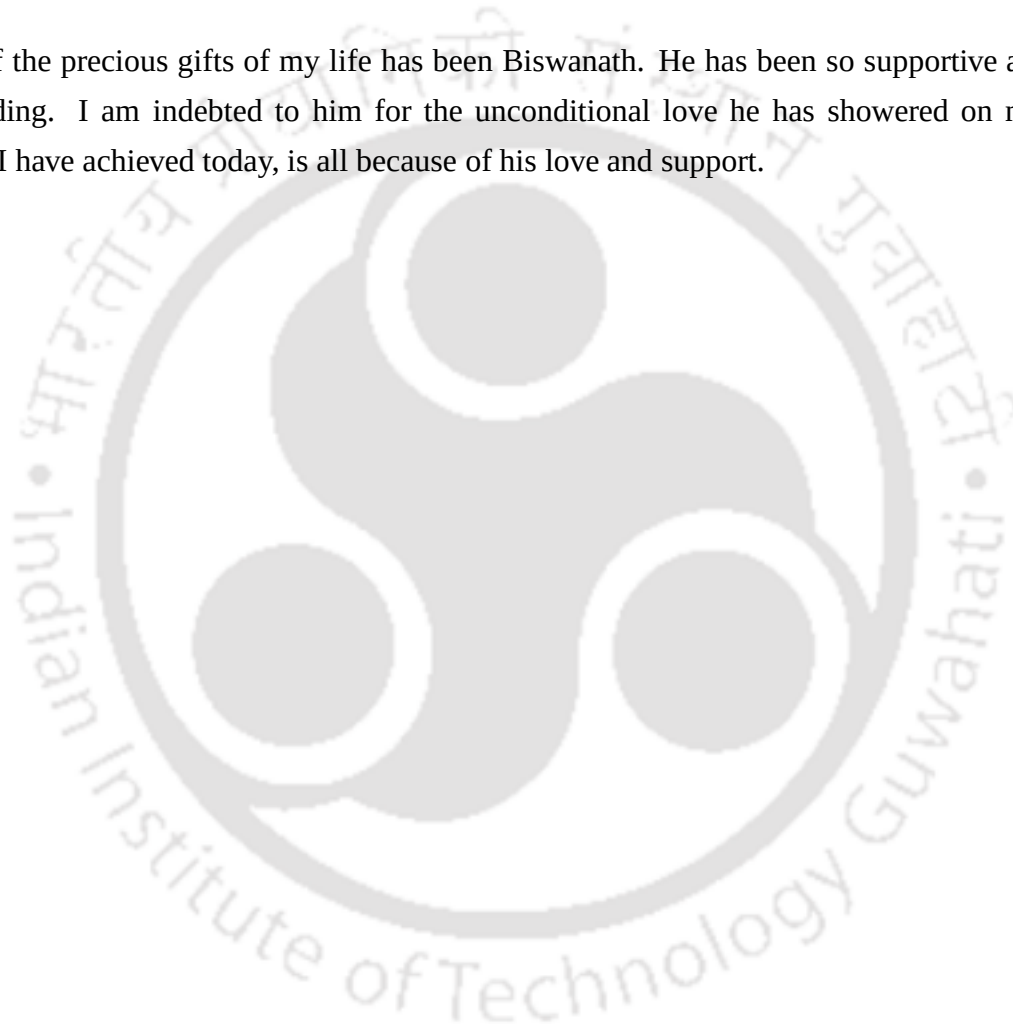
I take this opportunity to thank all my teachers. I am privileged to get a teacher like Mongal Saha. His intelligence, honesty and dedication towards work have inspired me immensely.

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Abstract

The first part of our work deals with a smooth crossover from a Bardeen Cooper Schrieffer (BCS) phase comprising of largely overlapping pairs to a Bose superfluid (BEC) with short ranged tightly bound pairs induced by a random onsite disorder potential, as opposed to tuning the interparticle attraction which is largely seen in literature. At small disorder concentration, Anderson theorem is known to be valid and in the large disorder regime, an insulating phase is favoured. We have convincingly shown that the intermediate disorder regime holds key to a more interesting phase, a paired phase having long range order, resembling a BEC. Quantities such as participation ratio and ground state fidelity are computed which further strengthen the claim of crossover to a Bose phase, when the starting point is a weak coupling BCS superconductor. Many physical quantities which are of experimental significance e.g. superfluid stiffness, off diagonal long range order, spectral gap etc are computed to characterize the exotic phase which emerges at intermediate values of disorder strength. Thus a detailed study is carried out to elucidate different physical properties associated with a BCS-BEC crossover.

The next problem deals with studying superfluidity in population imbalanced systems which are often thought to host an exotic Fulde-Ferrell-Larkin-Ovchinnikov phase (FFLO) characterized by finite momentum Cooper pairing. In spite of the extensive study of the phase, the unambiguous determination of the exotic phase both theoretically and experimentally, is still awaited. Recently, cursory evidences of the presence of FFLO phase has been obtained in trapped ultracold atoms in an optical lattice, which provided motivation for us to explore the FFLO phase in details. Our gap parameter and magnetization data show modulating profiles in real space, thereby providing support to the existence of FFLO phase, while we have noted the presence of various other ground states with close by energies. As confinement effects are technologically important for achieving the condensation phenomena in atomic systems, we have incorporated a harmonic trapping potential in our study and elaborately investigated the effects of harmonic confinement vis-a-vis the finite momentum pairing scenario. Further, we have computed different correlation functions that are of experimental importance. Finally, an interesting physics emerges that shows superfluid to insulator transition (SIT) as obtained by increasing the trapping potential, even in a model with attractive interactions.



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The figures in this thesis have been presented with different kinds of symbols *e.g.* with continuous line, broken line, bullets (viz. square, circle etc) and at times with a combination of them. It may be noted that all of them are used in the same sense, that is, usage of one kind of symbol (say, with a continuous line) for a given plot would have carried exactly the same meaning had we used another (say, with a broken line with filled circles). The error bars have been computed for the disorder problem which lies within the symbols used for representing the data.





Chapter 1

Introduction

Study of strongly correlated systems like transition metal oxides, heavy fermion compounds and the high- T_c superconductors has evolved into a very challenging task in the modern theoretical and experimental physics. At a fundamental level all these systems involve strongly coupled quantum degrees of freedom, such as spin and charge density fluctuations, which demonstrate interesting physical phenomena such as the quantum phase transitions, unconventional pairing mechanisms, very anomalous normal state properties, pseudogap (gap in the normal state) character etc. A collection of such novel phenomena observed in these systems generated an intense activity among the researchers. This has resulted in a tremendous progress in understanding the physics behind the occurrence of such exciting realizations.

Many of the correlated electron systems are intrinsically inhomogeneous and such inhomogeneity (along with disorder, defects etc) are known to lead to fundamentally new effects in interacting electronic systems. Generally, the simultaneous presence of interaction and inhomogeneity lead to a new coupling of the quantum degrees of freedom in one and two particle correlations that has no counterpart in noninteracting and inhomogeneous or interacting and isotropic systems.

Recently in the context of studying the high- T_c superconductors, the issue of inhomogeneous charge (and spin) order or "stripe" phase has become one of the most crucial issues in this field. The experimental demonstration of stripes is robust. Neutron scattering studies on Nd-doped La_2CuO_4 (viz. $\text{La}_{2-x-y}\text{Nd}_y\text{Sr}_x\text{CuO}_4$) show charge modulation in the CuO_2 plane for x (hole doping) covering the entire superconducting range[1]. More recently, Büchner

et al.[2] noticed that the above mentioned superconducting sample with charge modulation undergoes a structural phase transition from a low temperature orthorhombic (LTO) phase to a low temperature tetragonal (LTT) phase below a temperature $\sim 70\text{K}$. Thus it opened up another channel for investigation: the relationship between stripes, structure and superconductivity. On a more general tone, one can ask the question: do stripes 'help', 'hinder' or more radically, create pairing correlations? In fact, the dynamical stripes have been proposed as a pairing mechanism[3]. But such speculations are yet to be confirmed. Still there exists a general consensus that a close look at the issue of stripes may contain a plethora of unanswered questions regarding the pairing mechanism, anomalous normal state and importantly for us, if at all how are the stripes beneficial to the superconducting state?

On the other hand, the investigation of quantum degenerate gases has a long history. The latest step ahead in this direction has been the realization of Bose Einstein condensation (BEC) of alkali atoms, e.g. ^{87}Rb [4], ^7Li [5] and ^{23}Na [6] in a confined geometry created by the magneto optical traps. It is well known, in contrast with two-particle Cooper pairing in Fermi systems, the essence of superfluidity in Bose systems is one-particle BEC. This asymmetry between the Fermi and Bose systems (two-particle pairing vs. one-particle condensation) had remained a subject of interest since long time[7].

A system consisting of dilute mixture of Fermi and Bose gases has also generated considerable interest for studying superfluidity in ^3He - ^4He mixtures, fermionic superfluidity in magnetic traps etc in recent years. A detailed study in this field can make significant contribution to issues such as the submonolayers of ^4He , excitons in semiconductors, holons in high- T_c superconductors (where a possibility of two-holon pairing is proposed via slave-boson calculations) etc.

We now present a discussion on the high- T_c superconductors. We shall mostly restrict ourselves to the issues which are relevant for the thesis. The discovery of high- T_c cuprates by Bednorz and Müller[8] in 1986 triggered extensive studies on superconductivity in systems which are characterized by presence of copper oxide layers. The superconductivity is believed to originate from the strongly interacting charge carriers that move on the two-dimensional copper oxide layers in cuprates. There is a general consensus that these materials exhibit various exotic phases as the carrier concentration is varied[9]. The existence of a mysterious gap in the normal state highlights one such largely explored, though not well understood, phase of the underdoped cuprates known as the pseudogap. The pseudogap is defined as the partial

gap that opens at parts of the Fermi surface[10, 11]. In the underdoped phase of cuprates, pseudogap evolves smoothly into the superconducting gap as temperature is lowered. In particular, the amplitude and symmetry of the two gaps are very similar[11], thus leading many researchers to conclude that the explanation of the pseudogap state is very essential to understand the microscopics of superconductivity[12]. Strong pairing correlations without phase coherence hold key to a number of anomalies observed in the pseudogap regime and that it evolves smoothly into a superconducting condensate with phase coherence as temperature is decreased leads to the belief that the origin of the two gaps are quite closely knit. Thus the pseudogap is a precursor to the superconducting gap and the onset of superconductivity signifies the setting in of phase coherence among the pre-formed (fermionic) pairs below the critical temperature, T_c (Fig. 1.1). In this sense the two gaps may be seen as both sides of the same coin.

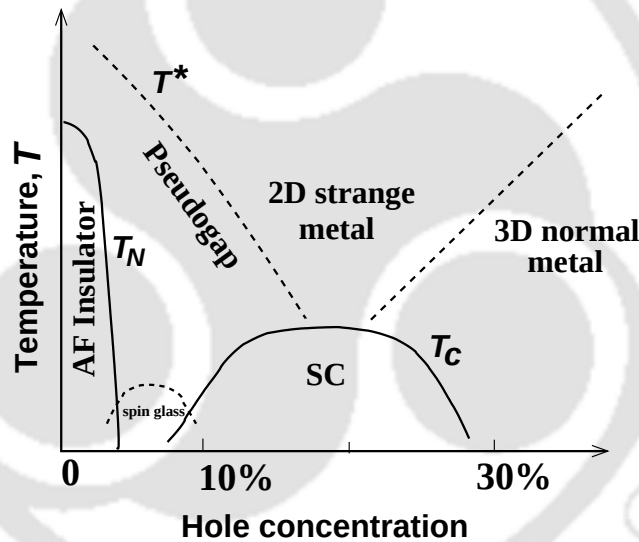


FIGURE 1.1: A schematic phase diagram of hole doped high- T_c superconductors.

There are a number of experiments which provide evidences in support of the existence and detailed understanding of the pseudogap namely, ARPES, NMR, μ SR, tunneling studies etc[10]. Among these ARPES is most commonly used and have proved to be most informative in terms of providing a detailed structure and symmetry of the pseudogap. The ARPES spectra shows anomalous features above T_c where the sharp quasiparticle peaks become broad and incoherent thereby indicating absence of single particle excitations in the normal state - a feature which signals breakdown of the Fermi liquid theory (FLT).

A number of possible mechanism leading to pseudogap state has been proposed. They include a RVB scenario[13], phase fluctuation of the superconducting order parameter[14, 15], a d -density wave theory[16] and preformed pairing ideas[17]. A deeper understanding of the physics governing the normal phase in the underdoped regime and subsequently how it evolves into the overdoped phase where normal behaviour is more prominent, is likely to help in providing a microscopic description of the cuprates.

Due to somewhat controversial nature of the experimental data available on the subject, the microscopic origin of the pseudogap phase is still questionable. A large section of the community has subscribed to the physics governing the BCS-BEC crossover as a potential candidate that describes the mechanism leading to the pseudogap phase[18]. The motivation obviously is derived from the fact that the above T_c excitation (bosonic) gap smoothly emerges into the (fermionic) superconducting gap below T_c . A number of experiments reveal that the pseudogap phase shares more in common with the superconducting phase than with the undoped insulating phase e.g. the small coherence length, (arguably) a d -wave symmetry as the superconducting gap (albeit with shifted nodes along the Fermi surface), fingerprints of pseudogap effects both above and below T_c (even if the effects are more widely studied above T_c) etc.

The fact that a condensate consisting of weakly interacting fermionic degrees of freedom smoothly evolves into one which is characterized by strongly interacting bosons is worth a problem to investigate. A controlled tuning of the attractive interaction between the carriers in presence of magnetic field for a system of ultracold fermionic atoms has facilitated the study of the crossover phenomenon in cold atom problem in laboratories[19–21]. The excitement is further intensified with the recent experiments on optical lattices and its associated practical applications[22, 23]. Interestingly, the subject relates to both atomic physicists and the condensed matter community.

So far we have discussed unconventional superfluidity in systems having equal spin populations. However, superfluidity in spin imbalanced systems has its own long history and has been seen to exhibit various exotic phases *e.g.* Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase[24, 25], the Sarma[26] phase, breached pair phase[27] and a mixed phase in which BCS superfluid coexists with an unpaired normal phase[28–30]. Of special importance among the above is the FFLO phase which is stabilized by a large Zeeman splitting between up and down-spin electrons which form pairs across the Fermi surface and subsequently condense to

give a state which has lower free energy than normal spin polarized state. These pairs have a non-zero total momentum as opposed to traditional zero momentum pairs in conventional BCS state. Interestingly, the finite momentum pairing results in an oscillating superconducting order parameter with a wave length of the order of superconducting coherence length. Several fascinating superconducting properties which have never been observed for the BCS pairing state, have been predicted for the FFLO state[31, 32].

1.1 BCS-BEC crossover

The BCS-BEC crossover is an old problem and has been studied in variety of contexts[17, 33–35] e.g. the crossover scenario has been contemplated to explain the physics of the pseudogap phase etc. The basic idea of the crossover problem is as follows. A weak interparticle attraction among fermionic degrees of freedom forms large overlapping Cooper pairs which is well described by the BCS (mean field) theory of superconductivity. In this limit, pairing is possible only in the presence of a filled Fermi surface and two fermions in vacuum is incapable of forming a bound state. As the attraction is increased beyond a point, two fermions with zero binding energy are formed which is the 'unitarity' point of the problem. Subsequently, at very large values of attraction strengths, tightly bound pairs with large binding energy emerge. A many body system of these bosons eventually undergo Bose Einstein condensation (BEC) as temperature is lowered beyond a threshold value. In this way, one describes smooth evolution of a BCS superconductor (the attractive strength is weak) to a BEC of short ranged tightly bound pairs (strongly interacting)[12, 18]. The challenge is then to find a single theory which can describe the entire regime from BCS to BEC limit. In this regard, it was first noticed by Eagles[33] and then by Leggett[34] that the BCS ground state wavefunction is capable of describing a continuous evolution from a BCS type condensate to a Bose phase as the interparticle interaction strength is varied. Thus it is likely that the crossover phenomena can be explained via a generalization of the standard mean field approach (BCS) to consider attractive interactions of arbitrary strengths.

Ultracold atomic gases provide an experimental playground for investigating the crossover scenario[19, 21, 36, 37]. A key feature of these atomic gases is that the effective interaction between atoms in different hyperfine states can be varied by applying an external magnetic

field using Feshbach resonance[38–40]. Thus a controlled tuning of the interaction among the atoms from weak to strong makes a smooth crossover from BCS to Bose superfluid feasible.

The transition between the two extreme ends (BCS and BEC) is smooth though the limits correspond to different physical situations. The following are some of the distinguishing features between them.

1. In the BCS limit, pairs form and condense simultaneously at the same temperature i.e. at superconducting transition temperature T_c . However, in the BEC regime, pairing occurs in the normal state at some temperature T^* and then these pre-formed pairs undergo condensation as temperature is lowered i.e. at $T_c (< T^*)$.
2. The excitations are of fermionic nature in BCS limit whereas the BEC phase is characterised by bosonic excitations. The intermediate regime is characterized by a mixture of fermions and fermionic pairs. Thus the excitations smoothly evolve from being fermionic (BCS) to bosonic (BEC) in nature. Fig. 1.2 can be referred to for a schematic description.
3. The superconducting order parameter Δ_{sc} and the excitation gap Δ are identical in the BCS limit as the pair formation (T^*) and condensation temperature (T_c) coincide. However, there exists a difference between Δ_{sc} and Δ in the BEC limit as $T_c \neq T^*$ (see Fig. 1.3).

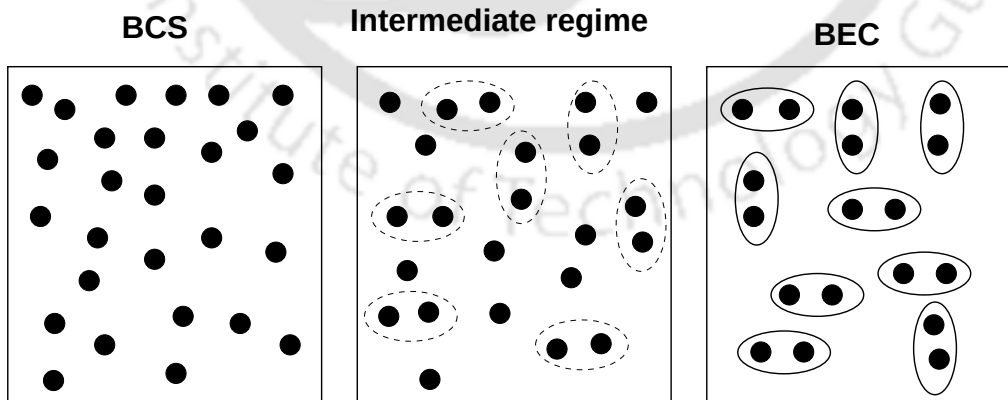


FIGURE 1.2: Schematic representation of the excitations in BCS, intermediate and BEC regimes. The excitations are fermions in BCS limit and bosons in BEC. The intermediate regime has a mixture of fermions and metastable (fermionic) pairs[18].

The largely explored but not well understood physics of the crossover phenomena lies in understanding the regime that lies intermediate to the two extreme limits (BCS and BEC). It is marked by strong fluctuation effects and shows significant digressions from the Fermi liquid behaviour because of the presence of fermionic pairs in the normal state. The breakdown of Fermi liquid theory in this regime is an outcome of a system undergoing smooth transition from fermionic to bosonic statistics.

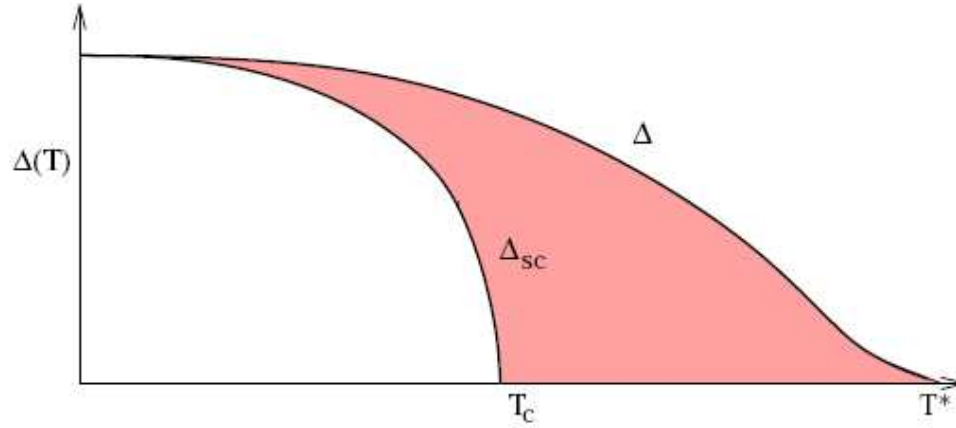


FIGURE 1.3: The superconducting order parameter Δ_{sc} and the excitation gap Δ differ in the BEC limit since pairs form (T^*) and condense (T_c) at considerably different temperatures. The shaded region comprises of pairs with no phase coherence[18].

1.1.1 Exploring a connection with high- T_c superconductors

There is probably some consensus that the crossover scenario may provide us a route to understand unusual features exhibited by the unconventional superconductors. Based on the μ SR and magnetic field penetration data, Uemura *et al.*[41] suggested that the unconventional or the 'exotic' superconductors belong to a separate class of materials characterised by high- T_c , short coherence length, ξ and low superfluid density, which are *unlike* their conventional counterparts. Further, the short ξ found in these materials, generate a scenario which is akin to a system consisting of local bosons. Finally, the boson condensation temperature, T_B at which the noninteracting Bose gas condenses (T_B is analogous to T^* at which local pairs form in the underdoped phase of cuprates), is almost one order of magnitude greater than the superconducting transition temperature T_c in these systems. The results encourage a generalisation of the BCS theory to be more suitable to the situation, rather than pursuing a search

for more exotic theories[42–44]. In fact the coherence length, ξ (or its dimensionless variant $k_F\xi$, k_F being the Fermi wave vector) is an appropriate quantity that tracks the crossover phenomenon[45], such that at $k_F\xi \simeq 2\pi$, the system becomes unstable against bosonization and the concept of Fermi surface gets wiped out since the onset of pairing instability no longer demands presence of a filled Fermi surface in this limit. Further, a meaningful connection to the Uemura plot is obtained as the unconventional materials are found to lie near the $k_F\xi \simeq 2\pi$ line in the plot and hence are closer to Fermi surface instability.

The unusual features of the normal state observed in the context of these high- T_c superconductors have also put a special focus on the physics governing the crossover. It has been argued that a BCS-BEC crossover induced pseudogap is the origin of the mysterious gap in the normal state observed in high T_c superconductors[46–48]. The above idea though highly contentious, is strongly believed by a section of the scientific community as it is based on the rationale that the gap in the normal state smoothly evolves into the superconducting gap as temperature is lowered. This in turn suggests that the pseudogap phase bears resemblances with the superconducting phase and not with the insulating phase exhibited by the parent compound.

The appearance of pseudogap in form of depletion of single particle spectral weight around the Fermi level below a certain critical temperature T^* in the underdoped regime of cuprates[17, 49–53] demonstrates the most comprehensive deviation from the mean-field (BCS) scenario for superconductors. The BCS picture may be viewed as a very special case where the pair formation and the condensation occur simultaneously i.e. at the same temperature while at moderate values of the interaction strength, the pairs form and condense at different temperatures, as energetics favour pair formation within the normal phase. Finally the system comprising of such bosonic degrees of freedom condenses at a different temperature, say T_c (below T^*). The two temperature scales (T_c and T^*) signal the presence of two different gap parameters, one of them being the superconducting gap (related to T_c) and the other corresponding to the excitations of the normal state or pseudogap at temperature $T > T_c$. Thus the bosonic excitations in the pseudogap phase smoothly evolves into fermionic ones in the BCS regime, thereby proving the inextricable connection between the crossover phenomenon and the pseudogap.

1.1.2 Kinetic energy driven vs Potential energy driven pairing

The signature of strong electron correlations in deciding the physical properties of the cuprate superconductors are robust and well studied. Thus the energy considerations in the normal and the superconducting phases, i.e. the condensation energy must involve the occupied part of the single particle spectral function - a quantity measured by ARPES. Consequently the energy gain that drives the system from a normal to a superconducting phase should be closely related to the renormalization of the spectral weight while lowering the temperature through T_c . The fact that the gap in the ARPES spectra opens at temperatures considerably larger than T_c while the quasiparticle peaks only emerge below T_c [54, 55], strongly suggests that there is an intimate connection between the phase coherence in pair degrees of freedom and the onset of coherence in the single particle spectrum. Further, the incoherent part of the spectral function should be carefully accounted for in calculating the condensation energy as the whole of the spectral intensity, not just the quasiparticle peak, is responsible for contributing to the total condensation energy.

Not too long back, the optical measurements on $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ [56] have shown a continuous transfer of spectral weight from higher energies to the lower energy part of the in-plane optical conductivity as the temperature is lowered. The above effect is observed in both the underdoped and overdoped phases. A characteristic energy scale has been identified, above which the integrated optical conductivity as a function of temperature behaves differently than that below the scale. In a $t-J$ model, roughly the same energy scale differentiates two regions, the one below, where the integrated optical weight is proportional to the kinetic energy, and the one above, where the same is proportional to the superexchange energy. This indicates (starting well above and persisting below T_c) that the normal to superconductor transition is accompanied by a continuous lowering of the kinetic energy, while the superexchange energy is increased as temperature is lowered. The rise in the interaction energy as the system evolves into the superconducting phase seems strange and contrasts the conventional BCS picture. Believing that the $t-J$ model is relevant to the discussion of cuprates, the kinetic energy drives the system both in the normal (pseudogap) and the superconducting phase. Thus the kinetic energy driven pairing may hold an important clue to the formation of pseudogap and more generally, the high- T_c problem.

Finally, to make the discussion free from loose ends, it is wise to investigate whether a BCS-BEC crossover scenario supports the condensation energy to flip from being potential energy driven (BCS) to kinetic energy driven (BEC).

1.1.3 Experimental realization of the crossover in ultracold atoms

We have seen in the previous discussion that a BCS-BEC crossover can be obtained by tuning the interparticle attraction strength. In this regard, the ultracold atomic gases has recently emerged as a potential candidate to study the crossover scenario. In this section, we digress from the main focus of the thesis so as to understand the experiments carried on ultracold atoms to achieve superfluidity. The most commonly used atoms for these experiments are the alkali atoms which have only one electron occupying the outermost shell. In the ground state, the inner shells are closed and thus they have no net angular momentum, and the outermost electron is in an s -orbit, also with no angular momentum. The outermost electron is the reason to the common use of alkali atoms in the experiments since these atoms have suitable transitions with optical wavelengths, that can be utilized for cooling. A typical trapping scheme utilizes the hyperfine interaction, which is the coupling between the electronic spin and the spin of the nucleus. The dependence of the energies of these hyperfine states on the external magnetic field is the well known Zeeman effect. The hyperfine states are characterized by their total spin F , which can take the values $I \pm 1/2$, where I is the nuclear spin and their hyperfine magnetic moment, m_F ranges from $-F$ to F . There is an energy difference between states $F = I - 1/2$ and $F = I + 1/2$ which is known as hyperfine splitting. In the absence of magnetic field, the states with same F are degenerate but as the magnetic field is turned on, it couples to both nuclear and electron spins resulting in splitting of the levels called Zeeman sublevels. The magnetic trapping makes use of the Zeeman coupling of magnetic field to energy levels of atoms in order to ensure trapping of atoms. Atoms can also be trapped in an optical lattice which is a one-, two-, or three-dimensional periodic potential obtained from superposition of counterpropagating laser beams. It operates on the principle of atom polarizability and its interaction with the electric field. The most commonly used trap based on the above techniques is the magneto optical trap (MOT) which helps in achieving temperatures of the order of $10 - 100 \mu K$. In order to cool the sample further, a technique called evaporative cooling is employed. This can be understood as lowering the 'edge' of the trapping potential, causing the atoms with the most kinetic energy, i.e. the hottest atoms, to

escape and letting the gas thermalize. The repetition of this process allows the cooling of the sample to very low temperatures of the order of 10 *nK*.

The ultracold atom gases have an essential feature of being dilute with densities below 10^{20} m^{-3} and the interparticle distance being larger than 100 *nm*. The extreme diluteness condition in turn results in two-body interactions playing dominant role while other processes involving higher order interactions are neglected. Thus, the underlying physics is mostly based on the two-body scattering theory. The attractive potential between the cold atoms is provided by the van der Waals interaction which is described by an interatomic potential which is repulsive at very small distances, r but has a weak attractive tail that goes as $1/r^6$ as $r \rightarrow \infty$. This interaction potential between the atoms depend on their internal states (spin- singlet or spin triplet). The effective interaction in the triplet channel can be tuned by changing the energy of a bound state in the singlet channel (with respect to the scattering states in the triplet channel) with a magnetic field. This phenomenon is known as Feshbach resonance in which one of the bound states (in triplet channel) is made to coincide with the collision energy of two free atoms in a different scattering channel (singlet channel). The energy difference between the free state and the molecular state which is controlled by the magnetic field, makes the scattering length in the singlet channel, a_s change from the BCS value ($1/k_F a_s \rightarrow -\infty$) to the BEC ($1/k_F a_s \rightarrow \infty$) through the strongly interacting unitary point ($1/k_F a_s = 0$).

a_s near Feshbach resonance (shown in Fig. 1.4), varies with magnetic field, B as[57]

$$a_s(B) = a_0 \left(1 - \frac{w}{B - B_0} \right) \quad (1.1)$$

Here a_0 is the triplet background scattering length for atoms scattering in the open channel, B_0 is the magnetic field position at which the bound state is just formed at the threshold and w is the magnetic field width of the Feshbach resonance, defined as the distance between B_0 and the magnetic field at which $a_s = 0$. A number of recent experiments have yielded detailed insights on the BCS-BEC crossover issue using Feshbach resonance[21, 36, 58–61].

1.1.4 Theoretical developments

Here we provide a brief outline of the variational mean field approach introduced by Eagles[33] and later by Leggett[34] to investigate BCS-BEC crossover at zero temperature. It was pointed

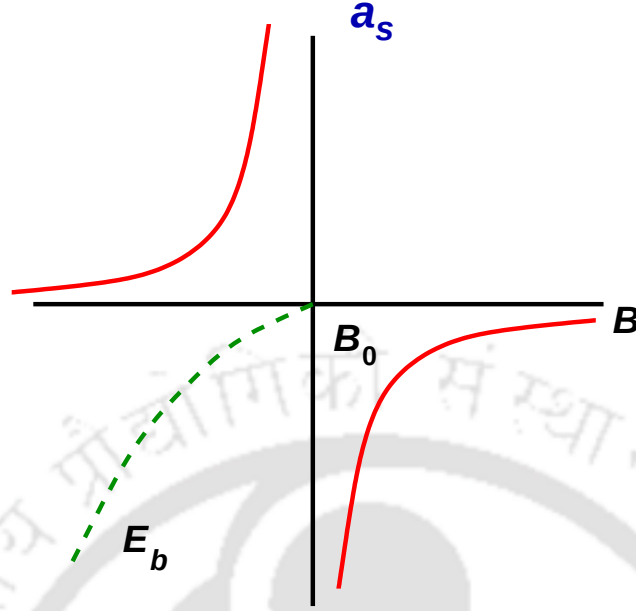


FIGURE 1.4: Schematic diagram showing variation of the scattering length, a_s (solid red line) with the magnetic field, B . The field corresponding to unitarity is marked by B_0 . The green dashed line is the energy of the two-body bound state, E_b in vacuum.

out by them that the BCS ground state wavefunction

$$\Psi_0 = \prod_k (u_k + v_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger) |0\rangle \quad (1.2)$$

is capable of describing a continuous evolution from a BCS superconductor to a Bose system of tightly bound pairs, provided the chemical potential, μ is self-consistently computed as the interparticle attraction strength is varied.

The self-consistent conditions that need to be solved are the BCS gap equation[62],

$$\Delta_k = - \sum_{k'} U_{kk'} \Delta_{k'} \frac{1}{2E_{k'}} \quad (1.3)$$

and number equation,

$$n = \sum_k \left[1 - \frac{\epsilon_k - \mu}{E_k} \right] \quad (1.4)$$

where $E_k = \sqrt{\xi_k^2 + \Delta_k^2}$ is the quasiparticle excitation energy with $\xi_k = (\epsilon_k - \mu)$. In the BCS approach, the interparticle attraction strength $U_{kk'}$ is assumed to be of the form,

$$U_{kk'} = \begin{cases} -U & \text{if } |\xi_k| \text{ and } |\xi_{k'}| \leq \hbar\omega_D \\ 0 & \text{otherwise} \end{cases} \quad (1.5)$$

Thus, the interaction strength is constant within the Debye energy, $\hbar\omega_D$, of Fermi energy, E_F . Using the above $U_{kk'}$ in Eq. (1.3), we find that it is satisfied by

$$\Delta_k = \begin{cases} \Delta & \text{for } |\xi_k| < \hbar\omega_D \\ 0 & \text{for } |\xi_k| > \hbar\omega_D \end{cases} \quad (1.6)$$

The gap parameter $\Delta_k = \Delta$ in this model and hence can be cancelled from both sides of Eq. (1.3) which yields

$$1 = \frac{U}{2} \sum_k \frac{1}{E_k} \quad (1.7)$$

It is however found that the above equation diverges as k assumes large values. For BCS superconductors, this problem is resolved by replacing the summation by an integration over $\hbar\omega_D$ and assuming the density states to be constant at the Fermi level. Both these conditions together give

$$-\frac{1}{N(0)U} = \int_{-\hbar\omega_D}^{\hbar\omega_D} \frac{d\xi}{2\sqrt{\xi^2 + \Delta^2}} \quad (1.8)$$

where $N(0)$ is the density of states at Fermi level. Solving Eq. (1.8), we obtain the BCS result,

$$\Delta = 2\hbar\omega_D e^{-1/N(0)|U|} \quad (1.9)$$

The extension of the BCS theory to large values of interaction strengths in order to investigate the BCS-BEC crossover phenomena, results in breakdown of the $\hbar\omega_D$ cut off. The divergence problem is then taken into account using a renormalization procedure[17] which yields a 'renormalized' gap equation

$$-\frac{m}{4\pi\hbar^2 a_s} = \frac{1}{V} \sum_k \left(\frac{1}{2E_k} - \frac{1}{2\epsilon_k} \right) \quad (1.10)$$

where the interaction is now replaced by a single parameter i.e. the s -wave scattering length,

a_s (in place of U) and V is the volume of the system. The above gap equation is then self-consistently solved with Eq. (1.4) for computing Δ and μ as a function of the dimensionless parameter $k_F a_s$ where $k_F = \sqrt{2mE_F}/\hbar$.

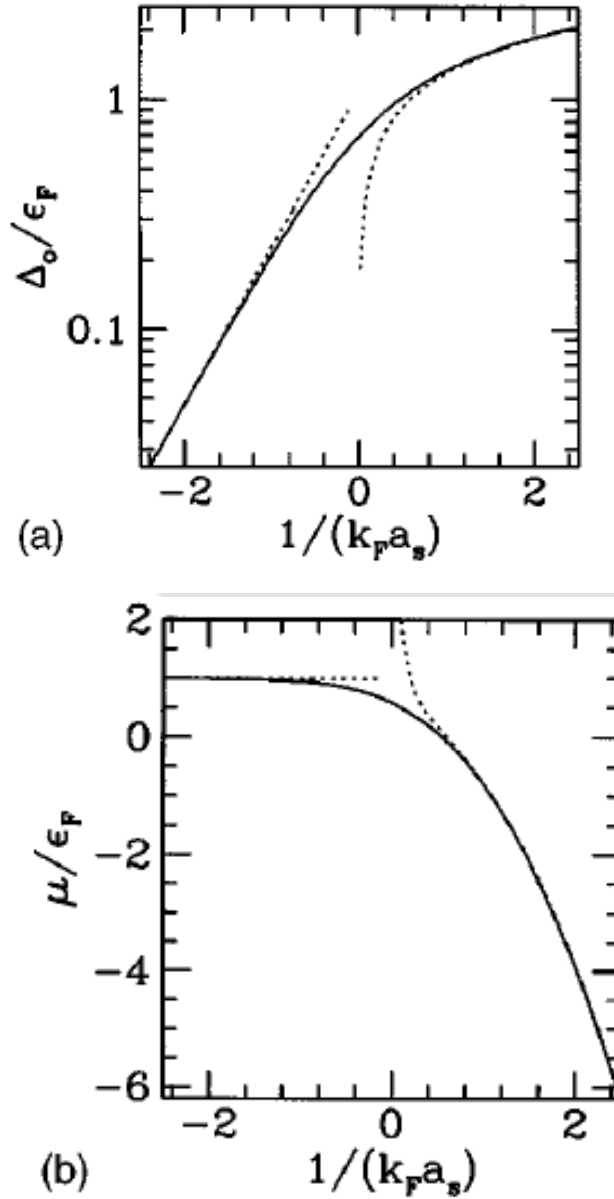


FIGURE 1.5: (a) The order parameter, Δ and (b) the chemical potential μ as a function of $1/k_F a$ [63].

Fig. 1.5 shows the result of Δ and μ obtained from the above analysis along with the analytic results of the two asymptotic limits (BCS and BEC) shown by the dashed line in the

figure[63]. It is clear from the Δ and μ plots that the crossover occurs in a small region of the parameter $1/k_F a_s$ i.e. $-1 \leq 1/k_F a_s \leq 1$.

Let us now analyze the definition of μ and Δ in the two limits. In the weak coupling limit where BCS theory holds, μ is solely determined by the Fermi energy, E_F . It shows a continuous decrease and eventually becomes negative ($\approx -E_b/2$ where E_b is the binding energy of a pair) in the BEC regime as a function of $1/k_F a_s$. Thus as coupling strength is increased, μ varies from being positive (in BCS) to negative (in BEC) and thus μ changing sign bears the signature of a crossover which is known as the 'Leggett criterion'. Δ also differs significantly in the extreme limits. For example,

$$\Delta = \exp\left(\frac{-\pi}{k_F |a_s|}\right) E_F \quad (1.11)$$

in the BCS limit while it is given by

$$\Delta = E_F \sqrt{\frac{16}{3\pi} \frac{1}{k_F a_s}} \quad (1.12)$$

in the BEC[64].

Further work on the crossover subject was done by Nozieres and Schmitt-Rink (NSR)[35] who extended the study to finite temperatures and in lattice systems. They resorted to a diagrammatic approach at finite temperatures. T_c determined by them in the continuum case, shows a monotonous increase in the weak BCS regime where it is determined by the breaking of pairs and eventually saturates at strong coupling where T_c is controlled by the center of motion of bound pairs. Further, their work on fermions in a lattice described by an attractive Hubbard model, had similar implications of T_c being a continuous function of interparticle attraction strength. They had shown that T_c undergoes an exponential increase ($\ln T_c \sim (-1/U)$, where U is the interparticle attraction strength) in the BCS regime, goes through a maximum when U is of the order of the band width ($\sim W$) and finally decreases at strong coupling.

Among many other attempts to describe the crossover scenario, an approach based on Ginzburg-Landau theory was followed by Drechsler and Zwirger[65] in order to determine the transition temperature in two dimensional systems. In a separate work by Sá de Melo *et al.*[66], a time dependent Ginzburg Landau theory was proposed to calculate the transition temperature which exhibited a small maximum in the crossover regime. It is important to

note here that all these theories were based on an approximation which used free-fermion Green's function to describe the fermionic degrees of freedom and the superfluid transition was marked by the rise of bosonic properties. This analysis yielded correct results in the two limiting cases of weak (BCS) and strong (BEC) coupling. However, its applicability failed in the crossover region where the fermionic quasiparticles were no longer free particles. An improved theory was then introduced by Haussmann[67] in which the fermion Green's function was determined self-consistently leading to qualitatively new results. Their work suggested a monotonically increasing T_c as a function of interparticle attraction strength in three dimensional systems and non-existence of maximum of T_c in the crossover regime.

Since the discovery of short coherence length superconductors (*e.g.* the cuprates), which are believed to occur in between large coherence length conventional superconductors (BCS) and a phase with extremely short (of the order of one lattice spacing) pairing correlations, the crossover phenomenon has received renewed attention. Attempts were made to interpolate between the two extreme limits so as to visit the physics that is operative for these superconductors. In this regard, Randeria and coworkers[68] initiated formal studies on the conditions for a pairing instability in two dimensional systems and also investigated the evolution of the superconducting ground state from large overlapping Cooper pairs to a Bose condensate of tightly bound pairs. They considered a two dimensional continuum of Fermi gas interacting with a given two body potential for investigating the conditions under which a pairing instability takes place in various angular momentum channels in the many body problem. In addition to a hard core at short distances, the potential is assumed to have an attractive part with a finite range R . The system is taken to be dilute i.e. $k_F R \ll 1$ which allows the analytical results independent of the shape of the potential and with the interaction energy completely characterized by the low energy phase shifts $\delta_l(E)$ of the two body scattering problem. The results are obtained by analyzing the energy dependence of the scattering phase shifts, starting with the Cooper problem.

In two dimensions, for the s -wave channel which is of interest to us, it is possible to obtain[68]

$$\pi \cot \delta_0(E) = \log(E/E_a) + O(E/\epsilon_R) \quad (1.13)$$

where $\epsilon_R = (\hbar^2/2mR^2)$ and the low energy s -wave T -matrix can be expressed in terms of the s -wave scattering phase shift as,

$$\frac{1}{\tau_0(E)} = (m/4\hbar^2) [-\cot\delta_0(E) + i] \quad (1.14)$$

It may be noted that $\tau_0(E)$ has a logarithmic divergence at $E = -E_a$ thereby indicating formation of a two bound state with E_a being the binding energy of the bound state. It is found that onset of pairing instability necessarily requires the existence of a two-body bound state. Note that in presence of strong repulsion at short distances, the attractive part of the effective potential must cross a threshold value before a bound state exists (beyond which the energy scale E_a above is the binding energy). In addition to this, they have also found that existence of such a two body bound state in a higher angular momentum channel ($l > 0$) is not a necessary condition for a many body pairing instability.

Randeria *et al.*[68] had then studied the many body ground state within a variational approach to investigate the evolution of a state with largely overlapping Cooper pairs to a Bose phase in a system with s and p -wave pairing instabilities. For this, they had chosen an ansatz for the ground state wavefunction as,

$$\Psi(1, 2, \dots, N) = \mathcal{A} [\phi(1, 2)\phi(3, 4)\dots\phi(N-1, N)] \quad (1.15)$$

which is an antisymmetrized product of pair wave functions. There is significant rearrangement of the occupation probability in the momentum space with increasing attraction strength and it no longer looks like a rounded step function. Consequently, the chemical potential μ for the fermions is not just E_F and needs to be determined self-consistently[34] along with gap function Δ_k .

An interesting feature of the 2D dilute system as obtained in Ref. [68] is that the coupled integral equations for $\Delta_k = \Delta$ (for $kR \ll 1$) and μ can be solved exactly for the s -wave pairing instability. The gap function and chemical potential thus obtained is as simple as $\Delta = (2E_F E_a)^{1/2}$ and $\mu = E_F - E_a/2$, where the interaction enters only via E_a , the binding energy of a pair in vacuum. The physical quantities e.g. the pair size, ξ_0 and the condensation energy which characterize a superconducting condensate, were computed as a function of E_a/E_F . The results obtained shows a smooth crossover from a BCS state with $k_F \xi_0 \gg 1$ for $E_a/E_F \ll 1$ to a Bose condensed state with $k_F \xi_0 \ll 1$ for $E_a/E_F \gg 1$.

The crossover scenario in a triplet superconductor i.e. in a p -wave channel is interesting, though not a focus of this thesis. It was found that the above variational analysis is considerably more complicated in p -wave channel than the s -wave case because of the appearance of ultraviolet divergences in the integral equations of the gap function and the chemical potential. The problem was then solved by regulating the divergences using corresponding results from the two body problem in vacuum. The results thus obtained show a continuous interpolation between the two extreme limits i.e. BCS and Bose phase. However, a weak singularity was found in the ground state results at $\mu = 0$.

In separate works by Strinati and coworkers[69, 70], the crossover effects were underscored by identifying a more significant variable than the coupling strength i.e. $k_F\xi$ which made the crossover study independent of the details of the interaction potential. Subsequently a great deal of work using diagrammatic approach[71–76] followed which have extensively investigated the normal and superconducting states (both above and below T_c). In Ref. [72], a fermionic system interacting through an effective nonretarded potential of the type introduced by Nozieres and Schmitt-Rink is considered to calculate the phase coherence length phase associated with the spatial fluctuations of the superconducting order parameter by exploiting a functional integral formulation for the correlation functions and the associated loop expansion. The phase coherence length phase, ξ_{phase} thus obtained is compared with the coherence length, ξ_{pair} for two-electron correlation, which distinguishes the weak coupling limit ($k_F\xi_{pair} \gg 1$) from the strong coupling limit ($k_F\xi_{pair} \ll 1$). It is shown that ξ_{phase} coincides with ξ_{pair} till $k_F\xi_{pair} \approx 10$ where ξ_{pair} is equivalent to the Pippard coherence length. The above condition breaks down in the strong-coupling limit where $\xi_{phase} \gg \xi_{pair}$, with ξ_{pair} coinciding with the radius of the bound state.

The fermionic self-consistent T-matrix approximation is widely utilized to describe crossover above the superconducting critical temperature. However it fails to yield the correct behavior of the system in the strong-coupling limit where pairs are tightly bound. This problem was solved in Ref. [74] by setting up the correct approximation for a 'dilute' system of composite bosons and had shown that a class of diagrams has to be considered in the place of the fermionic T-matrix approximation for the self-energy. This class of diagrams correctly described the interpolation between the weak and strong coupling limits. In this context, they had also provided a systematic mapping between the corresponding diagrammatic theories for the composite bosons and the constituent fermions. The scattering length obtained from

the above diagrammatic approach shows a considerable modification from the result obtained within the self-consistent fermionic T-matrix approximation in the strong-coupling limit.

In a separate work by Pieri *et al.*[77], the crossover scenario is studied in a broken-symmetry phase between zero temperature and the critical temperature by adopting a fermionic self-energy in the broken-symmetry phase that represents fermions coupled to superconducting fluctuations at weak coupling and to bosons described by the Bogoliubov theory in the strong coupling regime. The extension of the theory beyond mean field becomes crucial at finite temperatures in order to connect with the results of the normal phase. The order parameter, the chemical potential and the single-particle spectral function numerically computed for a wide range of values of coupling and temperature enables the assessment of the quantitative importance of superconducting fluctuations in the broken-symmetry phase across the entire crossover regime.

Other works on the crossover phenomenon include the numerical studies such as Quantum Monte Carlo[78, 79]. In Ref. [78], an extended quantum Monte Carlo study for various static and dynamic properties of the attractive Hubbard model are presented. The various observables investigated include magnetic susceptibilities, energies, specific heat, order parameters and spectral properties. In their work, they have shown appearance of tightly bound pairs far above the superconducting transition temperature in the crossover regime and have been able to quantify the separation of the formation of pairs and the condensation of the pairs into a coherent state with increasing coupling strength.

Further, the BCS-BEC crossover has been investigated using the dynamical mean field (DMFT) theory[80, 81]. It casts the lattice problem into a single correlated site positioned in a 'mean field' produced by the neighbouring sites. In doing so, the DMFT freezes all spatial fluctuations analogous to the usual classical mean field approach. But the main difference with the classical mean field theory is that here the mean field is a function of time and thus it retains the important quantum (temporal) fluctuations of the underlying problem. In the crossover studies, DMFT is used to explore the intermediate coupling regime and also allows study of the (metastable) normal phase down to zero temperature. The nature of the normal phase underlying the superfluid state is expected to strongly affect the properties of the state. The ground state properties of the normal phase has been studied in[82] as a function of the attractive strength.

The superfluid ground state for quarter filling on the Bethe lattice has been investigated in Ref. [83], where the authors compared the DMFT approach with the static mean-field results. The mean-field results are recovered in both the extreme limits (weak and strong coupling). However, the inclusion of local quantum fluctuations results in a reduction of the gap, which is particularly relevant for the intermediate-coupling regime. The ground state now evolves smoothly with the coupling and the transition found in the normal phase is washed out by the symmetry breaking. The same smooth evolution is found in [84, 85] where the authors have used DMFT to study the finite temperature phase diagram of the model in the superconducting phase. In particular, explicitly allowing the superconducting order to take place at finite temperature, the first order transition line of the normal phase is completely hidden by the superconducting state because the critical temperature for the transition to the normal state is higher than the pairing transition temperature. The evolution of the critical temperature and of the energetic balance as a function of the interaction strength is studied in Ref. [85]. It is remarkable that, in striking contrast with the static approach, the DMFT correctly reproduces both the extreme limits of the crossover also for zero temperature. Indeed both in the weak-coupling and strong-coupling, the BCS and BEC limit for the critical transition temperature are respectively recovered using DMFT.

The crossover effects induced by density has been also widely studied. In fact, the combined effects of density and interparticle potential [86] have been investigated which yields important conclusions like the robustness of the crossover scenario for all densities in case of s -wave pairing, however the same is not true for d -wave pairing at large densities. The reason being, at large densities, there is a substantial overlap between the spatially extended (d -wave) pairs even for strong attractive interactions. An elaborate discussion on density induced crossover in presence of different types of fermionic interaction potentials has also been done by Andrenacci *et al.* [87]. They have shown that absence of a threshold (for the formation of a two body bound state) in d -wave systems and the existence of a finite range of potential favour density driven crossover in two dimensional lattice systems. In addition, they have found out the essential criterion for the presence of crossover (as a function of density) in the continuum case.

The role of structural disorder in inducing a smooth evolution from a BCS superconductor to a BEC superfluid was put forward earlier [88]. More recently, a strongly disordered attractive Hubbard model with infinite range hopping (where mean field theory is exact) is shown to emulate a smooth BCS-BEC crossover as the range of hopping is varied [90]. Further, the

ground state properties of a superfluid Fermi gas is studied across a BCS-BEC crossover in presence of random disorder at $T = 0$ [91]. The main observation in Ref. [91] is the superfluid order parameter shows a non-monotonic behaviour as a function of interaction strength with a pronounced dip near the crossover regime. The renormalization effects are more pronounced as one moves towards the BEC limit.

The various works listed above do not put emphasis on evolution from a BCS to a BEC as a function of the strength of disorder (and density) alone. In this thesis, we have put forward that random onsite disorder can be an efficient agent to induce a crossover scenario. The investigation of the effect of disorder on the superconducting properties of dirty metals has a long history dating back almost to the advent of BCS theory[92, 93]. Renewed efforts during eighties[94–97] have revealed that in the strong disorder regime, the pairs loose their large spatial extension and get localized. A nice review on the subject may be found in Ref. [98]. From the ongoing discussion, it is clear that disorder crucially affects superconductivity, however at low densities, as we shall show later, it induces a crossover from a homogeneous (BCS) phase to a BEC superfluid.

Numerics, to investigate disorder effects on superconductivity, were used extensively[98–102]. Since the main objective was to study how superconducting properties respond to disorder and because the superconducting correlations are strongest at large electron densities, these studies were mostly restricted to large densities (and weak coupling). In any case, the main observation was that the spectral gap persists in presence of disorder, as is evident from the formation of superconducting islands, characterized by large pairing amplitudes and separated by regions which are insulating in nature. As the strength of disorder is enhanced, the islands shrink, making room for the intervening insulating seas. At small electron densities, the islands (or what we call '*droplets*' here) are more localised and thus bear fingerprints of a BEC phase which has very short and local pairs. In presence of strong disorder, quantum fluctuations, importance of which is underscored in literature[98, 100], plays a crucial role and may modify the scenario drastically. We provide our opinion on the effects of phase fluctuations in this thesis.

1.2 Spin imbalanced superfluid phases

In fermionic systems, the formation of pairs between two constituent components is the essential ingredient of superfluidity and superconductivity. When the populations of the two participating species are equal then superfluidity arises out of complete pairing between the species and thus the entire system contributes to superconductivity. This is the scenario in conventional BCS superconductors in which pairing occurs between equal number of fermions in momentum state k and spin $\uparrow$ with those in momentum state $-k$ and spin $\downarrow$. The important question which arises next is that how is the superfluidity affected when the populations of the participating species are unequal? One possible way of creating an imbalance in the densities of spin up and spin down electrons is by using magnetic field which makes the Fermi surfaces (corresponding to up- and down- spin states) shift away with respect to each other. It was proposed by Clogston[103] in 1962 that there exists an upper limit to this externally applied magnetic field beyond which superconductivity vanishes. The breakdown of superfluidity by such population imbalance can be understood by realizing that deep in the Fermi sea, particles cannot form a pair or even scatter off one another because their motion is 'frozen' by the exclusion principle. Pairing requires partially empty energy states that are found only near the Fermi surface. But if the populations of the two different spin components are different, the two Fermi surfaces no longer match up in momentum space i.e. there are no partially occupied states in which both atoms have the opposite momentum and can form a zero-momentum pair. This makes pairing energetically less favourable and eventually causes superfluidity to break down.

The 'ferromagnetic superconductors' are a class of superconductors in which an intrinsic magnetic field is produced by the ferromagnetic alignment of the paramagnetic impurities in the sample which in turn causes spin imbalance between different species of electrons[31, 32]. Thus in these materials, ferromagnetism coexists with superconductivity. The first experimental evidence of the existence of these ferromagnetic superconductors came recently with the discovery of UGe_2 [104] and URhGe [105] compounds. Neutron scattering experiments on UGe_2 have revealed that the same electrons are responsible for ferromagnetism and Cooper pair formation leading to superconductivity. It is also proposed that spin-triplet Cooper pairs

(*p*-wave) with non-zero net magnetic moment are most likely candidates of being ferromagnetic superconductors. In case of spin-singlet superconductors, the coexistence of ferromagnetism and superconductivity can be easily achieved in artificially fabricated layered ferromagnetic/superconductor (*F/S*) systems. This is possible because of the penetration of the Cooper pairs into the *F* layer thereby inducing superconductivity there. Thus, it provides a unique possibility to study the interplay between superconductivity and magnetism by changing the relative strengths of the two competing factors by varying the thickness of the *F/S* layers.

Various kinds of exotic phases were proposed to explain superconductivity in spin imbalanced systems. For example, Fulde and Ferrell[24] and independently Larkin and Ovchinnikov [25] proposed pairing between Zeeman splitted parts of the Fermi surface giving rise to an unconventional pairing state ($k \uparrow, -k + q \downarrow$), comprising of pairs having finite center of mass momentum, q . Another kind of non-BCS superfluid phase proposed is the breached pair (BP) phase. The general idea of BP superfluidity arises from standard BCS superfluidity, but with the two spin species participating in pairing being unequal. The interesting feature of the superfluid state is the presence of gapless fermionic excitations. The dominant interactions in these superfluids are the *s*-wave interactions because of which the states are homogeneous and isotropic. As a consequence, the gapless modes occupy entire Fermi-surface and not just nodal points as is the case with several other 'gapless' superfluids. Thus the coexistence of superfluidity with gapless excitations is a novel feature of the BP phase.

The origin of these states goes back to as early as 1960's when Sarma considered a gapless Schwinger-Dyson solution for a superconductor in an external magnetic field[26] in order to investigate the coupling between the field and the spins of the conduction electrons. These studies by Sarma and also by Maki *et al.*[106] were motivated from the unusual critical temperature versus magnetic field curve along with the existence of the Clogston-Chandrasekhar limit[103, 107] which showed that the critical field in some superconductors was set by Pauli paramagnetism. The inference drawn from the above studies was that the second order phase transition which exists between superconducting to normal phases becomes a first order transition at a critical value of temperature and magnetic field, making the critical value a tricritical point.

The interest in the phenomenon of gapless superfluidity was renewed by the works of Liu and Wilczek[27], where they considered a shift in the chemical potentials of the two spin states

due to a large mass ratio. They introduced the term 'interior gap' superfluidity to describe the scenario where the primary pairing takes place about the inner Fermi-surface. However their study was contested by Wu and Yip[108], who argued that the state is unstable to quantum fluctuations.

Further possibilities for gapless superfluids were reconsidered in the QCD and neutron stars where different quark flavours have different chemical potentials because of their different masses and charges[109, 110]. Motivated by these discoveries, Bedaque *et al.*[28] showed that a third possibility exists that can compete energetically with the BP state. They considered a heterogeneous mixed phase consisting of an inhomogeneous mixture of BCS and normal states and have found that the energy of such a mixed phase is lower than that of the BP state in several cases.

1.2.1 Understanding of the FFLO phase

The study of superconductivity in presence of magnetic field commenced nearly half a century ago with the works of Clogston and Chandrasekhar[103, 107]. In their work, they had considered pair breaking only by Pauli paramagnetic effect and the orbital component was assumed to be negligibly small. Later it was observed by Sarma[26] that the uniform state with population imbalance is unstable as magnetic field is increased (till $h = \frac{\Delta_0}{\sqrt{2}}$, where h is magnetic field and Δ_0 is the superconducting order parameter) at zero temperature which was confirmed by comparing the free energies of the normal and superconducting phases. Thus there is an indication of phase separation of the two spin species at $h > \frac{\Delta_0}{\sqrt{2}}$. The subject was intermittently revived to discuss about the bounds on the upper critical field and its effect on the phase boundary where the paramagnetic effect governs the physics. More abounding implications of the presence of an external magnetic field is elucidated by Fulde and Ferrell[24] and by Larkin and Ovchinnikov[25] where a possibility of finite momentum pairing between the different participation species of electrons is explored.

The relevant discussion on the effect of magnetic field on superconductivity is as follows. The Fermi surfaces of the spin up and down electrons split apart when an external magnetic field is turned on resulting in an imbalance of the two electron species. Under such circumstances, along with the conventional BCS state, the spin polarized state (normal state) and possibly more states compete for the ground state. The imbalance of the two electron species

inturn leads to breaking of a portion of the Cooper pairs. If the number of broken pairs is small, than the energy gap, Δ_0 is not affected. It may be noted that an energy of $2H$ (where H is the strength of the magnetic field) is gained from the new spin orientation at a cost of $2\Delta_0$ in breaking a Cooper pair, while attaining a spin polarized state. A continuous increase in the number of the broken Cooper pairs demand H to be larger than Δ_0 in order to make the spin polarized state eventually energetically more favored over the BCS state. But the spin polarized state has a lower energy when $H = 1/\sqrt{2}\Delta_0$ which is known as the 'Pauli limit'[103, 107]. Thus the BCS state with large number of broken Cooper pairs is unstable and an alternative solution exists for the ground state. This unusual phase is known as the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase which is stabilized by a large Zeeman splitting between up and down-spin electrons which form pairs across the Fermi surface and subsequently condense to give a state which has lower free energy than normal spin polarized state. These pairs have a non-zero total momentum ($2q = k_\uparrow - k_\downarrow$) as opposed to traditional zero momentum pairs in conventional BCS state (refer to Fig. 1.6) since the paired electrons have different momenta ($k_\uparrow$ and $k_\downarrow$). Interestingly, the finite momentum pairing results in an oscillating superconducting order parameter with a wave length of the order of superconducting coherence length, ξ . The FFLO phase thus breaks spontaneously translational symmetry and resembles the unconventional superconductivity in strongly correlated systems[111], where the order parameter changes sign in the momentum space. It is worthwhile to mention at this stage that FFLO phase is possible in the case of condensation (mass polarized) quarks (color superconductivity). Astrophysical objects, e.g. neutron stars or pulsars can be a good candidate to realize such a phenomena[112, 113]. A good introduction to the subject is obtained in reviews by Casalbuoni and Nardulli[31] and by Buzdin[32].

The orbital (diamagnetic) pair breaking is a crucial mechanism that limits realization of the FFLO state. It is a dominating pair breaking mechanism that destroys superconductivity for magnetic fields much weaker than the Clogston-Chandrasekhar limit (H_c). The significance of the diamagnetic pair breaking is usually described in terms of the Maki parameter $\alpha = \sqrt{2}H_{c2}^{orb}/H_c$, where H_{c2}^{orb} is the upper critical field calculated without the Zeeman splitting. Thus the paramagnetic effect (due to the exchange field) responsible for FFLO has to dominate over a competing orbital effect which annihilates superconductivity due to the formation of screen currents arising from vortices's. The above requirement demands few stringent conditions which must be satisfied for the realization of the FFLO phase such as ultra-clean type

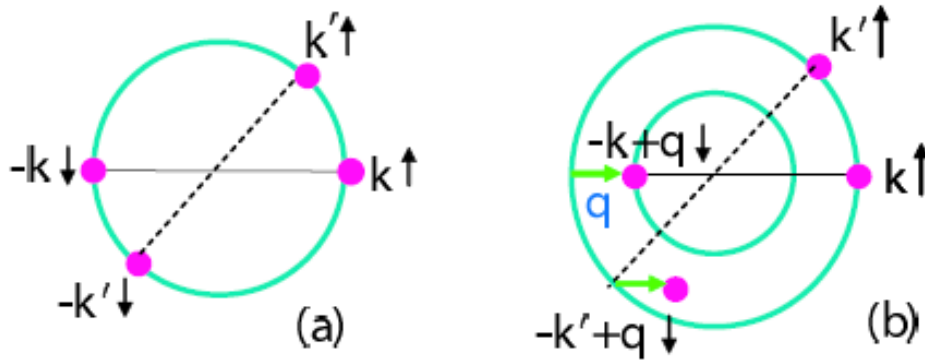


FIGURE 1.6: Schematic view of pairing states. (a) BCS pairing state, (b) FFLO pairing state. The inner and outer circles represent the Fermi surface of the spin down and up bounds respectively[111].

II superconductor, such that the pairing correlations survive at a finite magnetic field and the electronic mean free path, $l \gg \xi$ where ξ is the superconducting coherence length.

In spite of a robust theoretical possibility for the existence of FFLO, the experimental scenario remained bleak mainly due to the lack of phase space available for pairing to occur. Thus FFLO occupies very small space in the phase diagram. There exist two general possibilities to reduce the destructive role of the orbital pair breaking. In the layered superconductors, formation of Landau orbits should be suppressed for magnetic fields applied parallel to the layers. This may explain possible observations of the FFLO state in some organic superconductors. The role of the orbital pair breaking should also be limited in systems with narrow energy bands, like heavy fermion systems.

1.2.2 Experimental signatures

The experimental studies of FFLO in heavy fermion compounds e.g. Ce and U based materials started in the early nineties as some of the prerequisite conditions for observing FFLO is met in these systems[114–116]. Notable of them is CeRu₂ which is usually in a metallurgically clean state (defects and impurities easily destroy superconductivity) and exhibits extreme type-II behaviour (large $\kappa = \lambda/\xi$). Besides, UPd₂Al₃ (large Maki parameter), UBe₁₃ (high quality single crystals are grown and large upper critical field). However the findings on the FFLO phase has been inconclusive[117]. Among the heavy Fermion systems, the most explored one is CeCoIn₅ which receives strong support as a candidate with a FFLO phase.

These are essentially quasi two-dimensional structures and the magnetic field is applied parallel to the ab plane. The experiments on CeCoIn_5 , has shown the heat capacity (see Fig. 1.7) to undergo two phase transitions, a second order one within the superconducting (SC) state at low field values and a higher field first order transition at H_{c2} [118], the intervening regime acquiring a nonuniform nature. With the external magnetic field acquiring an angle with the ab -plane, the orbital effect starts playing a role and the large field transition goes away rendering an absence of the nonuniform or the FFLO state.

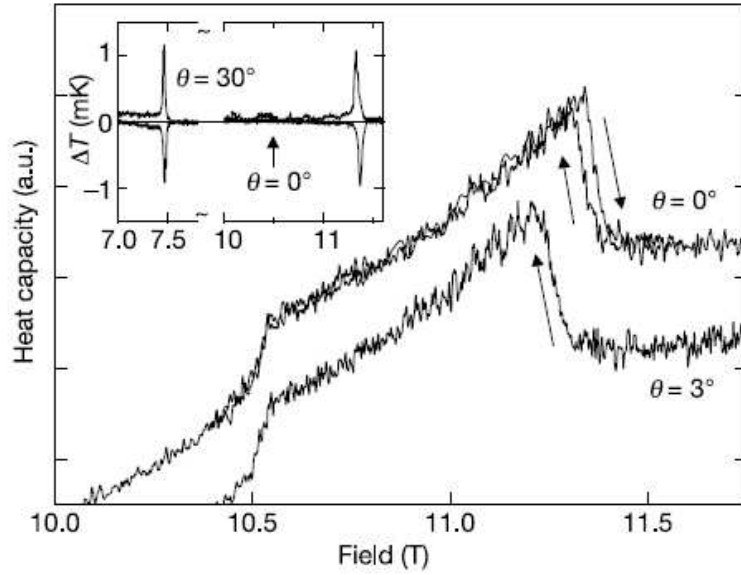


FIGURE 1.7: Heat capacity data obtained for CeCoIn_5 as a function of magnetic field which acquires an angle θ with the ab -plane[118].

The enhancement of penetration depth (as a function of magnetic field)[119], anomalous thermal and magneto-thermal conductivity (a discontinuous jump) in the vicinity of the upper critical field[120] and a structural transformation with vortices's appearing in the flux line lattice observed via ultrasound measurements[121] have provided reasonable though not robust support for CeCoIn_5 to host a FFLO phase.

Other experiments such as anisotropic magnetothermal measurements[120, 122] ultrasound velocity measurements[121] etc provide only indirect and cursory evidences supporting the presence of FFLO state.

More recently, ^{115}In NMR studies on CeCoIn_5 with the applied field parallel to ab plane reveals a dramatic asymmetry in the NMR spectrum for a field greater than the upper critical

field when compared with the one less than that[123]. Further, an unusual temperature dependence of the knight shift of ^{115}In is noted for the latter case. These facts are correlated with a direct evidence of the FFLO phase and a simulation of the NMR spectrum with a spatially modulated gap function seems to satisfactorily explain the experimental findings[124]. These results were challenged in the light of other NMR studies[125].

The main factors that act in favour of the organic superconductors as possible candidates for observing FFLO is that their layered structures (with the magnetic field parallel to the layers) thereby making orbital H_{c_2} to be extremely high and hence the Pauli paramagnetic effect becomes supremely important. The reduced dimensionality or the planar structure of these materials is conjectured to be a facilitator for observing the FFLO phase[126–128]. Recent critical field measurements[129] in the quasi-two-dimensional organic superconductor $\kappa(\text{BEDT} - \text{TTF})_2\text{Cu}(\text{NCS})_2$ strongly suggest that a state of the FFLO type exists in this material. The agreement between experiment[129] and existing theories has been successfully verified[130] both in view of the angle-dependence[131] and the temperature dependence[132, 133] of the upper critical field. In Ref. [130], a comparison between the experimental[129] temperature dependence of the plane parallel upper critical field with the theoretical results for $\kappa(\text{BEDT} - \text{TTF})_2\text{Cu}(\text{NCS})_2$ has been reported (refer to Fig. 1.8). This is the first time since the original predictions of the FFLO phase that quantitative agreement between theory and experiment with regard to the FFLO phase boundary has been established.

The increase of the critical field at low temperatures with positive d^2H_c/dT^2 was observed in $(\text{TMTSF})_2\text{PF}_6$ [134]. Such behavior of the critical field is very similar to the behavior that is theoretically obtained in low dimensional FFLO superconductors[126, 128, 135–137]. This might suggest the possibility of the FFLO state in this material or similar organic compounds, although this is not a conclusive evidence of the existence of the FFLO phase.

There have also been exciting development in recent years in achieving exotic superfluidity in ultracold atoms, e.g. ^6Li which have been trapped and cooled via magnetic means[138, 139]. An important issue of the study of the cold atoms is preparation of systems with imbalanced spin state populations. The population imbalance in different spin states is created by radio frequency (RF) sweeps where the relative number of the two states can be controlled by the RF power. The derivative of the study of trapped ultracold atoms yields the realization of BCS-BEC crossover at the Feshbach resonance[140]. Interaction between the atoms in different hyperfine states is strongly enhanced around a wide Feshbach located at

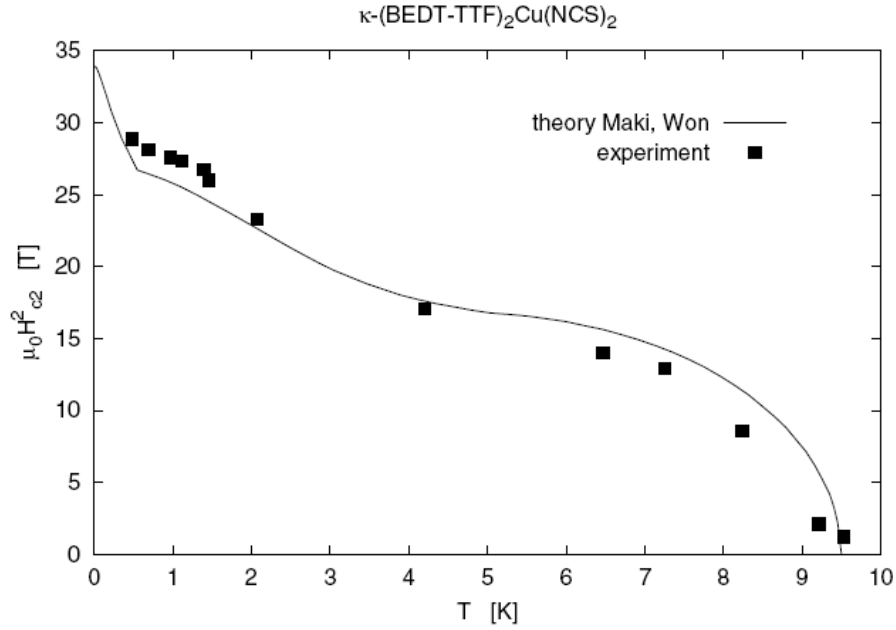


FIGURE 1.8: Upper critical magnetic field as a function of temperature as obtained from experiments and theory[130].

$B_c = 834\text{G}$. Below B_c , one sees a molecular superfluidity BEC (characterised by positive a_s , a_s is the s -wave scattering length) and above B_c , there occurs a gas of paired atoms (a_s being negative)[141]. The above cases are studied as a function of population imbalance between the participating up and down spins which show a coexistence of superfluid component (characterised by the presence of vortices's) with unpaired atoms. In a separate work, Partridge *et al.*[142] have reported quantum phase transition in a strongly interacting Fermi gas with imbalanced spin populations. The study claims evidence for a homogeneous superfluid state with unequal densities below a critical population imbalance and a phase separated state with a core of superfluid pairs surrounded by a shell of excess spin-up atoms above a critical population imbalance. The transition from the superfluid to the normal state in an imbalanced Fermi gas has been also seen by Zwierlein *et al.*[143] where the fermion pair condensates and the normal state were detected through sudden changes in the shape of clouds of fermionic atoms.

There has been considerable speculation about the nature of the spin imbalanced superfluid phase. For example, the FFLO phase[24, 25], breached pairing[27], Sarma superfluidity[26] and phase separated phase in which BCS superfluid coexists with an unpaired normal phase[28–30]. However, the consensus on the true ground state of a spin polarized Fermi system is yet

to be reached.

1.2.3 Theoretical works on the FFLO physics

A theoretical analysis of the FFLO state requires, in general, a self-consistent calculation of the amplitude of the spatially varying order parameter. Such calculations are within the reach of present computation capacities but were not possible in the early years of discovery of the FFLO phase. Early theoretical works on this problem were mostly centered around studying the region near the second order phase transition to the normal state[25, 144, 145] or studied the Fulde-Ferrell state characterized by a spatially modulating order parameter[146],

$$\Delta(r) = \Delta_0 e^{i\vec{q} \cdot \vec{r}} \quad (1.16)$$

Although analytical solution of both the problems exist, it fails to provide a complete description of the spin imbalanced inhomogeneous phase. For example, the Fulde-Ferrell (FF) state is not the correct minimum energy state, as shown by Larkin and Ovchinnikov (LO) who considered the order parameter to be of the form $\Delta = \Delta_0 \cos(\tilde{q} \cdot \tilde{r})$. It may be noted that the amplitude of the order parameter is no longer a constant in real space in the LO phase. Various studies have been performed with decreasing magnetic field which have shown that the LO phase evolves into a state with a set of domain walls. This has been shown in one[147], two[148], three[149] dimensions and also for d -wave superconductors[150]. In the limit of small population imbalance, the order parameter is constant in real space with the value being equal to that in the state with no population difference, excepting near the domain walls. These are the locations where the magnetization concentrates and the phase of the order parameter changes by π when the walls are crossed. The physics of these domain walls is closely related to that of the π junctions in superconductor-ferromagnet-superconductor junctions[32].

A suitable framework for a numerical study of the problem is the quasiclassical theory of superconductivity, developed by Larkin and Ovchinnikov[25] and Eilenberger[151]. This theory can be interpreted as the generalization of Landau's theory of normal Fermi liquids for the superconducting state. Further, the phase transitions from BCS to FFLO and FFLO to normal states have been studied using Ginzburg Landau theory[152]. In another Ginzburg Landau study[153], the Josephson effect is used to detect the existence of the FFLO phase based on the suppression of the Josephson current in the junction between BCS and FFLO

superconductors due to the mismatch in the momenta of the order parameters. Their study also provides a way to directly measure the momentum of the order parameter. Other theoretical works mostly concentrated around investigating the stability of the FFLO states[154, 155], a comparison between FF and LO states in real materials[156–158] and the nature of phase transitions involved at the BCS-FFLO and FFLO-normal interfaces[159]. Doh *et al.*[160] in their work have proposed a unique way of stabilizing FFLO state by applying external currents in superconductors with Fermi surface nesting. A detailed study of the effect of dimensionality on the exotic FFLO phase has been also performed. In one dimensions, it was argued that the ground state of the homogeneous attractive Fermi gases with unequal spin populations is the one dimensional analogue of the FFLO phase[161].

An elaborate study of the scenario in two dimensional systems has yielded many intriguing results[162, 163]. In particular, a quasiclassical analysis in Ref.[164] using a Ginzburg-Landau expansion of the free energy in Fourier components of the superconducting order parameter, had shown that the FFLO transition in two dimensions is continuous at low temperatures. In a separate study of a two dimensional two-component atomic Fermi gas with population and mass imbalance, it was argued that the normal and homogeneous balanced superfluid phases are separated by an inhomogeneous FFLO-like phase[165]. The study of FFLO phase in three dimensional systems[156, 166], have predicted a narrow region of FFLO phase in the phase diagram as compared to one and two dimensional cases.

Various studies have shown that the system has to be in the ultraclean limit where the quasiparticle mean free path l is much longer than the coherence length ξ for the realization of the FFLO phase. This in turn demands that the Ginzburg Landau parameter, κ must be much larger than unity. These conditions are readily met in d -wave superconductors like high- T_c superconductors and organic superconductors e.g. $\kappa - (ET)_2$ salts and $\lambda - (ET)_2$ salts[129]. Thus the discovery of these new classes of superconductors have triggered an extensive search of FFLO state in d -wave superconductors[167, 168]. In this regard, some of the theoretical studies have predicted that the stability of the FFLO state in two dimensional d -wave superconductors is much more than in three dimensional s -wave superconductors[132, 169, 170]. Some other studies have been performed to investigate the effect of disorder on the FFLO state in d -wave superconductors. For example, Vorontsov and coworkers[171], have investigated the stability of the FFLO state in dirty d -wave superconductors using the quasiclassical theory based on the self-consistent t -matrix approximation for impurities. Their results are counterintuitive as it shows the FFLO state to be robust in 'dirty' d -wave superconductors. In

a separate study by Yanase[172], the spatial structure of the superconducting order parameter and the magnetic properties in the disordered FFLO state are investigated using Bogoliubov de Gennes method. The results show that the nature of the superconducting order parameter is strongly dependent on the kind of disorder taken into consideration.

The modulating superconducting order parameter which yields a direct evidence of the presence of FFLO phase, is very difficult to observe in experiments. In this context, the quasi particle local density of states (LDOS) is very useful as it can be directly detected using scanning tunneling microscopy (STM). The LDOS for a two dimensional d -wave superconductor has been computed by Vorontsov *et al.*[150] by solving quasiclassical Eilenberger equations. Wang *et al.*[173] have also investigated LDOS for both s and d -wave superconductors, along with the superconducting order parameter which is found to be stripe-like for s -wave superconductors and a square lattice for d -wave superconductors.

Most of the theoretical studies of the FFLO state are based on mean field approach which is counterintuitive as one expects the quantum and thermal fluctuation effects to play significant role in FFLO phase than in conventional BCS superconductors, as the FFLO phase breaks the translational symmetry. In this regard, Kun Yang[161] has studied the FFLO phase in quasi-one dimensional superconductors using bosonization for an exact treatment of the intrachain quantum fluctuations and had shown that the transition from the FFLO phase to BCS is a continuous transition of the commensurate-incommensurate type. The effect of thermal fluctuations has been discussed by Shimahara[111] which reveals that the mean field FFLO state is destabilized by the enhanced fluctuation effects. In all these studies for treating phase fluctuations for an FFLO superconductor, the most common method is to incorporate a fluctuation in the phase of the order parameter and hence construct a generalised Ginzburg-Landau (GL) action for the phase variable[152, 174]. Spatial correlations of the phase variable indicate a rapid suppression of the long range order (LRO). Further, the fluctuation driven transition from normal to FFLO is found to be first order that corroborates the experimental evidences in CeCoIn₅, however contradicts the mean field results[152].

The experimental realization of the phase has been illusive mainly because its occurrence requires several stringent conditions to be met simultaneously. In most type-II superconductors, destruction of superconductivity occurs through orbital pair breaking effect, leading to the emergence of vortex state. However, such an orbital effect is always detrimental to the FFLO state. Hence for the FFLO state to occur, the orbital pair breaking effect must be weak

relative to the Pauli paramagnetic effect. Moreover the system needs to be clean, since the FFLO state is readily destroyed by impurities. The cleanliness condition is met when the coherence length, ξ is very small as compared to the mean free path, λ . Thus, the superconducting materials fulfilling these necessary conditions are few. Some of these conditions are satisfied in heavy fermion superconductors with large orbital limiting fields[114–116].

An alternative route to achieve the supremacy of paramagnetic effect is to use a layered structure in a strong magnetic field applied parallel to the layers, thereby undermining the orbital pair breaking effect further and augmenting the parameter space where FFLO can exist[175]. The organic superconductors strongly fit into these requirements and hence are considered as ideal candidates for FFLO phase[126, 128]. Apart from these compounds, signatures of FFLO phases are also observed in neutron stars[176].

The cold atoms in optical lattices also offers the possibility to explore the novel superfluid phase of imbalanced fermions[141, 142, 177, 178]. Numerous proposals for the paired state have been suggested for the trapped spin polarized gas. For example, the FFLO phase, breached pairing[27], Sarma superfluidity[26] and phase separated phase in which BCS superfluid coexists with an unpaired normal phase[28–30]. The theoretical evidences of the presence of FFLO phase in a trapped gas have been reported earlier[155, 179, 180]. In a separate work by Liu *et al.*[181], a comparative study of zero-temperature quantum phases in a one-dimensional spin-polarized Fermi gas has been presented using three different theoretical methods viz. mean-field theory with an order parameter in a single-plane-wave form, a self-consistently determined order parameter using the Bogoliubov de Gennes equations and the exact Bethe ansatz method. Their results have shown that a spatially inhomogeneous FFLO phase lies between the fully paired BCS state and the fully polarized normal state. Further, the phase transition from the BCS to the FFLO phase has been found to be of second order in nature. They have also investigated the effect of a harmonic trapping potential on the phase diagram and confirmed that the presence of trap leads to phase separation. The investigation of the local fermionic density of states of the FFLO phase has shown appearance of a two energy gap structure and hence is useful as an experimental probe of the FFLO phase. The zero temperature study has then been extended to finite temperatures[182] using Bogoliubov de Gennes method which provides the density profiles of the system along with various thermodynamic properties e.g. entropy, energy and specific heat. The FFLO phase has been seen to exist in trapped three dimensional gases for small polarizations and weak attractive interactions[183]. However, the region occupied by it in the $T = 0$ phase diagram[155] is

found to be small which further diminishes with increasing temperature[184]. In another work by Parish *et al.*[185], they have shown that the two dimensional optical lattice enlarges the region of the FFLO phase in the phase diagram thereby making its experimental observation possible.

Various kinds of FFLO have been predicted in trapped gases. The most well studied among them is the radial FFLO which is characterized by an order parameter which changes its sign along the radial direction around the edge of the harmonic trap[179–181, 186, 187]. Chen *et al.*[188] have explored the superconducting order parameter of a two dimensional trapped gas by solving the Bogoliubov de Gennes equations and have found a radial FFLO at low densities. A more exotic angular FFLO is observed at high densities while the nature of the FFLO state becomes square lattice-like at intermediate densities. The angular FFLO has been also predicted in two dimensional population imbalanced gas trapped in a toroidal trap[189].

1.2.4 Superconductor to insulator transition in spin imbalanced superfluids

Excellent control over the interparticle interaction for the ultracold atoms in optical lattices in which the strength of the collisional interaction between atomic states of different spin species are controlled using Feshbach resonance[40, 190], can provide useful guide to study strongly correlated systems. It offers the unique possibility to examine a superfluid to insulator (SIT) transition which has been an intensely studied problem in condensed matter physics.

The interplay between localization and superconductivity is an old problem. The gradual vanishing of superconducting transition temperature as a function of the driving parameter and finally the emergence of the insulating phase signaled via enhanced resistivity represents a classic example for a phase transition. In many of the thin films, disorder plays the role of the driving parameter which at large values of disorder show considerable digression from early theories of dirty superconductors[191, 192]. The issue of SIT received renewed attention with the observation of inhomogeneous pairing with formation of isolated superconducting islands in a highly disordered s-wave superconductors[98, 100, 101, 193]. At the mean field level, the eigenstates of the system become localized and in the limit of large disorder, the superconducting regions reduce to small 'blobs' which are separated by extended insulating

strips. At extremely large disorder, superconductivity vanishes giving way to a homogeneous insulating phase.

It is important to realize the localization effects induced by disorder. Similar effects can also be produced by confining potential profiles. Creating such confinement effects for charge carriers on a crystal lattice is an impossible task as the wavelength of the electromagnetic wave that is needed to create such trap should be of the order of lattice spacing. However, the situation for atomic gases in optical lattices present are far more optimistic scenario to achieve such trapping effects. In fact the Mott-Hubbard transition in cold bosonic atoms has been observed experimentally[194] as the depth of the optical lattice potential is increased. The superfluid phase, where phase coherent atomic wavefunctions spread over entire lattice for low lattice potential strengths, transforms to an insulating phase with exact number of atoms at individual sites, thereby loosing phase coherence for higher values of lattice potential. The loss of phase coherence with increasing potential strength is studied in experiments by sudden turn off of the lattice potential thereby allowing free expansion of the atomic wavefunctions, where a high contrast interference pattern is obtained in the superfluid regime owing to maximum interference between the delocalized atomic wavefunctions possessing definite relative phases between different lattice sites. As the lattice potential is made larger, the interference maxima is completely lost due to the complete localization of atomic wavefunctions at a single lattice site and hence giving rise to an insulating phase. This is well understood with the framework of a Bose-Hubbard model on a lattice with hard core repulsive interaction[195, 196]. Such transition was also observed in ultracold Fermi gases where the vanishing of the compressibility of the system indicates emergence of a Mott insulating phase as the repulsive interaction between the Fermionic atoms is continuously tuned[197]. Similar signatures of transition to an insulating phase has also been observed as a function of harmonic trapping potential[198].

1.3 Outline of the thesis

In this thesis, we have performed an elaborate study on two of these exotic phases viz. the one that deals with a smooth evolution of a system of fermions with weak attractive interactions comprising of largely overlapping Cooper pairs (BCS) to a phase characterized by short ranged tightly bound molecules (BEC) driven by a random onsite disorder potential and the

second one explores FFLO phase induced by spin imbalance and the effects of a trapping potential on such a phase for weakly coupled superfluids.

Chapter 2 deals with the model and formalism used in this thesis to address different issues concerning BCS-BEC crossover and that of the FFLO phase in a weakly coupled, planar s -wave superconductor. While different tools and model systems are available in studying these subjects, we resorted to an attractive Hubbard model in two dimensions and solved the Bogoliubov de Gennes (BdG) equations for the model via numerical computation, which seems to be a suitable starting point for both the problems. As for the crossover issue, the evolution to a Bose phase is induced by a random distribution of onsite disorder potential (chosen from a random distribution e.g. Gaussian) and the onset of a FFLO phase is achieved by a constant magnetic field interacting with the electronic spins via Zeeman coupling and quantified by the density imbalance between up and down spin species. However, since the BdG approximation ignores phase fluctuations and an estimate of the effect of phase fluctuations about the inhomogeneous BdG state (pertaining to the disorder problem) is necessary, a scheme for incorporating fluctuation effects with specific emphasis to Gaussian fluctuations is discussed.

Chapter 3 contains a thorough investigation of the BCS-BEC crossover scenario in disordered superconductors. The existence of a crossover in the disordered model is first confirmed from the behaviour of the chemical potential as a function of disorder, which slips below the noninteracting electronic band minimum (Leggett criterion) at the onset of the Bose phase. An exotic phase characterized by short ranged pairs, is seen to emerge at intermediate values of disorder, sandwiched between the conventional BCS phase (corresponding to low disorder values) and an insulating phase (at large disorder values). Further, the role of carrier density on the crossover issue is highlighted. Hence, to understand the nature of the disordered phase, various physical quantities e.g. off diagonal long range order (ODLRO), spectral gap and superfluid stiffness (averaged over several different random configurations) are computed using the BdG eigenstates as a function of the disorder strength. Inclusion of the phase fluctuations about the inhomogeneous BdG state yields an exciting possibility of achieving a phase which bears resemblance with the pseudogap phase of cuprates.

In chapter 4, to convince ourselves about the proposed crossover picture driven by random onsite disorder, we next compute some crucial (real space) quantities e.g. the pairing amplitudes, electron occupancies, participation ratio and the fidelity. At moderate values of

disorder, we obtain clear signatures of the emergence of a superfluid phase which is characterized by short ranged and tightly bound pairing correlations. In particular, the fidelity data show a significant drop in overlap between the ground states in the vicinity of the proposed crossover regime. The implications of their results are discussed in details.

Chapter 5 introduces the second problem of the thesis where a thorough analysis of the FFLO phase induced by spin imbalance is presented. The local pairing amplitude and magnetization computed via solving BdG equations for all lattice sites, show spatial modulation (characteristic of the FFLO phase) with the modulation wavevector being a function of the spin polarization and hence the effective momentum of the Cooper pair. The above scenario is scrutinized for different interaction strengths and over a broad range of band filling. Further a careful study is presented to select between various competing ground states which are close by in energies, however show very different ground state correlations.

Chapter 6 discusses the effect of trapping potential on a spin imbalanced superfluid state as such confinement effects are of technological importance for the cold atomic gases in an optical lattice. While acknowledging the fact that engineering of such trapping effects is not possible in crystal lattices, we proceed without further hesitation, as either for electrons in a crystal or for a system of cold fermionic atoms in an optical lattice, the model and formalism discussed earlier all the while remain unaltered, thus a common description suits our purpose. Corresponding to a finite spin imbalance, the superconducting order parameter shows different modulation profiles for with and without a trapping potential. We propose that signatures of a FFLO phase is best obtained when the trap effects are switched off, as seen by computing various physical and experimentally accessible quantities, such as the pair-pair, density-density (double occupancy) correlations and local number density fluctuations.

Chapter 7 examines the possibility of a transition from a superconductor to an insulator (SIT) in a confined spin-imbalanced Fermi system. The signature of SIT is obtained via a non-monotonic behaviour of the spectral gap, while the order parameter that characterizes the superfluid phase vanishes as a function of trapping strength. This is a remarkable result as it signals a SIT in model with (weak) attractive interactions in two dimensions. While it is known that the large trapping potentials can induce localization effects, our work demonstrates that similar effects are also possible at relatively small trapping strengths.

Chapter 8 concludes with a summary of the main results of the thesis. The implications of these, alongwith the possible extensions are discussed thereafter.



Chapter 2

Attractive Hubbard model and the Bogoliubov de Gennes method

2.1 Introduction

In this chapter, we introduce the model used in this study for studying superconductivity. Previous results for this model in literature are discussed briefly. Next we describe the Bogoliubov de Gennes method (BdG) which we use for studying the model. Detailed derivations of the BdG equations both in the presence of disorder and magnetic field are presented.

2.2 The attractive Hubbard model

The attractive Hubbard model (AHM) is the simplest lattice model, using which one can study the pairing correlations and the evolution of superconductivity as a function of the attractive strength. As we will see below, it provides a very simple realization of the BCS-BEC crossover in a lattice model. In the past, this model has received enormous attention because of the possible connection between the BCS-BEC crossover and high- T_c superconductors. The repulsive counterpart of the AHM was introduced in 1963 independently by Hubbard[199], Kanamori[200] and Gutzwiller[201] in the context of strongly correlated electron system. It

has been proved to describe the physics of the Mott transition, i.e. the metal-insulator transition induced by the increasing repulsions between the electrons, while its relevance in the physics of high- T_c superconductors is still under debate. AHM on the other hand has the advantage that Quantum Monte Carlo simulations are not affected by the fermionic sign-problem as contrary to the repulsive case. It is a very useful tool for the study of the region with intermediate values of coupling strength where the crossover actually occurs.

2.2.1 General properties of the model

The grancanonical Hamiltonian of the Hubbard model is written as,

$$H = - \sum_{\langle ij \rangle, \sigma} t (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) + U \sum_i \left(n_{i\uparrow} - \frac{1}{2} \right) \left(n_{i\downarrow} - \frac{1}{2} \right) - \mu \sum_i (n_{i\uparrow} + n_{i\downarrow}) \quad (2.1)$$

where the operator $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) creates (destroys) a fermion with spin σ on the site i and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ is the number operator, t is the hopping amplitude between next-neighbor sites, U is the strength of the Hubbard on-site interaction ($U < 0$ for the attractive model) and the chemical potential, μ is shifted making the model explicitly particle-hole symmetric for $\mu = 0$, which corresponds to the half-filling case i.e. $\langle n_{i\sigma} \rangle = 1$.

The physical properties of the AHM depends upon $|U|/t$ and $\langle n \rangle$. Studies have shown that for dimensions $d \geq 3$ at half filling, there exists a finite critical temperature separating a disordered phase from a low temperature phase where charge density wave (CDW) order coexists with superconductivity[202–204]. The low temperature phase becomes completely superconducting away from half filling with a critical transition temperature that decreases with filling. At two dimensions $d = 2$, the critical transition temperature is zero at half filling. In a work by Scalettar *et al.*[205], it was argued that doping away from half filling leads to a finite superconducting transition temperature for the two dimensional attractive Hubbard model. Although the model is simple and widely studied, no exact solutions are available in two and three dimensions. It is thus necessary to adopt some kind of approximation or numerical approach. In our work, we have chosen explicitly the case of two dimensional superconductors.

The crossover physics is determined in this model by the competition of two energy scales: the first one represents the kinetic energy, t during the hopping processes and the second one is

the attractive potential energy U assumed to be local, i.e. particles interact only when they lie at the same site. The ratio U/t can be used to identify a weak coupling regime ($U/t \ll 1$) and a strong-coupling regime ($U/t \gg 1$). The presence of a local attraction favors the formation of fermionic pairs, which become local (on-site) for $U \gg t$, making the model particularly suitable for describing the evolution towards a bosonic superconductivity.

Weak-coupling limit ($U/t \ll 1$)

In the weak-coupling limit, the correlations between the fermions are not so significant and a mean field approach can safely be applied. Such a mean field calculation has been carried out, for a system with uniform DOS by Robaskiewicz *et al.*[206, 207]. Under the reasonable assumption (if $n = 1$) of neglecting the CDW phase, they have computed the analytical expression for the order parameter $\Delta(r_i) = -|U|\langle c_{i\downarrow}c_{i\uparrow} \rangle$ and the critical temperature T_c for the transition to the normal phase given by,

$$\Delta(T = 0) = -D \frac{\left(\sqrt{n(n-2)} \right)}{\left(\sinh \left(\frac{2D}{U} \right) \right)} \quad (2.2)$$

and

$$k_B T_c = 1.14D \sqrt{n(n-2)} \exp \left(-\frac{2D}{|U|} \right) \quad (2.3)$$

where D is the half-bandwidth. In the weak coupling limit ($U \ll t$) characterized by largely overlapping and loosely bound Cooper pairs, the gap $\Delta(T = 0)$ is exponentially small. Thus results become analogous to the standard BCS theory. It may be noted that in this regime the underlying lattice is not essential for the description of the superconductivity, since the coherence length ξ_0 , which roughly gives the size of the pairs, is much larger than the lattice spacing. The only relevant difference with the standard BCS results is that in this case the pairing takes place in the whole Brillouin zone, instead of being limited by a characteristic phonon frequency (ω_D). Therefore it is the fermionic bandwidth which plays the role of the relevant energy scale in this case which is evident from the proportionality of both $\Delta(T = 0)$ and T_c on D .

Strong-coupling limit ($U/t \gg 1$)

In the opposite limit of strong attraction ($U/t \gg 1$), tightly bound pairs are formed. The coherence length ξ_0 which is determined by the size of the pairs, decreases with increasing

attractive strength until the pairing becomes a local process and the bound pairs have a typical extension of the order of the lattice spacing of the underlying lattice. An useful insight on the strong-coupling limit of the model can be gained building the effective strong-coupling Hamiltonian by applying the standard degenerate perturbation theory for arbitrary band filling[202].

2.2.2 Attractive Hubbard model in presence of onsite disorder

Our first problem deals with studying BCS-BEC crossover in disordered superconductors. For studying this problem, we consider an attractive Hubbard model on a two-dimensional square lattice,

$$H = - \sum_{\langle ij \rangle, \sigma} (t + \delta t_{ij}) (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) - |U| \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_{i, \sigma} (V_i - \mu) n_{i\sigma} \quad (2.4)$$

To model random on-site disorder, we let $\delta t_{ij} = 0$ for all i and j and the onsite disorder, V_i to be chosen randomly from a Gaussian distribution of the form,

$$P[V_i(\sigma)] = \frac{1}{\sqrt{2\pi}\sigma^2} \exp\left[-\frac{V_i^2}{2\sigma^2}\right] \quad (2.5)$$

In a similar fashion, hopping disorder is modeled by letting $V_i = 0$ for all i and δt_{ij} to be chosen from a gaussian distribution, which may be obtained as one replaces V_i by δt_{ij} in Eq. (2.5). Here σ denotes the width of the distribution and parametrizes the strength of disorder in our computation, *i.e.* larger σ implies stronger disorder. The third kind of inhomogeneity, *i.e.* hopping anisotropy, which is a case of correlated disorder, is modeled trivially by choosing $\delta t_{ij} = V_i = 0$ and the hopping, t is defined as

$$t_{ij} = \begin{cases} t & \text{for } j = i \pm \delta x \\ rt & \text{for } j = i \pm \delta y \end{cases} \quad (2.6)$$

when δx and δy are neighbours along x and y -directions respectively, with r the anisotropy parameter ($0 < r \leq 1$).

2.2.3 Attractive Hubbard model in presence of magnetic field

We adhere to the weak coupling limit of the AHM, as a conventional (BCS) superfluid state is a suitable starting point for our next problem which deals with studying superconductivity in the presence of magnetic field. AHM for a two-dimensional s-wave superconductor in presence of magnetic field is given by

$$\mathcal{H} = -t \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) - |U| \sum_i \left(n_{i\uparrow} - \frac{1}{2} \right) \left(n_{i\downarrow} - \frac{1}{2} \right) + \sum_{i, \sigma} (\sigma h - \mu) n_{i\sigma} \quad (2.7)$$

h is the magnetic field which couples with spin, σ of electrons via Zeeman coupling and μ denotes the chemical potential.

2.3 Bogoliubov de Gennes method

The effect of strong disorder on superconductivity is a challenging theoretical problem, as it necessarily involves interplay of interactions and disorder. In disordered superconductors, electrons experience an arbitrary external potential (site-dependent), in addition to the attractive interactions between them. It is interesting to note that with increasing disorder, the local pairing amplitude shows a substantial reduction in amplitude, eventually becoming zero. However, the spectral gap in the one-particle density of states continues to exist even at high disorder[100]. This and many other interesting features have put a special focus on understanding the physics governing the disordered superconductors and necessitate a detailed study on the subject.

The Bogoliubov-de Gennes (BdG) method is appropriate in understanding the physics of inhomogeneous superconductors. The BdG framework provides crucial information regarding the spatial inhomogeneity of the pairing amplitude[208]. To obtain the pairing amplitudes in real space, the Bogoliubov equations need to be solved self consistently. It has previously been widely used to study problems of disordered superconductors, structure of vortices, metal superconductor interfaces, superconductivity in presence of magnetic field and various other problems where the spatial variation of the order parameter is of paramount importance. In presence of strong disorder, signatures of superconducting islands (characterised

by large gap amplitudes) separated by insulating sea (vanishing gap amplitude) have been obtained[100].

The BdG approach was first used to study vortices in BCS superconductors in the work by Caroli *et al.*[209, 210]. In the superfluid atomic Fermi gases, the BdG approach has been used in the BCS limit[211]. In another work by Machida *et al.*[212], the BdG equations are numerically solved in order to investigate the structure of a singly quantized vortex in a superfluid fermion gas near the Feshbach resonance in the boson-fermion model.

2.3.1 Bogoliubov de Gennes equations for disordered superconductors

The BdG equations for the BCS-BEC crossover are the generalization of the Leggett mean field theory of the crossover to the case of spatially inhomogeneous systems. The BCS coherence factors for the homogeneous case u_k and v_k are generalized to the BdG eigenfunctions $u_n(r_i)$ and $v_n(r_i)$. These are obtained by solving a set of coupled differential equations involving the spatially varying order parameter $\Delta(r_i)$ and density, n . The order parameter $\Delta(r_i)$ must obey a self-consistency condition in terms of the functions $u_n(r_i)$ and $v_n(r_i)$ which is analogous to the gap equation for the homogeneous system.

In order to understand the details of the BdG method, we present the derivation of the BdG equations. We begin with a mean field decoupling of the quartic term in the Hamiltonian given by,

$$\begin{aligned} n_{i\uparrow}n_{i\downarrow} &= c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} \approx \langle n_{i\uparrow} \rangle n_{i\downarrow} + \langle n_{i\downarrow} \rangle n_{i\uparrow} - \langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \rangle c_{i\uparrow} c_{i\downarrow} \\ &\quad - \langle c_{i\uparrow} c_{i\downarrow} \rangle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger - \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle + \langle c_{i\uparrow} c_{i\downarrow} \rangle \langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \rangle \end{aligned} \quad (2.8)$$

which yields the local pairing amplitudes and local density as,

$$\begin{aligned} \Delta(r_i) &= -|U| \langle c_{i\downarrow} c_{i\uparrow} \rangle \\ \langle n_{i\sigma} \rangle &= \langle c_{i\sigma}^\dagger c_{i\sigma} \rangle \end{aligned} \quad (2.9)$$

The effective quadratic Hamiltonian is then given by

$$H_{eff} = - \sum_{\langle ij \rangle, \sigma} (t + \delta t_{ij}) (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) + \sum_{i, \sigma} (V_i - \tilde{\mu}_i) n_{i\sigma} + \sum_i [\Delta(r_i) c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger - \Delta^*(r_i) c_{i\uparrow} c_{i\downarrow}] \quad (2.10)$$

where $\tilde{\mu}_i = \mu + |U| \langle n_i \rangle / 2$ and $\langle n_i \rangle = \sum_\sigma \langle n_{i\sigma} \rangle$. Hence we calculate the local pairing amplitudes and number density in terms of $u_n(r_i)$ and $v_n(r_i)$ using,

$$\Delta(r_i) = |U| \sum_n u_n(r_i) v_n^*(r_i) \quad \text{and} \quad \langle n_i \rangle = 2 \sum_n |v_n(r_i)|^2 \quad (2.11)$$

In order to find eigenstates and their corresponding energies, we perform following unitary transformations,

$$\begin{aligned} c_{i\uparrow} &= \sum_n [\gamma_{n\uparrow} u_n(r_i) - \gamma_{n\downarrow}^\dagger v_n^*(r_i)], \\ c_{i\downarrow} &= \sum_n [\gamma_{n\downarrow} u_n(r_i) + \gamma_{n\uparrow}^\dagger v_n^*(r_i)] \end{aligned} \quad (2.12)$$

where γ_n and $\gamma_n^\dagger$ are the quasiparticle operators satisfying the fermion anticommutation relations,

$$\begin{aligned} \{\gamma_{n\alpha}, \gamma_{m\beta}^\dagger\} &= \delta_{nm} \delta_{\alpha\beta}, \\ \{\gamma_{n\alpha}, \gamma_{m\beta}\} &= 0 \end{aligned} \quad (2.13)$$

$u_n(r_i)$ and $v_n(r_i)$ are the BdG eigenvectors satisfying $u_n^2(r_i) + v_n^2(r_i) = 1$ for all r_i .

Using eq. (2.12), the effective Hamiltonian may be diagonalized, that is,

$$H_{eff} = E_g + \sum_{n, \alpha} \epsilon_n \gamma_{n\alpha}^\dagger \gamma_{n\alpha} \quad (2.14)$$

where E_g is the ground state energy of H_{eff} and ϵ_n is the energy of excitation n . The above condition can also be written by taking the commutator of H_{eff} with $\gamma_{n\alpha}$ and $\gamma_{n\alpha}^\dagger$ given by,

$$\begin{aligned} [H_{eff}, \gamma_{n\alpha}] &= -\epsilon_n \gamma_{n\alpha} \\ [H_{eff}, \gamma_{n\alpha}^\dagger] &= \epsilon_n \gamma_{n\alpha}^\dagger \end{aligned} \quad (2.15)$$

We now proceed to derive the equations for u_n and v_n for which we first compute the commutator $[H_{eff}, c_{i\uparrow}]$ using eqn. (2.10) and the anticommutation properties of $c_{i\uparrow}$ which yields,

$$[H_{eff}, c_{i\uparrow}] = t \sum_{\hat{\delta}} c_{i+\hat{\delta}\uparrow} - (V_i - \tilde{\mu}) c_{i\uparrow} - \Delta(r_i) c_{i\downarrow}^\dagger \quad (2.16)$$

Here $\hat{\delta}$ denotes the nearest neighbours of lattice site i and $\delta t_{ij} = 0$. We then replace the c 's by γ 's using eq. (2.12) and apply the commutation relations eq. (2.15). Comparing the coefficients of $\gamma_{n\uparrow}$ and $\gamma_{n\downarrow}^\dagger$ on two sides of the equation, we obtain the BdG equations:

$$-t \sum_{\hat{\delta}} u_n(r_i + \hat{\delta}) + (V_i - \tilde{\mu}) u_n(r_i) + \Delta(r_i) v_n(r_i) = \epsilon_n u_n(r_i) \quad (2.17)$$

and,

$$t \sum_{\hat{\delta}} v_n(r_i + \hat{\delta}) - (V_i - \tilde{\mu}) v_n(r_i) + \Delta^*(r_i) u_n(r_i) = \epsilon_n v_n(r_i) \quad (2.18)$$

We rewrite eq. (2.17) as,

$$\hat{K} u_n(r_i) + \hat{\Delta} v_n(r_i) = \epsilon_n u_n(r_i) \quad (2.19)$$

where $\hat{K} u_n(r_i) = -t \sum_{\hat{\delta}} u_n(r_i + \hat{\delta}) + (V_i - \tilde{\mu}) u_n(r_i)$ with $\hat{\delta} = \pm\hat{x}, \pm\hat{y}$ and $\hat{\Delta} v_n(r_i) = \Delta(r_i) v_n(r_i)$.

Similarly eq. (2.18) is rewritten as,

$$-\hat{K}^* v_n(r_i) + \hat{\Delta}^* u_n(r_i) = \epsilon_n v_n(r_i) \quad (2.20)$$

where $-\hat{K}^* v_n(r_i) = t \sum_{\hat{\delta}} v_n(r_i + \hat{\delta}) - (V_i - \tilde{\mu}) v_n(r_i)$ and $\hat{\Delta}^* u_n(r_i) = \Delta^*(r_i) u_n(r_i)$.

Eqns. (2.19) and (2.20) can be compactly written in matrix form as,

$$\begin{pmatrix} \hat{K} & \hat{\Delta} \\ \hat{\Delta}^* & -\hat{K}^* \end{pmatrix} \begin{pmatrix} u_n(r_i) \\ v_n(r_i) \end{pmatrix} = E_n \begin{pmatrix} u_n(r_i) \\ v_n(r_i) \end{pmatrix} \quad (2.21)$$

The usual procedure for obtaining $\Delta(r_i)$ and $\langle n_i \rangle$ self-consistently consists of making initial guesses for $\Delta(r_i)$ and the renormalized chemical potential $\tilde{\mu}_i$ for all r_i , diagonalize Eq. (2.21) for the eigensolutions E_n and $(u_n(r_i), v_n(r_i))$, re-compute $\Delta(r_i)$ and $\langle n_i \rangle$ using Eq. (2.11). The process is iterated until self-consistency is achieved for these quantities at each site for a particular value of disorder strength.

2.3.2 Bogoliubov de Gennes equations in presence of magnetic field

The mean field decoupling of the interaction term of eq. (2.7) yields the effective Hamiltonian of the form,

$$\mathcal{H}_{eff} = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i\sigma} \left(\sigma h - \mu - U \left(n_{i\bar{\sigma}} - \frac{1}{2} \right) \right) \hat{n}_{i\sigma} + \sum_i \left(\Delta_i c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger + \Delta_i^* c_{i\downarrow} c_{i\uparrow} \right) \quad (2.22)$$

Following the algebra discussed in previous section, we get,

$$\begin{aligned} [\mathcal{H}_{eff}, c_{i\uparrow}] &= +t \sum_{\hat{\delta}} c_{i+\hat{\delta}\uparrow} - \xi_{i\uparrow} c_{i\uparrow} - \Delta(r_i) c_{i\downarrow}^\dagger \\ &= \sum_n \gamma_{n\uparrow} \left(t \sum_{\hat{\delta}} u_n(r_i + \hat{\delta}) - \xi_{i\uparrow} u_n(r_i) - \Delta(r_i) v_n(r_i) \right) \\ &\quad + \sum_n \gamma_{n\downarrow}^\dagger \left(-t \sum_{\hat{\delta}} v_n(r_i + \hat{\delta}) + \xi_{i\uparrow} v_n(r_i) - \Delta(r_i) u_n(r_i) \right) \end{aligned} \quad (2.23)$$

where $\xi_{i\uparrow} = (V_i - \mu - U\delta n_{i\downarrow} + h)$ with $\delta n_{i\downarrow} = n_{i\downarrow} - 1/2$.

Equating coefficients of $\gamma_{n\uparrow}$ and $\gamma_{n\downarrow}^\dagger$, we get two equations

$$\begin{aligned} t \sum_{\hat{\delta}} u_n(r_i + \hat{\delta}) - \xi_{i\uparrow} u_n(r_i) - \Delta(r_i) v_n(r_i) &= -\epsilon_n^{\gamma\uparrow} u_n(r_i) \\ -t \sum_{\hat{\delta}} v_n(r_i + \hat{\delta}) + \xi_{i\uparrow} v_n(r_i) - \Delta(r_i) u_n(r_i) &= -\epsilon_n^{\gamma\downarrow} v_n(r_i) \end{aligned} \quad (2.24)$$

And similarly, from $[\mathcal{H}_{eff}, c_{i\downarrow}^\dagger]$ expression, we get

$$\begin{aligned} -t \sum_{\hat{\delta}} v_n(r_i + \hat{\delta}) + \xi_{i\downarrow} v_n(r_i) - \Delta(r_i) u_n(r_i) &= -\epsilon_n^{\gamma\uparrow} v_n(r_i) \\ -t \sum_{\hat{\delta}} u_n(r_i + \hat{\delta}) + \xi_{i\downarrow} u_n(r_i) + \Delta(r_i) v_n(r_i) &= \epsilon_n^{\gamma\downarrow} u_n(r_i) \end{aligned} \quad (2.25)$$

From above four equations, we get,

$$\begin{aligned} -t \sum_{\hat{\delta}} u_n(r_i + \hat{\delta}) + \xi_{i\uparrow} u_n(r_i) + \Delta(r_i) v_n(r_i) &= \epsilon_n^{\gamma\uparrow} u_n(r_i) \\ t \sum_{\hat{\delta}} v_n(r_i + \hat{\delta}) - \xi_{i\downarrow} v_n(r_i) + \Delta(r_i) u_n(r_i) &= \epsilon_n^{\gamma\downarrow} v_n(r_i) \end{aligned} \quad (2.26)$$

And another set,

$$\begin{aligned} -t \sum_{\hat{\delta}} (-v_n(r_i + \hat{\delta})) + \xi_{i\uparrow} (-v_n(r_i)) + \Delta(r_i) u_n(r_i) &= -\epsilon_n^{\gamma\downarrow} (-v_n(r_i)) \\ t \sum_{\hat{\delta}} u_n(r_i + \hat{\delta}) - \xi_{i\downarrow} u_n(r_i) + \Delta(r_i) (-v_n(r_i)) &= -\epsilon_n^{\gamma\uparrow} u_n(r_i) \end{aligned} \quad (2.27)$$

Note that the matrix on lhs is same for all equations given by,

$$\begin{pmatrix} \mathcal{H}_{ij\sigma} & \hat{\Delta} \\ \hat{\Delta}^* & -\mathcal{H}_{ij\bar{\sigma}}^* \end{pmatrix} \begin{pmatrix} u_n(r_i) \\ v_n(r_i) \end{pmatrix} = \epsilon_n^{\gamma\uparrow} \begin{pmatrix} u_n(r_i) \\ v_n(r_i) \end{pmatrix} \quad (2.28)$$

here $\mathcal{H}_{ij\sigma} = -t\delta_{i\pm 1j} - (\mu + U\delta n_{i\bar{\sigma}} - \sigma h)\delta_{ij}$ and $\epsilon_n^{\gamma\uparrow}$ are the eigenvalues. As discussed earlier, we start with initial guesses for the pairing amplitude, $\Delta(r_i)$ and the density of up and down-spin electrons, $\langle n_{i\uparrow} \rangle$ and $\langle n_{i\downarrow} \rangle$ respectively. Subsequently, the eigenvalues, $\epsilon_n^{\gamma\uparrow}$ and the eigenvectors $(u_n(r_i), v_n(r_i))$ are determined numerically from Eq. (2.28). The local pairing amplitudes at sites r_i in terms of $u_n(r_i)$ and $v_n(r_i)$ are hence calculated from,

$$\Delta(r_i) = -|U| \sum_n [u_n(r_i) v_n^*(r_i) f(E_{n\uparrow}) - u_n(r_i) v_n^*(r_i) f(-E_{n\downarrow})] \quad (2.29)$$

and alongwith the density of up and down-spin electrons using,

$$\langle n_{i\sigma} \rangle = \sum_n [|u_n(r_i)|^2 f(E_{n\sigma}) + |v_n(r_i)|^2 f(-E_{n\bar{\sigma}})] \quad (2.30)$$

where $f(E_{n\sigma})$ is the Fermi distribution function. The entire process is iterated with new guesses for the above quantities until self-consistency is achieved for all of them simultaneously.

A number of self consistent solutions may exist for the pairing amplitude, $\Delta(\mathbf{r}_i)$ corresponding to one set of parameters. In order to decide the ground state among the various solutions, the energy of the superconducting state is computed using,

$$E_0 = \langle \text{GS} | \mathcal{H} | \text{GS} \rangle - \langle 0 | \mathcal{H} | 0 \rangle \quad (2.31)$$

Here $|\text{GS}\rangle$ is the ground state of the system (obtained from BdG analysis) and $|0\rangle$ is the vacuum state. Now,

$$\mathcal{H} = \mathcal{H}_{eff} - U \sum_i \left(\hat{n}_{i\uparrow} - \frac{1}{2} \right) \left(\hat{n}_{i\downarrow} - \frac{1}{2} \right) + \sum_{i\sigma} U \left(n_{i\bar{\sigma}} - \frac{1}{2} \right) \hat{n}_{i\sigma} - \sum_i \left(\Delta_i c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger + \Delta_i^* c_{i\downarrow} c_{i\uparrow} \right) \quad (2.32)$$

We now proceed to calculate $\langle \text{GS} | \mathcal{H} | \text{GS} \rangle$ of eqn. (2.31) term by term. The quartic term in the expectation is non-trivial and is given by,

$$\begin{aligned} \langle \text{GS} | \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} | \text{GS} \rangle &= \langle \text{GS} | c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} | \text{GS} \rangle \\ &= \frac{1}{U^2} |\Delta_i|^2 + n_{i\uparrow} n_{i\downarrow} \end{aligned} \quad (2.33)$$

The other expectation value is,

$$\left\langle \text{GS} \left| \sum_{i\sigma} U \left(n_{i\bar{\sigma}} - \frac{1}{2} \right) \hat{n}_{i\sigma} \right| \text{GS} \right\rangle = 2 \sum_i U n_{i\downarrow} n_{i\uparrow} - \frac{U}{2} \sum_i n_i \quad (2.34)$$

And,

$$\left\langle \text{GS} \left| \sum_i \left(\Delta_i c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger + \Delta_i^* c_{i\downarrow} c_{i\uparrow} \right) \right| \text{GS} \right\rangle = - \sum_i \frac{2\Delta_i^2}{U} \quad (2.35)$$

Finally,

$$\langle \text{GS} | \mathcal{H}_{eff} | \text{GS} \rangle = \sum_n \epsilon_n f(\epsilon_n) \quad (2.36)$$

Eqns. (2.33), (2.34), (2.35) and (2.36) are used to get

$$\langle \text{GS} | \mathcal{H} | \text{GS} \rangle = \sum_n \epsilon_n f(\epsilon_n) + \sum_i U n_{i\uparrow} n_{i\downarrow} + \sum_i \frac{\Delta_i^2}{U} - \frac{U}{4} N_s \quad (2.37)$$

Subtracting the contribution from energy of the superconducting state in vacuum, we get

$$E_0 = \sum_{n\sigma} \epsilon_{n\sigma} \left[f(\epsilon_{n\sigma}) - \sum_i |v_n(r_i)|^2 \right] + U \sum_i n_{i\uparrow} n_{i\downarrow} + \frac{1}{U} \sum_i \Delta_i^2 - \frac{UN_s}{4} \quad (2.38)$$

The winner among the various solutions corresponding to a particular set of parameters is the one with lowest value of E_0 .

The mean field calculations that we have presented in this thesis can raise discussion on its validity, especially since our calculations are done in two dimensions. We argue that the usage of mean field theory (BdG calculations) helps us to identify the crossover scenario from a BCS superconductor to a BEC superfluid and produces spatial fluctuations in different correlation functions for the spin imbalanced phase. However it certainly gets worse for strongly disordered superconductors, which is why we attempt to include the effects of phase fluctuations, at least for the crossover problem.

2.4 Beyond mean field theory: phase fluctuations

The effect of fluctuations in superconductors has been studied extensively. Ginzburg-Landau (GL) theory allows description of the superconducting transition in terms of a complex superconducting order parameter, $\Psi(r)$ which is non-zero below the transition temperature T_c but vanishes in the normal state (above T_c). Most of the theoretical studies are focused on the transition point between superconducting and normal phases where the superconducting order parameter undergoes fluctuations as T_c is approached from above. The interest in the field is further accentuated by the discovery of high- T_c superconductors. A number of different experiments indicate a suppression of low-frequency spectral weight in the underdoped cuprates below a characteristic temperature T^* which is higher than the superconducting (SC) transition temperature T_c . As discussed earlier, this striking scenario is referred to as pseudogap that is a gap in the normal phase. A variety of proposals have been made to understand its origin as the answer to this may hold the key for understanding high- T_c superconductivity. One of these proposals is that the pseudogap arises from phase fluctuations of the superconducting gap[213].

The phase fluctuations and hence the pseudogap for the cuprates resembles the intermediate regime between the BCS and BEC limits. In the weak coupling limit, the radius of the Cooper pair, ξ_0 is much larger than the distance, d between the pairs ($\xi_0 \gg d$). Due to the strong overlap between a large number of pairs, pairing fluctuations are unimportant and the transition to the superconducting state can be described by the BCS (mean-field) theory. However, the pairing fluctuations become crucial in the BEC limit (strong coupling) where the pairs are tightly bound and hence the pair size is much smaller than the distance between the pairs ($\xi_0 \ll d$). The pair fluctuations are usually treated in a perturbative way by taking into account diagrams beyond the BCS mean-field approximation. These are the famous Aslamazov-Larkin diagrams which describe short-time Cooper-pair fluctuations above T_c [214]. In the intermediate coupling regime ($\xi_0 \sim d$), the dominating fluctuations are that of the phase fluctuations of the Cooper pairs.

The phase fluctuation scenario has been explored by various approaches. For example, Franz *et al.*[215] calculated the single-particle spectral weight by a semi-classical coupling of the supercurrent to the quasiparticles, which leads to a Doppler-shifted excitation spectrum. A similar perturbative approach has been used by Kwon *et al.*[14] to calculate several single-particle properties. In another work by Franz *et al.*[216], a connection between the phase action of a phase fluctuation model for the cuprates and quantum electrodynamics has been explored to obtain the single particle excitation spectrum and quantum critical behavior of their model. Herbut in his work[217] has shown that the topological vortex defects in a phase fluctuation model can lead to an incommensurate spin-density wave using the same approach. Clearly the entire literature relevant to the discussion of phase fluctuations in cuprates is beyond the scope of this thesis. However, we felt a short introduction is necessary (a may be sufficient) for our purpose.

In this thesis, we have investigated the effect of inclusion of classical phase fluctuations in two dimensional disordered superconductors. In the BdG approximation, the spatial fluctuation of the pairing amplitude is obtained, however, it neglects phase fluctuations altogether, and all regions with non-vanishing pairing amplitude are thus phase-correlated. The approximation becomes questionable in the limit of large disorder where the mean field pairing amplitudes become spatially inhomogeneous at large values of disorder owing to the system breaking up into superconducting islands with large pairing amplitudes, separated by insulating strips. Hence, the superconducting condensate display deviations from mean field

behaviour at large disorder and phase fluctuations, both classical and quantum, have a significant influence on the physical properties in the limit of large disorder and hence must be taken into account.

2.4.1 Phase fluctuations: the formalism

The most common approach to incorporate the phase fluctuation effects is by computing the partition function[218] given by,

$$\mathcal{Z} = \int D[c_i, c_i^\dagger] e^{-S} \quad (2.39)$$

where $c_i^\dagger$ (c_i) are the fermion operators and S is the action which is defined as,

$$S = \int_0^\beta d\tau \left[\sum_{i\sigma} c_{i\sigma}^\dagger(\tau) (\partial_\tau + V_i - \mu) c_{i\sigma}(\tau) - t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger(\tau) c_{j\sigma}(\tau) - |U| \sum_i c_{i\uparrow}^\dagger(\tau) c_{i\downarrow}^\dagger(\tau) c_{i\downarrow}(\tau) c_{i\uparrow}(\tau) \right] \quad (2.40)$$

Here V_i is the random onsite potential and rest of the symbols have usual meanings.

It is usual to apply a Hubbard-Stratonovic transformation in which Δ_i is the local Hubbard-Stratonovic field, with amplitude $|\Delta_i|$ and phase θ_i . The partition function thus becomes,

$$\mathcal{Z} = \int D[\Delta_i, \theta_i] D[c_i, c_i^\dagger] \exp \left[- \int_0^\beta d\tau (H_0 + H_I) \right] \quad (2.41)$$

where

$$H_0 = \sum_{i\sigma} c_{i\sigma}^\dagger(\tau) (\partial_\tau + V_i - \mu) c_{i\sigma}(\tau) - t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger(\tau) c_{j\sigma}(\tau) \quad (2.42)$$

and

$$H_I = \sum_i \left[\frac{|\Delta_i(\tau)|^2}{U} - \left(\Delta_i(\tau) e^{-i\theta_i(\tau)} c_{i\uparrow}^\dagger(\tau) c_{i\downarrow}^\dagger(\tau) + c.c. \right) \right] \quad (2.43)$$

We shall henceforth work within the BdG approximation. The thermal phase fluctuations are taken into account which ignores the time dependence of Δ , i.e. the quantum fluctuations in Eq. (2.41) that yields

$$\mathcal{Z} = \int \prod_i d|\Delta_i| d\theta_i \exp \left(- \frac{\beta}{U} \sum_i |\Delta_i|^2 \right) \text{Tr} \exp(-\beta H_{BdG}) \quad (2.44)$$

where H_{BdG} is the mean field Hamiltonian.

Subsequently, the phase correlations are obtained as,

$$\langle \cos(\delta\theta_i - \delta\theta_j) \rangle = \frac{1}{Z} \int \prod_i d|\Delta_i| d\theta_i \exp\left(-\frac{\beta}{U} \sum_i |\Delta_i|^2\right) \text{Tr} \exp(-\beta H_{BdG}) \cos(\delta\theta_i - \delta\theta_j) \quad (2.45)$$

The above integral can be numerically evaluated using Monte Carlo scheme. In our work, we decided to resort to a harmonic approximation where we have adopted a different approach to calculate the above correlation function. The details of our method is presented in the following discussion.

To incorporate phase fluctuations on the order parameter, we have chosen the classical XY model which defines phase variable (of the order parameter) with two dimensional planar degree of freedom at each lattice site with a Josephson type coupling between them. It thus describes the dynamics of the phase variable on a lattice.

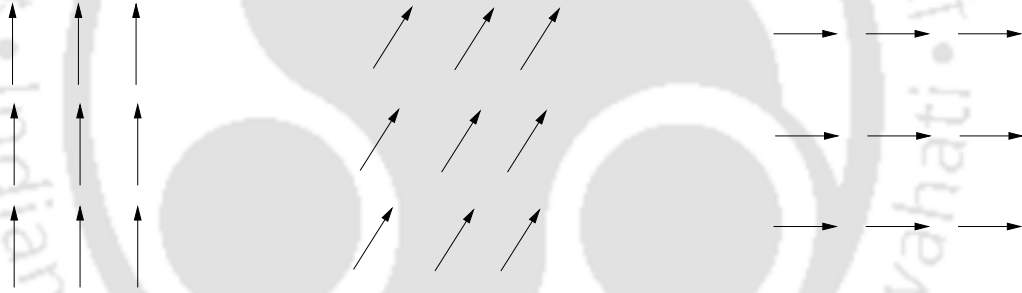


FIGURE 2.1: Different ground states for the XY Hamiltonian. The phase variable of the order parameter can point towards any direction in the two dimensional plane.

Let us discuss how this model can be relevant in the present context. The Josephson term plays a crucial role in establishing phase ordering between various superconducting islands which emerge in the limit of large disorder. Thus the phase variable continues to be a smoothly (and slow) varying function with the phase difference between the superconducting islands being negligibly small. The fluctuation in the phase is then introduced by adding a coulombic term to the model which restricts hopping of pairs from one superconducting island to another. Combining the above two terms, we get a phase-only Hamiltonian[97, 98, 219, 220] given by

$$\begin{aligned} H_\theta &= \frac{U'}{2} \sum_i \hat{n}_i^2 + J \sum_{\langle ij \rangle} [1 - \cos(\theta_i - \theta_j)], \\ &= E_c + E_J. \end{aligned} \quad (2.46)$$

Here $\hat{n}_i$ is the number operator for Cooper pairs on the i th grain and U' is related to the inverse of the capacitance of the assembly of superconducting islands. The second term is specified by the Josephson coupling strength J , with θ_i being the phase angle on the i th grain. It may be noted that the charging energy, E_c favors insulating behaviour as it arises due to the fact that it costs energy to transfer a Cooper pair from one superconducting island to another. However, the Josephson coupling energy, E_J establishes a (global) phase coherence among the islands and thus gives rise to a superconducting ground state.

The harmonic approximation of the cosine term in Eq. (2.46) gives the trial Hamiltonian as,

$$H_0 = \frac{U}{2} \sum_i \hat{n}_i^2 + \sum_{\langle ij \rangle} \frac{D_s}{8} (\theta_i - \theta_j)^2. \quad (2.47)$$

Here D_s is the renormalised superfluid density which is to be determined by a variational approach. In order to get D_s , the Gibbs-Bogoliubov[219] inequality is applied which states that the Helmholtz free-energy, F_θ for a system described by a Hamiltonian, H_θ satisfies the inequality,

$$F_\theta \leq F_0 + T \langle S_\theta - S_0 \rangle_0, \quad (2.48)$$

where F_0 is the free energy of the system described by the trial Hamiltonian given in Eq. (2.47). S_θ and S_0 are the Euclidean actions corresponding to H_θ and H_0 respectively. F_θ is then minimized to obtain D_s as,

$$D_s(\kappa, \xi, T, \sigma) = D_s^0 \exp \left[\frac{-\phi(\kappa, \xi, T, \sigma)}{\xi \sqrt{\kappa D_s}} \right]. \quad (2.49)$$

Here κ is the compressibility ($= \frac{dn}{d\mu}$) and ξ is the coherence length. ϕ in the above expression is given by

$$\phi = \frac{1}{N} \left[\sum_k \left(\sqrt{f(k)} \coth \left(\frac{\beta}{2\xi} \sqrt{\left(\frac{D_s f(k)}{\kappa} \right)} \right) \right) \right] \quad (2.50)$$

and $f(k) = 4 - 2(\cos k_x + \cos k_y)$. Note that ξ is computed using the BCS relation $\xi(T) = \frac{\hbar v_F}{\pi \Delta(T)}$, where $\Delta(T)$ is chosen from BdG results for the pure case. Thus the effect of disorder on ξ is neglected. Eq. (2.49) is solved to determine the renormalized $D_s(T)$ for various values of disorder strengths, using the mean field superfluid stiffness, D_s^0 as an input from the BdG results. A detailed derivation of Eqns. (2.49) and (2.50) is presented in appendix A.

We now introduce the Nelson-Kosterlitz (NK) relation[221],

$$\lim_{T \rightarrow T_{KT}^-} D_s(T) = \frac{2}{\pi} T_{KT}, \quad (2.51)$$

where the Kosterlitz-Thouless (KT) transition temperature, T_{KT} is marked by the precipitous drop of the fully renormalised D_s . KT theory[222] defines T_{KT} as the critical temperature below which long range order prevails because of the presence of vortex-anti-vortex pairs in the system. D_s (obtained from SCHA) is substituted in Eq. (2.51) to get T_{KT} which is obtained from the intersection point of the straight line and D_s (as a function of temperature) for a particular value of disorder.

2.5 Choice of parameters

Since our starting point is a weakly interacting BCS superconductor, we need to be careful about the value of the attractive potential that we use. Usually an U less than the bandwidth (say by a factor of half) can be regarded as a weak interaction. In this thesis, we have taken U to be $1.5t$ and $2.5t$ which is almost a quarter of the bandwidth in two dimensions and should be satisfactory for our purpose.

Regarding the value of density, it may be noted that the BCS-BEC crossover problem studied in chapters 3 and 4 restrict our choice of density to be low, where we have taken $n = 0.1$. However we have investigated the relevant physics at other smaller densities as well which may not have always been included for discussion. With regard to the FFLO physics (chapters 5, 6 and 7), the density effect is quite insignificant (except for very low densities) but the manifestation of the FFLO phase is more lucid at larger densities. Thus we have chosen n as $\frac{2}{3}$ ($= 0.66$) for this purpose.

We have used a two dimensional system of size 24×24 for our numeric computation in this thesis unless stated otherwise *e.g.* a lattice of size 32×16 is used to study FFLO physics (chapters 5, 6 and 7). We have confirmed that the physical quantities computed here are qualitatively unaltered for larger system sizes (data not shown here).

A brief mention of the choice of parameters is included in all the chapters containing our results.

2.6 Summary

In this chapter, we have introduced the attractive Hubbard model which is the underlying model for both our problems. We have studied our first problem which deals with disorder driven BCS-BEC crossover by incorporating disorder effects in the attractive Hubbard model. The second problem which investigates superconductivity in presence of external magnetic field is studied by including an additional magnetic field term to the attractive Hubbard model.

We have described the Bogoliubov de Gennes (BdG) method which is used to solve both the problems. A detailed derivation of the BdG equations both in the presence of disorder and magnetic field are presented. These equations are then subsequently solved to get the eigensolutions of the system for the respective cases. Thus BdG provides detailed information about the spatial fluctuations of the order parameter. However, phase fluctuations of the order parameter which grow significantly in the presence of large disorder, are completely ignored. In order to incorporate the effects of phase fluctuation of the order parameter about the mean field (BdG) results, we resort to self-consistent harmonic approximation of the 'phase only' model for the problem dealing with disordered superconductors.

Chapter 3

BCS-BEC crossover

3.1 Introduction

Disorder effects in interacting electronic systems[92, 97, 223, 224] have generated excitement among researchers spanning over several decades. Superconductors are good examples of systems where electron correlations are prominent and hence disorder induced effects are interesting [225, 226]. Apart from a strong reduction in the superconducting transition temperature T_c , the disordered superconductors display spatial inhomogeneity of the pairing amplitude in the strong disorder limit, leading to striking effects such as persistence of the spectral gap at large disorder etc[100] as discussed before. Related studies suggest that the unconventionality which is operative at large values of disorder begets a *new* phase which shows less or no similarity with the (pure) superconducting condensate. A deeper understanding of the crossover to the new phase and the underlying features is still lacking. The system though resembles a BCS condensate for no (or weak) disorder, behaves very differently at intermediate values of disorder. In the latter limit, the condensate comprises of short and local pairs which is reminiscent of a BEC phase. Thus disorder is capable of inducing a crossover from a BCS superconductor characterised by largely overlapping Cooper pairs to a Bose Einstein condensate (BEC) of tightly bound short ranged pairs - the *new* phase mentioned earlier. The smooth evolution from a BCS superconductor to a BEC superfluid in presence of structural disorder was put forward earlier by Micnas and coworkers[88]. More recently, a strongly disordered attractive Hubbard model with infinite range hopping (where mean field theory is exact) is shown

to emulate a smooth BCS-BEC crossover as the range of hopping is varied[90]. Further, the ground state properties of a superfluid Fermi gas is studied across a BCS-BEC crossover in presence of random disorder at $T = 0$ [91]. Although, the role of disorder in inducing such a crossover remains to be resolved precisely.

In the present work, we study superconductivity in presence of onsite disorder using Bogoliubov de Gennes[208] (BdG) method on a negative- U Hubbard model in two dimensions. The main objective is to investigate the unconventional features which arises in the system at larger values of disorder. The emergence of these features is confirmed by computing various important physical quantities *viz.* the spectral gap which not only persists but also shows an increase with increasing disorder, thereby behaving differently from the order parameter of the system. The behaviour of the off-diagonal long range correlations in the presence of disorder, also bears signature of unconventionality as it predicts existence of two different temperature scales for pair formation and its subsequent condensation. An important consequence of the reduction in pair size from large (of the order of few thousands of lattice spacing) to small (of the order of a lattice spacing), is the enormous increase in fluctuation effects of the order parameter and thus can not be neglected in the strong disorder limit. Hence, we proceed to incorporate the fluctuations about the inhomogeneous BdG state using phase only model[97, 219, 220]. The results obtained are striking as they suggest opening of a large region between the mean field transition temperature (obtained from the vanishing of the superfluid stiffness) and the actual transition temperature, which is characterized by the presence of pairs with no phase coherence, a reminiscent of pseudogap phase[49] observed in cuprates.

3.2 Results and discussion

In the beginning, we review the underlying model and also the method which is used to solve the model Hamiltonian for disordered superconductors. For further details, one can refer to chapter 2.

The model considered here is an attractive Hubbard model on a two-dimensional square lattice,

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

Here t is the transfer integral, $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) is the creation (destruction) operator for an electron with spin σ at a site $\mathbf{r}_i$, $|U|$ is the magnitude of onsite interaction, $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ and μ denotes the chemical potential. To model random on-site disorder, V_i is chosen randomly from a Gaussian distribution of the form,

$$P[V_i(\sigma)] = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{V_i^2}{2\sigma^2}\right]. \quad (3.2)$$

Here σ denotes the width of the distribution and parametrizes the strength of disorder in our computation, *i.e.* larger σ implies stronger disorder. The random disorder potential thus generated are included in the last term of Eq. (3.1). Other random distributions such as a rectangular distribution has been studied and does not render any qualitative difference from the results discussed in the next section.

To solve Eq. (3.1), we resort to the mean field decoupling of the interacting term that yields the local pairing amplitudes and local density as,

$$\Delta(\mathbf{r}_i) = -|U|\langle c_{i\downarrow} c_{i\uparrow} \rangle \quad \text{and} \quad \langle n_{i\sigma} \rangle = \langle c_{i\sigma}^\dagger c_{i\sigma} \rangle. \quad (3.3)$$

The effective Hamiltonian is given by,

$$H_{eff} = -t \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) + \sum_{i, \sigma} (V_i - \tilde{\mu}_i) n_{i\sigma} + \sum_i [\Delta(\mathbf{r}_i) c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger - \Delta^*(\mathbf{r}_i) c_{i\uparrow} c_{i\downarrow}], \quad (3.4)$$

where $\tilde{\mu}_i = \mu + |U|\langle n_i \rangle / 2$ and $\langle n_i \rangle = \sum_\sigma \langle n_{i\sigma} \rangle$. The following transformations are used to diagonalize Eq. (3.4)[98],

$$c_{i\uparrow} = \sum_n [\gamma_{n\uparrow} u_n(\mathbf{r}_i) - \gamma_{n\downarrow}^\dagger v_n^*(\mathbf{r}_i)] \quad \text{and} \quad c_{i\downarrow} = \sum_n [\gamma_{n\downarrow} u_n(\mathbf{r}_i) + \gamma_{n\uparrow}^\dagger v_n^*(\mathbf{r}_i)], \quad (3.5)$$

where γ_n and $\gamma_n^\dagger$ are the quasiparticle operators, $u_n(\mathbf{r}_i)$ and $v_n(\mathbf{r}_i)$ are the BdG eigenvectors satisfying $\sum_n [u_n^2(\mathbf{r}_i) + v_n^2(\mathbf{r}_i)] = 1$ for all $\mathbf{r}_i$. In terms of these amplitudes, Eq. (3.4) is written as,

$$\begin{pmatrix} \hat{K} & \hat{\Delta} \\ \hat{\Delta}^* & -\hat{K}^* \end{pmatrix} \begin{pmatrix} u_n(\mathbf{r}_i) \\ v_n(\mathbf{r}_i) \end{pmatrix} = E_n \begin{pmatrix} u_n(\mathbf{r}_i) \\ v_n(\mathbf{r}_i) \end{pmatrix}, \quad (3.6)$$

where $\hat{K} u_n(\mathbf{r}_i) = -t \sum_\delta u_n(\mathbf{r}_i + \hat{\delta}) + (V_i - \tilde{\mu}_i) u_n(\mathbf{r}_i)$, with $\hat{\delta} = \pm \hat{x}, \pm \hat{y}$ and $\hat{\Delta} u_n(\mathbf{r}_i) = \Delta(\mathbf{r}_i) u_n(\mathbf{r}_i)$ and similarly for $v_n(\mathbf{r}_i)$.

Hence we calculate the local pairing amplitudes and number density in terms of $u_n(\mathbf{r}_i)$ and $v_n(\mathbf{r}_i)$ using,

$$\Delta(\mathbf{r}_i) = |U| \sum_n u_n(\mathbf{r}_i) v_n^*(\mathbf{r}_i) \quad \text{and} \quad \langle n_i \rangle = 2 \sum_n |v_n(\mathbf{r}_i)|^2. \quad (3.7)$$

The usual procedure for obtaining $\Delta(\mathbf{r}_i)$ and $\langle n_i \rangle$ self-consistently consists of making initial guesses for $\Delta(\mathbf{r}_i)$ and the renormalized chemical potential $\tilde{\mu}_i$ for all $\mathbf{r}_i$, diagonalize Eq. (3.6) for the eigensolutions E_n and $(u_n(\mathbf{r}_i), v_n(\mathbf{r}_i))$, re-compute $\Delta(\mathbf{r}_i)$ and $\langle n_i \rangle$ using Eq. (3.7). The process is iterated until self-consistency is achieved for these quantities at each site.

At the outset we discuss the size dependence issues related to our computation. We have carried out our computation on a 24×24 lattice. Next we comment on the choice of physical parameters. We perform studies for a few choices of the Hubbard interaction parameter, U and electron density, n . The choice of U is expectedly small, as our starting point is a weak coupling (BCS) superconductor. As for the density, Fig. 3.1 shows that the chemical potential slips below the noninteracting band only at small n (for moderate values of U). It is important to note that, the chemical potential, μ (in fact, a scaled value, viz. $\mu' = \mu/4t$ is useful for discussion) does not fall below the band edge ($\mu' = -1$) for $|U|$ less than $\sim 5.5t$ even for density as low as 0.1. In the next section we shall show that disorder can induce a crossover at much smaller values of U , i.e. $|U| = 1.5t$ at the same density ($n = 0.1$). At large densities viz. $n \simeq 0.8$, as is transparent from Fig. 3.1, there is no crossing of μ' below -1 even at reasonably large coupling, thereby making it impossible for disorder to induce a crossover at weak coupling. Thus we have chosen $|U| = 1.5t$, $n = 0.1$ and all the plots (except for Fig. 3.1) are generated for these values of the parameters. Further, we have investigated disorder strengths till $\sigma/t = 3$ and all the results for various physical quantities that we obtained are averaged over ten different disorder configurations.

In the subsequent discussion, we present the results of various physical quantities viz. the spectral gap, off-diagonal long range order and superfluid stiffness, to gain insight into the emergence of unconventional behaviour with increasing disorder. Further, the BCS-BEC crossover scenario is investigated by calculating the chemical potential as the crossover analysis has mostly concentrated on exploring how the chemical potential evolve as a function of the interaction strength between the fermions[34, 227]. For the continuum case, it can be shown that the chemical potential changing sign can be regarded as the signature of crossover, at least at low densities. The explanation can be given as follows: at very weak interaction strengths (or large particle density), the binding energy of a pair is extremely small, thus the

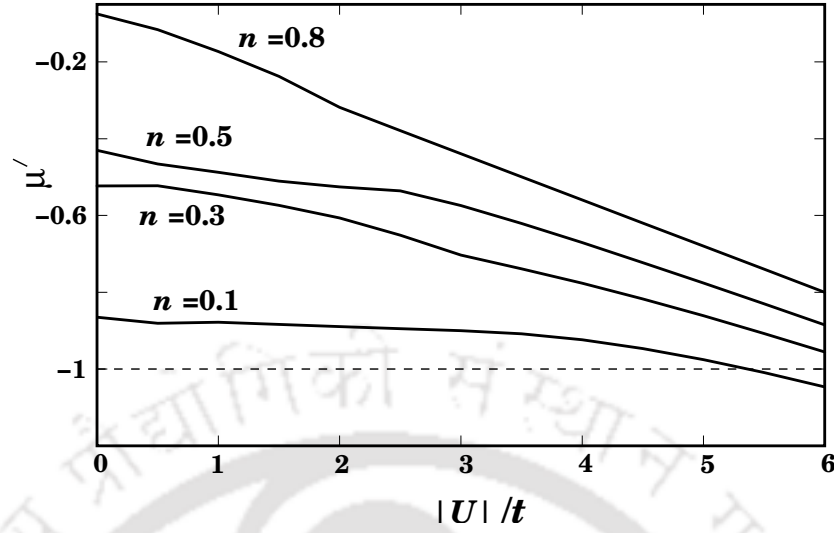


FIGURE 3.1: The (scaled) chemical potential, μ' ($= \mu/4t$, $4t$ being the noninteracting bandwidth) is shown as a function of $|U|$. The slipping below the band occurs for low densities and at best moderate couplings, *i.e.* $|U| \sim 5.5t$ for $n = 0.1$.

chemical potential is decided by the Fermi energy alone. In the other limit of strong inter-particle interaction (or low density), the binding energy of the pair dominates and sets the scale for the chemical potential. The corresponding behaviour for the lattice case shows up as the chemical potential slips below the noninteracting band minimum, suggesting formation of bound pairs and marks the onset of the Bose phase.

We then include the effects of (phase) fluctuations about the inhomogeneous BdG state, an interesting consequence of which is the emergence of pseudogap-like phase, characterised by the presence of pairs with *no* phase coherence.

3.2.1 Unconventional features

We begin with the notion of the spectral gap, E_{gap} which provides an estimate of the affect of the presence of disorder on superconductivity. It is the energy gap in the one-particle density of states, obtained as the lowest eigenvalue of the BdG theory. We plot the disorder dependence of E_{gap} along with the off-diagonal long range order parameter, Δ_{OP} which is defined by the long distance behaviour of the disorder averaged off-diagonal correlation given by,

$$\langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_{j\downarrow} c_{j\uparrow} \rangle \rightarrow \Delta_{OP}^2 / |U|^2 \quad \text{for } |\mathbf{r}_i - \mathbf{r}_j| \rightarrow \infty \quad (3.8)$$

$|U|$ being the onsite attractive potential. The results presented in Fig. 3.2, clearly show that E_{gap} and Δ_{OP} are same in absence of disorder ($\sigma = 0$). However the two show progressively different behaviour as a function of disorder, thereby showing digressions from the conventional behaviour. The reason behind the decrease in E_{gap} in the weak disorder regime, lies in the reduction in average density of states near Fermi energy with increasing disorder. The anomalous behaviour (upturn of E_{gap} as a function of disorder) in the opposite limit can be explained on the basis of the progressive localization of extended wave functions, leading to the emergence of a phase with tightly bound pairs, which in turn gives rise to a large spectral gap. Similar behaviour has been observed by Ghosal *et al.*[98] and alluded to the decrease in localization length of the noninteracting eigenstates.

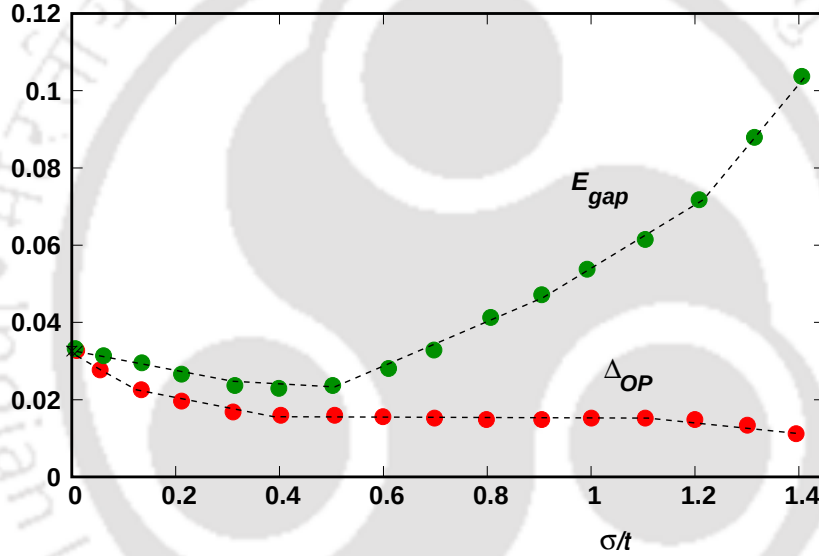


FIGURE 3.2: The spectral gap, E_{gap} and the ODLRO order parameter Δ_{OP} (defined in text) are shown as a function of disorder. Here $U = -1.5t$ and the density n is chosen to be 0.1. Note that they coincide for small σ/t but progressively differ with increasing disorder. Here E_{gap} and Δ_{OP} are in units of t .

3.2.2 The crossover scenario

We confirm the presence of crossover in our model by computing the chemical potential, μ as a function of disorder for a density as low as 0.1 and $U = -1.5t$ (see Fig. 3.3). μ' crosses below the noninteracting band edge at $\sigma \simeq 1.2t$ separating a BCS-like superconductor (at lower σ) and a BEC phase (intermediate σ)[193].

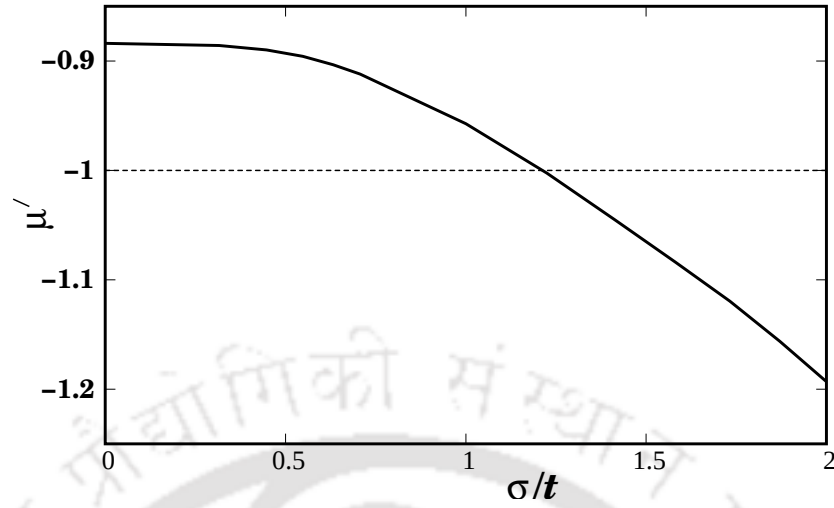


FIGURE 3.3: The scaled chemical potential, μ' ($= \mu/4t$) is plotted as a function of disorder. μ' crosses the band minimum $\mu' = -1$ (shown by the dashed line) at $\sigma/t \simeq 1.2$. Here $U = -1.5t$ and $n = 0.1$.

To remind ourselves, the disorder has been chosen from a Gaussian distribution in the above case. We have also investigated the crossover issue when the disorder is randomly chosen from a rectangular distribution and our study has shown that the crossover point continues to be the same i.e. $\sigma \simeq 1.2t$.

In what follows, we provide further evidences of the emergence of unconventional features in the system with disorder. The system possesses long range phase coherence when a definite phase relationship exists between pairs which are spatially separated in a superconductor. The decrease in superfluidity is signalled by the reduction in the off-diagonal long range order (*ODLRO*), a quantity which is a measure of correlations between pairs. We plot the temperature dependence of *ODLRO* and the double occupancy $n_d (= \langle n_{i\uparrow} n_{i\downarrow} \rangle)$ between the BdG states with and without disorder in Fig. 3.4. The temperature at which they vanish (or become negligible) is same for the pure system, while they differ considerably in the presence of disorder (for $\sigma/t = 1$). The result is important in the sense, it shows pair formation (indicated by n_d) and condensation (indicated by *ODLRO*) are same for the pure system, however the two processes happen at different temperatures in disordered systems. The existence of two different temperature scales is indicative of deviations from conventional superfluidity.

Next, we focus on the superfluid stiffness, D_s^0 given by the Kubo formula[228]

$$\frac{D_s^0}{\pi} = \langle -K_x \rangle - \Lambda_{xx}(q_x = 0, q_y \rightarrow 0, i\omega = 0). \quad (3.9)$$

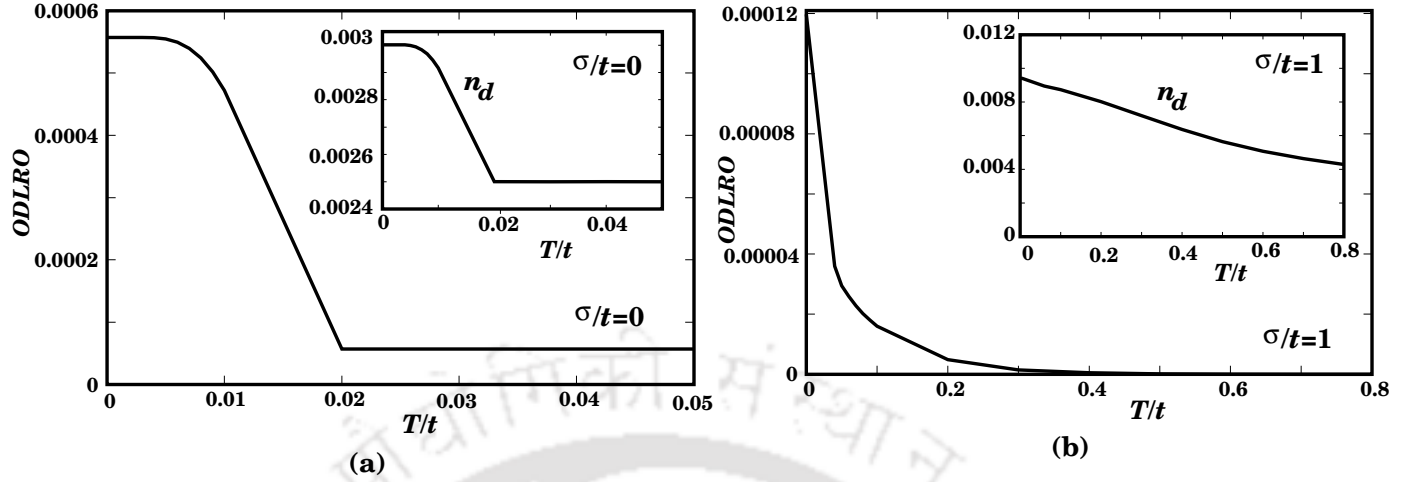


FIGURE 3.4: The off-diagonal long range order, $ODLRO$ and double occupancy, n_d (for $U = -1.5t$ and $n = 0.1$) are shown as a function of temperature, T for $\sigma/t = 0$ (a) and 1 (b). The pure case shows an unique temperature scale for them to become negligible, while they occur at considerably different temperatures for the disordered case.

The first term $\langle -K_x \rangle$ is the (diamagnetic) kinetic energy along the x-direction and is defined as,

$$\langle -K_x \rangle = -t \left\langle \sum_i \left[c_{i+\hat{x}}^\dagger c_i + c_i^\dagger c_{i+\hat{x}} \right] \right\rangle. \quad (3.10)$$

The paramagnetic response is given by the second term which is the disorder averaged transverse current-current correlation at different times and is given by,

$$\Lambda_{xx}(\mathbf{q}, i\omega_n) = \sum_{\mathbf{r}_i} \int_0^\beta d\tau \langle j_x(\mathbf{r}_i, \tau) j_x(0, 0) \rangle e^{i\mathbf{q} \cdot \mathbf{r}} e^{i-\omega_n \tau}. \quad (3.11)$$

D_s^0 is a measure of density of superelectrons, viz n_s ($D_s^0/\pi = n_s/m^*$, m^* being the effective mass).

The details of the derivation of the Eq. (3.9) is presented below.

The kinetic energy term in Hamiltonian is given by,

$$K = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) \quad (3.12)$$

In the presence of external vector potential, the kinetic energy term is modified as[229],

$$K_A = -te^{ieA_x(i)} \sum_{\langle ij \rangle \sigma} \left(c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right) \quad (3.13)$$

Expanding the phase factor in Eq. (3.13), we get

$$K_A = K - \sum_i \left[e j_x^P(i) A_x(i) + \frac{e^2 k_x(i)}{2} A_x^2(i) \right] \quad (3.14)$$

where j_x^P is the paramagnetic current given by,

$$j_x^P(i) = it \sum_{\sigma} \left(c_{i+x\sigma}^\dagger c_{i\sigma} - c_{i\sigma}^\dagger c_{i+x\sigma} \right) \quad (3.15)$$

and k_x is the kinetic energy along x-direction defined as,

$$k_x(i) = -t \sum_{\sigma} \left(c_{i+x\sigma}^\dagger c_{i\sigma} + c_{i\sigma}^\dagger c_{i+x\sigma} \right) \quad (3.16)$$

The total current density, $J_x(i)$ is given by,

$$J_x(i) = - \frac{\delta K_A}{\delta A_x(i)} = e j_x^P(i) + e^2 k_x(i) A_x(i) \quad (3.17)$$

where the first term is the paramagnetic contribution and the second one is the diamagnetic term. We thus get,

$$\langle J_x(i, t) \rangle = e \langle j_x^P(i, t) \rangle + e^2 \langle k_x \rangle A_x(i, t) \quad (3.18)$$

The vector potential can be written as,

$$A_x(i, t) = A_x(q, \omega) e^{i(q \cdot i - \omega t)} \quad (3.19)$$

The linear response theory yields,

$$\langle j_x^P(i, t) \rangle = \sum_{i'} \Lambda_x(ii', \omega) A_x(i', t) \quad (3.20)$$

where

$$\Lambda_x(ii', \omega) = - \frac{i}{\hbar} \int_{-\infty}^0 d\tau e^{i\omega\tau} \langle GS | [j_x^P(i, \tau), j_x^P(i', 0)] | GS \rangle \quad (3.21)$$

Thus Eqn. (3.20) can be written as,

$$\langle j_x^P(i, t) \rangle = \sum_{i'} \frac{-i}{\hbar} \int_{-\infty}^0 d\tau e^{i\omega\tau} \langle GS | [j_x^P(i, \tau), j_x^P(i', 0)] | GS \rangle A_x(q, \omega) e^{i(q \cdot i' - \omega t)} \quad (3.22)$$

Now, we have

$$j_x^P(q, 0) = \sum_{i'} j_x^P(i', 0) e^{-i(q \cdot i')} \quad (3.23)$$

which yields

$$\langle j_x^P(i, t) \rangle = \frac{-i}{\hbar} \int_{-\infty}^0 d\tau e^{i\omega\tau} \langle GS | [j_x^P(i, \tau), j_x^P(-q, 0)] | GS \rangle A_x(q, \omega) e^{-i\omega t} \quad (3.24)$$

Eqn. (3.24) can be rewritten as

$$\begin{aligned} \langle j_x^P(i, t) \rangle &= \frac{-i}{\hbar} \int_{-\infty}^t dt' \langle GS | [j_x^P(i, t), j_x^P(-q, t')] | GS \rangle A_x(q, \omega) e^{-i\omega t'} \\ &= \frac{-i}{\hbar} \int_{-\infty}^t dt' \langle GS | [j_x^P(i, t), j_x^P(-q, t')] | GS \rangle A_x(i, t) e^{-iq \cdot i} e^{i\omega(t-t')} \\ &= \frac{-i}{\hbar} A_x(i, t) e^{-iq \cdot i} \int_{-\infty}^t dt' \langle GS | [j_x^P(i, t), j_x^P(-q, t')] | GS \rangle e^{i\omega(t-t')} \end{aligned} \quad (3.25)$$

Now,

$$\begin{aligned} \Lambda_x(iq, \omega) &= \frac{-i}{\hbar} \int_{-\infty}^t dt' \langle GS | [j_x^P(i, t), j_x^P(-q, t')] | GS \rangle e^{-iq \cdot i} e^{i\omega(t-t')} \\ &= \frac{-i}{\hbar} \int_{-\infty}^t dt' e^{-i\omega t'} \langle GS | [j_x^P(i, t), j_x^P(-q, t')] | GS \rangle e^{-i(q \cdot i - \omega t)} \end{aligned} \quad (3.26)$$

Average over space variable i gives,

$$j_x^P(q, t) = \sum_i j_x^P(i, t) e^{-i(q \cdot i)} \quad (3.27)$$

Thus,

$$\Lambda_x(q, \omega) = \frac{-i}{\hbar} \int_{-\infty}^t dt' \langle GS | [j_x^P(q, t), j_x^P(-q, t')] | GS \rangle e^{i\omega(t-t')} \quad (3.28)$$

Say, $t - t' = \tau$, then

$$\Lambda_x(q, \omega) = \frac{i}{\hbar} \int_0^\infty d\tau \langle GS | [j_x^P(q, \tau), j_x^P(-q, 0)] | GS \rangle e^{i\omega\tau} \quad (3.29)$$

Eqn. (3.25) thus becomes,

$$\langle j_x^P(i, t) \rangle = A_x(i, t) \Lambda_x(q, \omega) \quad (3.30)$$

We now substitute above expression in Eqn. (3.31) which yields,

$$\begin{aligned} \langle J_x(i, t) \rangle &= e A_x(i, t) \Lambda_x(q, \omega) + e^2 \langle k_x \rangle A_x(i, t) \\ &= -e^2 \left[\langle -k_x \rangle - \frac{\Lambda_x(q, \omega)}{e} \right] A_x(q, \omega) e^{(q \cdot i - \omega t)} \\ &= \langle J_x(q, \omega) \rangle e^{(q \cdot i - \omega t)} \end{aligned} \quad (3.31)$$

So,

$$\langle J_x(q, \omega) \rangle = -e^2 \left[\langle -k_x \rangle - \frac{\Lambda_x(q, \omega)}{e} \right] A_x(q, \omega) \quad (3.32)$$

It may be noted that current response of a superconductor in a static $\omega = 0$, long wavelength $q_y \rightarrow 0$, transverse vector potential $q \cdot A$ is given by

$$J_x(q_y) = -\frac{1}{4\pi\lambda^2} A_x(q_y) \quad (3.33)$$

where the penetration depth, λ is given by

$$\frac{1}{\lambda^2} = \frac{4\pi n_s e^2}{mc^2} \quad (3.34)$$

Here n_s is the superfluid density which is related to the superfluid stiffness, D_s as

$$\frac{n_s}{m} \equiv \frac{D_s}{\pi e^2} \quad (3.35)$$

c is set to unity.

Now from linear response relation Eqn. (3.32) and Eqns. (3.33) and (3.35), we have

$$\frac{D_s}{\pi e^2} = \langle -k_x \rangle - \Lambda_x(q_x = 0, q_y \rightarrow 0, i\omega = 0) \quad (3.36)$$

Fig. 3.5 shows a considerable decrease in D_s^0 (or equivalently n_s , as m^* is negligibly affected) as σ is increased.

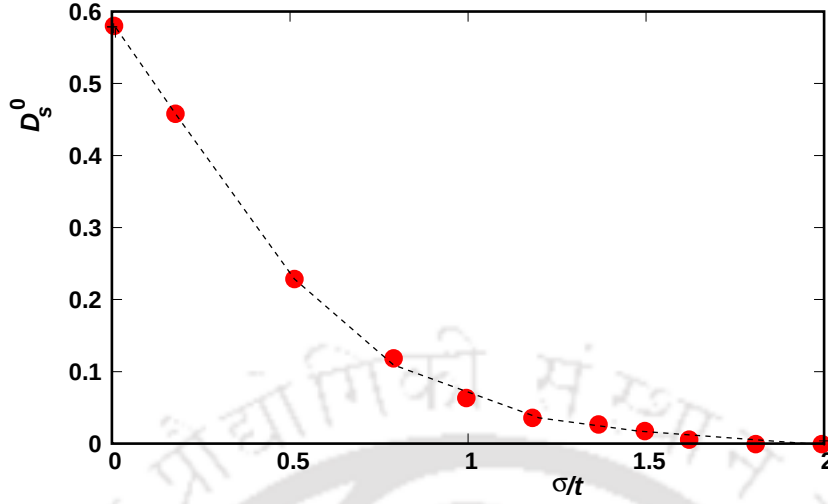


FIGURE 3.5: The superfluid stiffness, D_s^0 (in units of t) is shown as a function of disorder for $U = -1.5t$ and $n = 0.1$. At large disorder, D_s^0 becomes very small, implying a sharp decrease in superfluid density, n_s .

3.2.2.1 Phase fluctuations within self-consistent harmonic approximation (SCHA)

We investigate the effect of inclusion of (thermal) phase fluctuations on the interplay between disorder and superconductivity. We use the following expression for renormalized superfluid stiffness which is obtained using self-consistent harmonic approximation (for details refer to chapter 2)

$$D_s(\kappa, \xi, T, \sigma) = D_s^0 \exp \left[\frac{-\phi(\kappa, \xi, T, \sigma)}{\xi \sqrt{\kappa D_s}} \right]. \quad (3.37)$$

Here κ is the compressibility ($= \frac{dn}{d\mu}$), ξ is the coherence length and

$$\phi = \frac{1}{N} \left[\sum_k \left(\sqrt{f(k)} \coth \left(\frac{\beta}{2\xi} \sqrt{\left(\frac{D_s f(k)}{\kappa} \right)} \right) \right) \right] \quad (3.38)$$

where $f(k) = 4 - 2(\cos k_x + \cos k_y)$. Note that ξ is computed using the BCS relation,

$$\xi(T) = \frac{\hbar v_F}{\pi \Delta(T)} \quad (3.39)$$

where $\Delta(T)$ is chosen from BdG results for the pure case. Thus the effect of disorder on ξ is neglected. We then solve Eq. (3.37) to determine the renormalized $D_s(T)$ (shown in Fig. 3.6)

for various values of disorder strengths, using D_s^0 as an input from the BdG results.

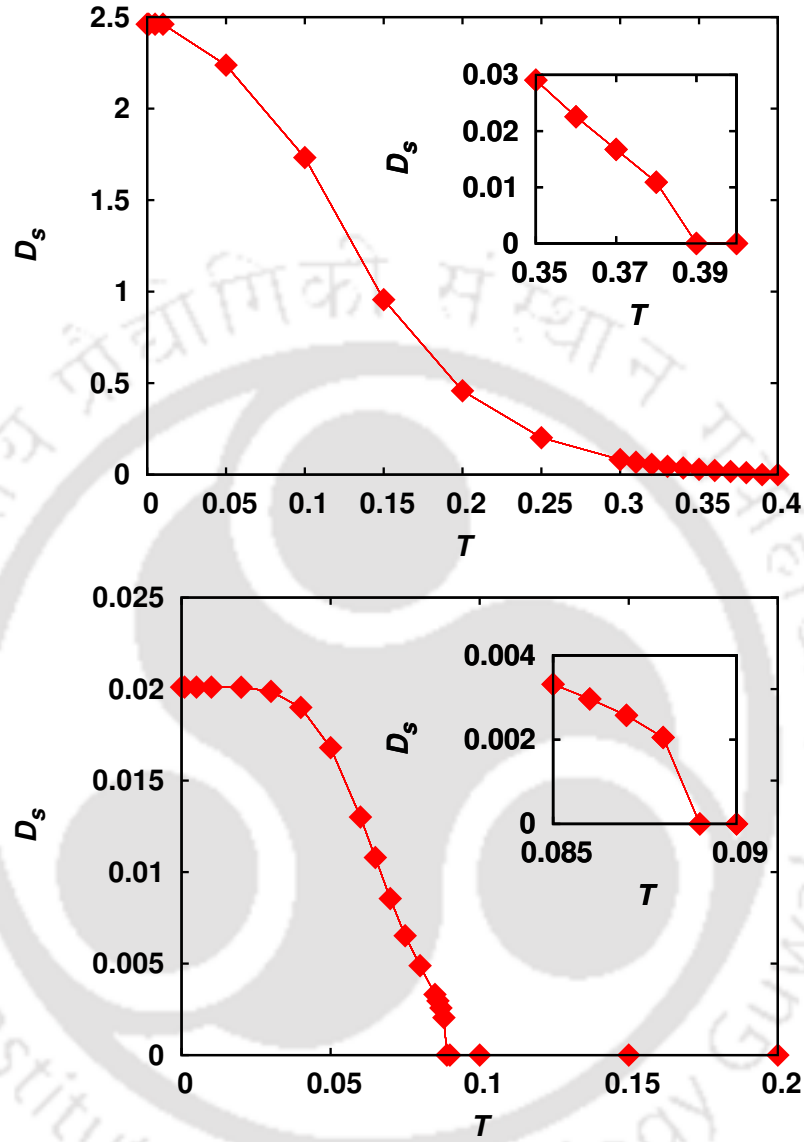


FIGURE 3.6: D_s (in units of t) is shown as a function of temperature for pure ($\sigma/t = 0$) and disordered ($\sigma/t = 3$) cases respectively. Here $U = -1.5t$ and $n = 0.8$. The inset shows sharp drop in D_s as the critical transition temperature, T_c is reached.

3.2.2.2 Pseudogap-like behaviour

The renormalised D_s obtained from SCHA, is indicative of the fact that the phase fluctuations lower the stiffness and beyond a certain critical temperature T_c , drive it to zero. It may be noted that D_s undergoes a jump as T_c is approached.

The Nelson-Kosterlitz (NK) relation is,

$$\lim_{T \rightarrow T_{KT}^-} D_s(T) = \frac{2}{\pi} T_{KT}, \quad (3.40)$$

where the Kosterlitz-Thouless (KT) transition temperature, T_{KT} is marked by the precipitous drop of the fully renormalised D_s . D_s (obtained from SCHA) is substituted in Eq. (3.40) to get T_{KT} which is obtained from the intersection point of the straight line and D_s (as a function of temperature) for a particular value of disorder. One of the cases (for $\sigma/t = 3$) is presented in Fig. 3.7) for reference.

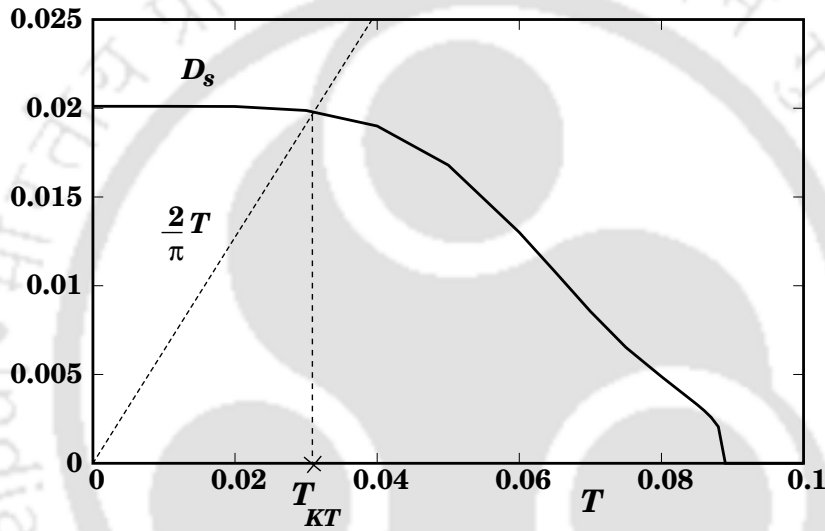


FIGURE 3.7: D_s and $\frac{2}{\pi}T$ are plotted vs temperature for $U = -1.5t$ and $n = 0.8$. Note that the intersection between the two gives T_{KT} , which is marked on the x -axis.

T_{KT} thus obtained is plotted with increasing disorder strength (along with mean field transition temperature, T_c^0 in Fig. 3.8). Our result clearly point towards opening of a large region between T_c^0 and T_{KT} where there is no phase coherence between pairs, though amplitude correlations continue to exist. Thus, pairs form at T_c^0 which is analogous to T^* and condense at T_{KT} analogous to T_c , where T_c^0 and T_{KT} correspond to sufficiently different temperatures. Note that T^* and T_c are commonly used in the context of underdoped cuprates. Importantly, the intervening region is characterised by the presence of incoherent pairs, thereby resembling the pseudogap phase in cuprates[230].

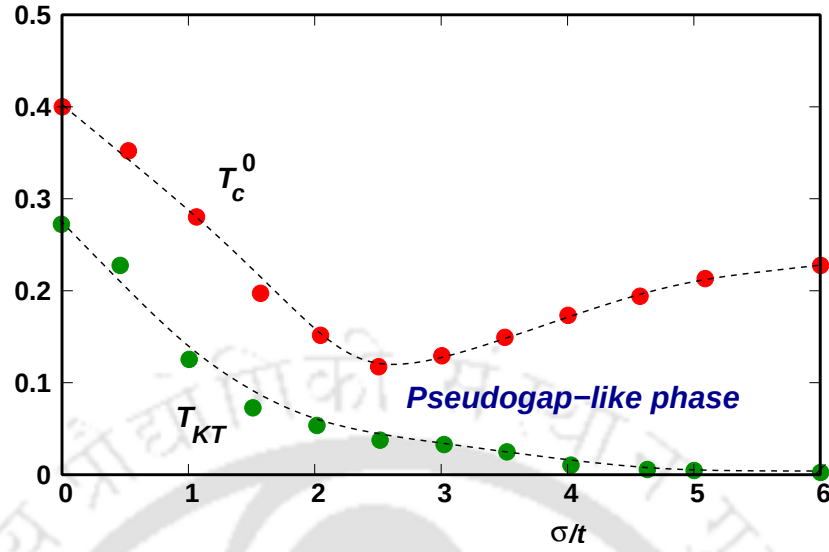


FIGURE 3.8: T_c^0 and T_{KT} shown as a function of disorder for $U = -1.5t$ and $n = 0.8$. Both the temperatures are in units of t .

3.2.3 Other agencies of BCS-BEC crossover

3.2.3.1 Hopping (off-diagonal) disorder

In the presence of hopping disorder, the attractive hubbard model gets modified as,

$$H = - \sum_{\langle ij \rangle, \sigma} (t + \delta t_{ij}) (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) - |U| \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_{i,\sigma} (V_i - \mu) n_{i\sigma} \quad (3.41)$$

where hopping disorder is modeled by letting $V_i = 0$ for all i and δt_{ij} to be chosen from a gaussian distribution, which may be obtained as one replaces V_i by δt_{ij} in Eq. (3.2). The Hamiltonian is then solved using BdG method as discussed before.

The ability of hopping disorder to induce a crossover phenomenon is under suspect. The reason is as follows - random hopping events of the electrons cause delocalisation, rather than a localised charge distribution, as was the case for onsite disorder. To confirm the presence of delocalisation effects as contrary to localisation in the case of onsite disorder, we present the variation of average kinetic energy along x -axis *i.e.* $\langle K_x \rangle$ for both kinds of disorder in Fig. 3.9. It may be noted that the localisation process for onsite disorder is further supported by the increase in potential energy (shown in Fig. 3.10(a)) as a function of disorder. Similar

behaviour of potential energy (Fig. 3.10(b)) is seen for hopping disorder also but the delocalization caused by the randomised hopping of charge carriers completely overshadows the localisation effect.

Further, superfluid stiffness (Fig. 3.11) also behaves differently than the onsite disorder case, *i.e.* D_s^0 is found to increase with disorder. The explanation for this behaviour is contained in Eq. (3.9), where the first term on the left ($\langle -K_x \rangle$) dominates the behaviour of D_s^0 in presence of disorder and at large disorder, D_s^0 is entirely governed by this term. However, D_s^0 falls initially at smaller values of disorder where an increase in the paramagnetic response offsets the rise in the diamagnetic term (see Eq. (3.9)). Expectedly, μ' [231] in Fig. 3.12 does not slip below the band edge and hence does not qualify to be a candidate for the crossover scenario. The enhancement of the noninteracting bandwidth owing to hopping disorder accommodate the chemical potential inside the band for all values of disorder[193].

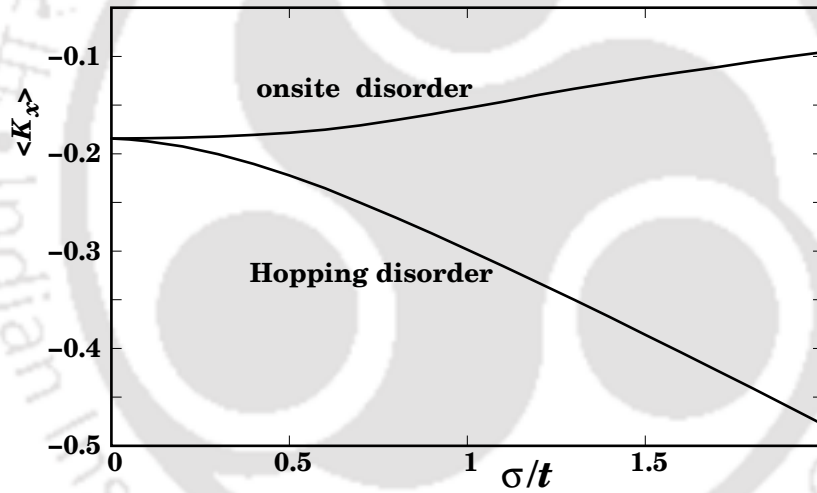


FIGURE 3.9: Average kinetic energy (negative of the expression used in Eq. (3.10)) for both hopping and onsite disorder as a function of disorder strength, σ . Here K_x is in units of t .

3.2.3.2 Hopping anisotropy

We now consider another situation where the carriers are allowed to move preferentially in one particular direction (say x -direction), while the movement is strongly restricted in the other direction (y -direction) owing to anisotropic hopping frequencies. The third kind of inhomogeneity, *i.e.* hopping anisotropy, which is a case of correlated disorder, is modeled trivially by choosing $\delta t_{ij} = V_i = 0$ in Eq. (3.41) and the hopping is t when i and j are

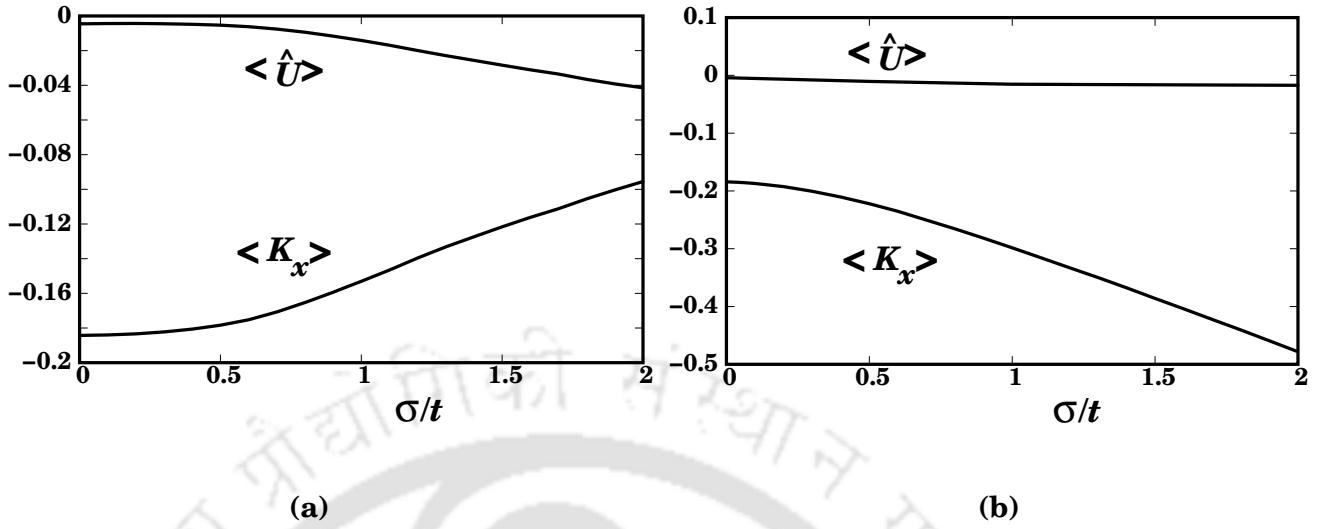


FIGURE 3.10: Average potential ($|U| \sum_i \langle n_{i\uparrow} n_{i\downarrow} \rangle$) and kinetic energies (both in units of t) are plotted as a function of disorder for (a) onsite and (b) hopping disorder.

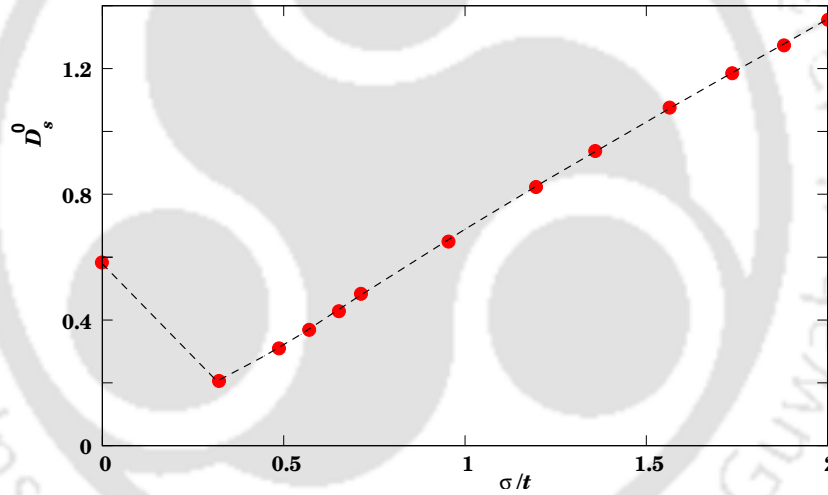


FIGURE 3.11: D_s^0 (in units of t) is shown vs disorder strength for hopping disorder. It shows a gradual increase because the diamagnetic contribution (average kinetic energy) dominates the behaviour of D_s^0 .

neighbours in x -direction, while it is rt when j is y -neighbour of i , with r being the anisotropy parameter ($0 < r \leq 1$).

The significant role played by anisotropy in stabilizing a superconducting condensate, has been previously studied in details. Studies reveal that the hopping anisotropy facilitates pair formation with an infinitesimal attractive interaction in the extreme anisotropy limit[232]. Moreover, it was found that a bound state becomes favourable for two electrons moving along

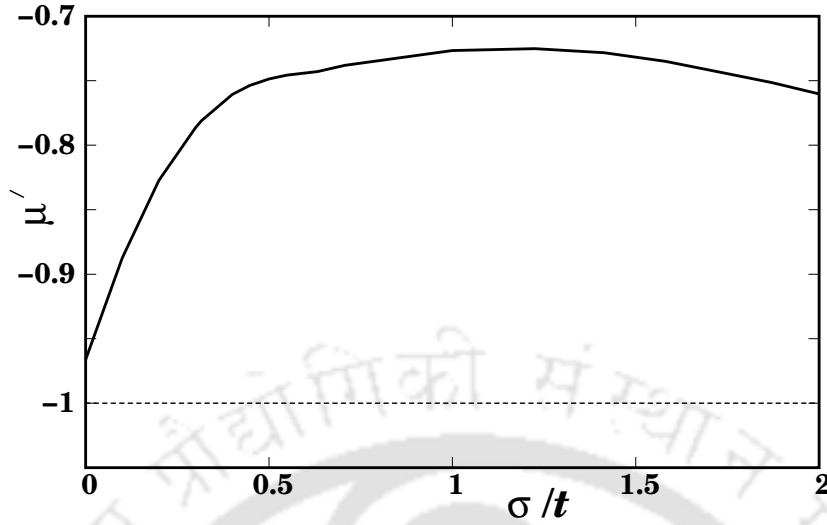


FIGURE 3.12: The scaled chemical potential is plotted as a function of σ for the case of hopping disorder. μ' does not cross the band edge, thereby ruling out a crossover scenario.

different chains of a two-leg ladder (rather than along the chain) and hence form a stable pair when anisotropy is large. Further an enormous enhancement of the superconducting transition temperature T_c , is also observed in this limit[233]. Thus anisotropy in hopping frequency of charge carriers may emerge as a potential candidate for inducing a crossover.

The neutron and X-ray diffraction studies[234] have confirmed the presence of stripes in cuprates. These stripes are the segregation of doped charge carriers into periodically spaced linear rivers of charges[234]. Many arguments have been put forward supporting the fact that these stripes play crucial role in the pairing mechanism in these materials and thus it demands special attention. This motivated us to incorporate an anisotropy in hopping frequencies of the charge carriers as it provides the simplest description of stripe-like inhomogeneities by inducing higher conductivity in one direction as opposed to another. These inhomogeneities may be experimentally realized by applying uniaxial pressure on materials so as to achieve restricted motion of charge carriers in a particular direction.

To confirm the presence of crossover in the anisotropic case, we compute the (scaled) chemical potential, $\mu' (= \mu/2t(1 + r))$ as a function of the anisotropy parameter r (see Fig. 3.13). μ' slips down the band minimum at a small value of r , *i.e.* in the extreme anisotropy limit, following band narrowing effects and thus present a case for the crossover scenario[193].

A similar problem has been investigated by us[235] in the context of BCS-BEC crossover, where an anisotropic hopping is considered in the strong coupling limit of the (repulsive)

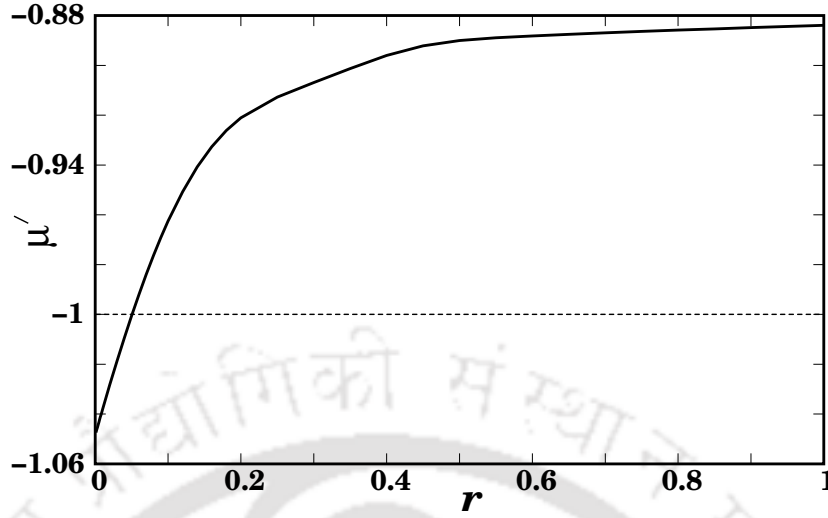


FIGURE 3.13: μ' is plotted vs anisotropy parameter $rt (= \frac{t_y}{t_x})$ shows a crossing below the band minimum at very small values of r (extreme anisotropy limit).

Hubbard, *i.e.* the $t - J$ model for a square lattice given by,

$$H = - \sum_{\langle ij \rangle \sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + h.c) + J \sum_{\langle ij \rangle} \left(S_i \cdot S_j - \frac{n_i n_j}{4} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (3.42)$$

The onsite potential U may be set to infinity to project out double occupancy of sites[236, 237]. This establishes a close correspondence with the familiar variant, *viz* $t - J$ model. We allow our t_{ij} and J to be non zero for near neighbours only. It may be noted that the exchange interaction is taken to be isotropic as we found no qualitatively new physics emerging out with anisotropic exchange.

Owing to the anisotropy, the electronic dispersion is given by,

$$\epsilon_k = -2t (\cos k_x + r \cos k_y) \quad (3.43)$$

where $r (= \frac{t_y}{t_x})$ is the anisotropy parameter. The isotropic limit ($r = 1$) corresponds to a square lattice but in the $r \rightarrow 0$ limit the lattice symmetry is that of an one dimensional chain. The effective interaction is decoupled in the form,

$$V_{kk'} = -J [\Gamma_s(k) \Gamma_s(k') + \Gamma_d(k) \Gamma_d(k')] \quad (3.44)$$

with,

$$\Gamma_s(k) = \cos k_x + \cos k_y \quad \text{and} \quad \Gamma_d(k) = \cos k_x - \cos k_y \quad (3.45)$$

as the irreducible symmetry factors for a square lattice. It may be noted that the symmetry factors of the point group (C_{4v}) of the square lattice undergoes a mixing owing to the hopping anisotropy.

We make the following ansatz for the gap amplitude Δ_k ,

$$\Delta_k = \Delta_s \Gamma_s(k) + e^{i\theta} \Delta_d \Gamma_d(k) \quad (3.46)$$

where Δ_s and Δ_d are gap parameters in the s - and d -wave channels respectively and θ is the mixing angle between the two contributions. The gap amplitudes are then obtained by substituting Eq. (3.44) and Eq. (3.46) into BCS gap equation at finite temperature given by,

$$\Delta_k = -\frac{1}{N} \frac{\sum_{k'} V_{kk'} \Delta_{k'} (1 - 2f(E_{k'}))}{2E_{k'}} \quad (3.47)$$

where, $E_k = \sqrt{(\epsilon_k - \mu)^2 + |\Delta_k|^2}$, $f(E_k)$ is the Fermi distribution function, μ is the chemical potential which controls filling. The coupled equations of the gap amplitudes are as follows,

$$\Delta_s = \frac{J}{N} \left[\Delta_s \sum_{k'} \frac{\Gamma_s(k') \Gamma_s(k') (1 - 2f(E_{k'}))}{2E_{k'}} + e^{i\theta} \Delta_d \sum_{k'} \frac{\Gamma_s(k') \Gamma_d(k') (1 - 2f(E_{k'}))}{2E_{k'}} \right] \quad (3.48)$$

$$e^{i\theta} \Delta_d = \frac{J}{N} \left[\Delta_s \sum_{k'} \frac{\Gamma_s(k') \Gamma_d(k') (1 - 2f(E_{k'}))}{2E_{k'}} + e^{i\theta} \Delta_d \sum_{k'} \frac{\Gamma_d(k') \Gamma_d(k') (1 - 2f(E_{k'}))}{2E_{k'}} \right] \quad (3.49)$$

The above coupled equations are solved self-consistently along with the equation for electron density,

$$n = 1 - \frac{1}{N} \sum_k \frac{(\epsilon_k - \mu) (1 - 2f(E_k))}{E_k} \quad (3.50)$$

We study the effect of r , the anisotropic hopping, on the gap amplitudes, Δ_s and Δ_d , with $J (= 1/3)t$, a value that is realized for cuprates) and for different values of θ .

Equations (3.48), (3.49), (3.50) are solved self-consistently to obtain Δ_s , Δ_d and μ as a function of temperature for various values of anisotropy. The gap amplitudes as a function of temperature for $r = 0.001$ is shown in Fig. 3.14. Interestingly, the d -wave correlations are enhanced as much as 10^4 times as $r \rightarrow 0$ compared to the isotropic limit (not shown here). Both the gap amplitudes grow as higher anisotropic limit is approached, signaling a stability of the superconducting state in that limit. Thus the hopping anisotropy helps in achieving a more robust superconducting condensate with equal amplitudes for s - and d -wave correlations[238].

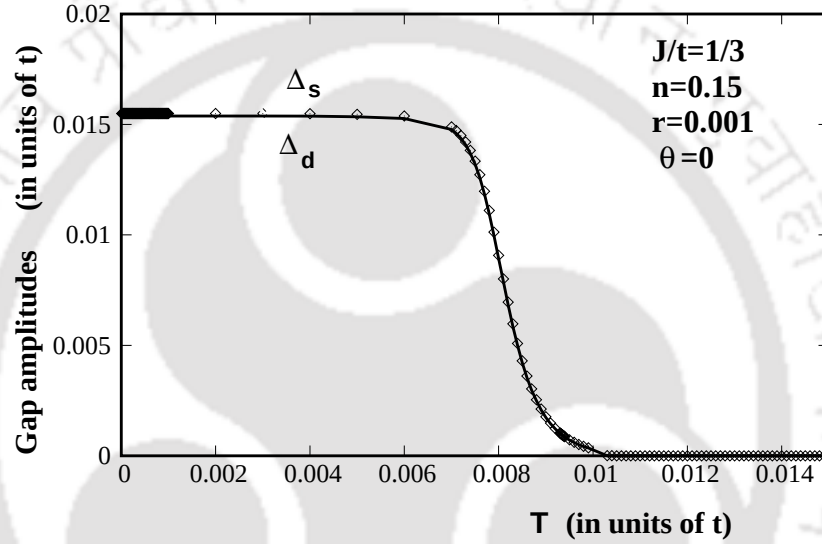


FIGURE 3.14: The gap amplitudes, Δ_s (solid line) and Δ_d (dotted line), are plotted vs temperature, T for $r = 0.001$. Both the axes are in units of t . The electron density, n , is taken to be 0.15 and $J/t = 1/3$. θ is the relative phase difference between the two gap amplitudes.

3.2.4 Mean pair radius

In conventional superconductors, the internal part of the pair wave function corresponds to a spherically symmetrical bound state whose radius is defined as the mean pair radius. It is defined by the following relation[239],

$$\xi_{pair}^2 = \frac{\int |f(r)|^2 r^2 d^3r}{\int |f(r)|^2 d^3r} = \frac{\sum_k |\nabla_k g_k|^2}{\sum_k |g_k|^2} \quad (3.51)$$

where $f(r)$ ($g(k)$) is the wave function for a cooper pair in real (momentum) space.

Eq. (3.51) is solved for ξ_{pair}^x and ξ_{pair}^y and the results are presented in Fig. 3.15 as a function of the anisotropy parameter r . It is interesting to note that $\xi_{pair}^{x,y}$ decreases from a few thousands of lattice spacing with increase in anisotropy and becomes very small (order of one lattice spacing) as $r \rightarrow 0$. Thus the system smoothly evolves from a large number of overlapping Cooper pairs to a condensate of tightly bound pairs carrying signature of a BCS-BEC crossover.

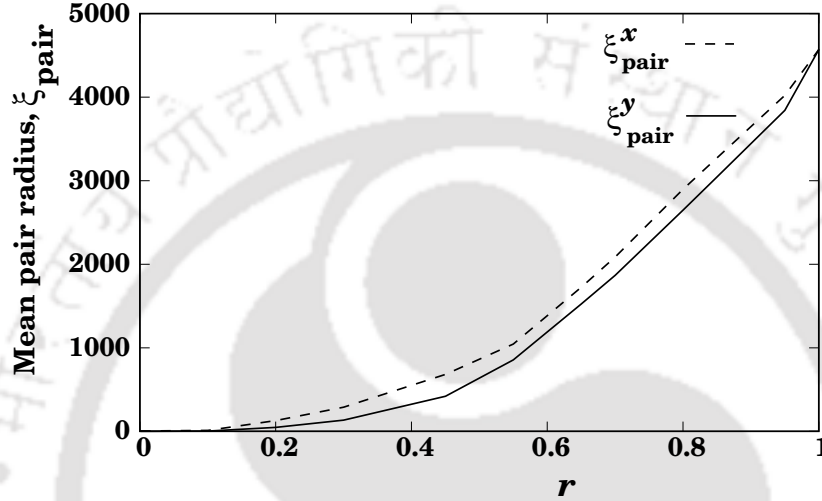


FIGURE 3.15: The mean pair radii, ξ_{pair}^x and ξ_{pair}^y , are plotted as a function of anisotropy parameter, r . Here $n = 0.15$, $J/t = 1/3$ and $U/t = \infty$ respectively. The temperature T is very small and chosen to be $0.1T_c$, T_c being the superconducting transition temperature. ξ_{pair} is in units of lattice spacing.

3.2.5 Penetration depth

The other important quantity, viz the penetration depth, signifies the distance over which an applied magnetic field is exponentially screened from the interior of a superconductor. The linear response of the current density to the magnetic field defines the penetration depth[62] and hence the superfluid density, the latter having an inverse square dependence on the penetration depth.

$$\mathbf{J}_\delta(\mathbf{q}) = -\frac{1}{4\pi} K_\delta(\mathbf{q} \rightarrow 0) \mathbf{A}_\delta(\mathbf{q}); \quad \delta = x, y \quad (3.52)$$

where,

$$K_\delta = \frac{1}{\sqrt{\lambda_\delta}} \quad (3.53)$$

$\mathbf{J}$ and $\mathbf{A}$ are current density and the vector potential respectively. Eq. (3.53) is used to obtain λ where λ_x and λ_y are penetration depths in x and y -directions respectively (shown in Fig. 3.16 as a function of the anisotropy parameter r). It is seen that λ_x remains almost constant in the entire interval whereas λ_y diverges as $r \rightarrow 0$. This implies that there is an efficient screening (Meissner effect) in x -direction where the carriers move unhindered while the field penetrates to the interior of the sample along y -direction due to a severely restricted motion. More importantly, the results point towards the emergence of a condensate having smaller number of superconducting electrons as the penetration depth is inversely proportional to the square of the superfluid density, thereby bearing fingerprints of a BE phase.

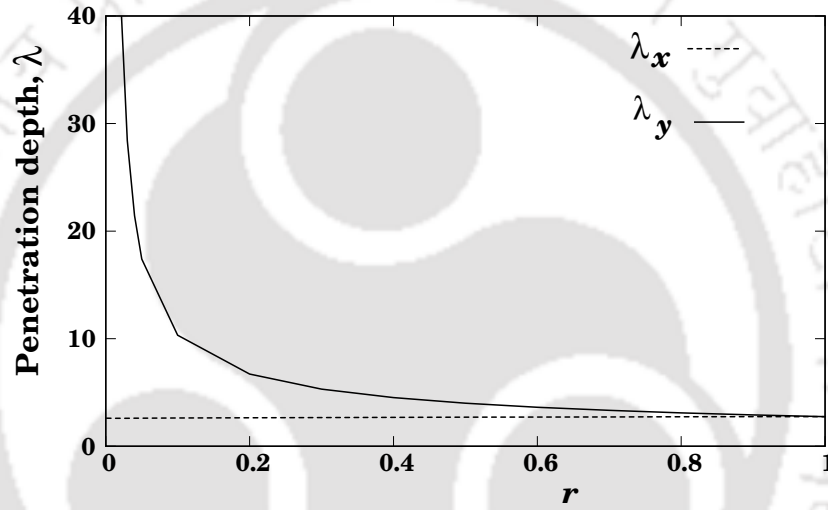


FIGURE 3.16: The penetration depth along x and y axis are plotted vs r . The parameters chosen are same as that of Fig. 3.15. λ_y shows a divergence in the limit $r \rightarrow 0$ while λ_x remains constant. λ is in units of lattice spacing.

3.2.6 Chemical potential

To further strengthen the claim for the existence of crossover scenario in our model, we consider the chemical potential, μ (obtained by solving Eq. (3.47)) which when slips below the band edge as a function of the anisotropy parameter, r (the Leggett condition), the system evolves into a Bose superfluid. We investigate the variation of the (scaled) chemical potential $\mu' (= \mu/2t(1+r))$ as a function of r for different values of n corresponding to a few representative values of J , *e.g.* $J/t = 1/3, 1$ and 2 . This sheds light on the dependence of crossover on electronic density and the interaction strength. The results obtained are presented in table 3.1.

TABLE 3.1: BCS-BEC crossover is investigated by computing μ as a function of anisotropy parameter, r for a few values of density, n and interaction strength, J . The value of r at which μ falls below the lower band edge ($= -2t(1 + r)$) and thus signal a crossover is denoted by r_c . The empty slots represent absence of a crossover for the corresponding parameter values.

	$J/t = 1/3$	$J/t = 1$	$J/t = 2$
n	r_c	r_c	r_c
0.02	0.007	0.11	0.57
0.1	-	0.006	0.08
0.15	-	-	0.026
0.2	-	-	-

The results clearly indicate absence of crossover for larger values of n for any value of J . The reason behind this being larger overlapping of pairs leads to an increase in the correlation energy at higher densities. To compensate for this, the system organizes itself with a larger average pair size so as to minimize the total energy of the system[86]. Thus at higher densities, the system bears fingerprints of BCS condensate even for larger values of J/t . It may be noted that there is no crossover for the isotropic case for J to be as large as $2t$. Thus the hopping anisotropy drives the system from a BCS phase to a Bose regime at lower densities[235].

3.2.7 Kinetic vs Potential energy driven pairing

The recent experimental data on optical conductivity[56] are consistent with a picture that pairing in cuprates is kinetic energy driven and thus contrasts the conventional BCS theory. These experiments have shown that the pairing in high- T_c superconductors is driven by a reduction in the kinetic energy and not by an attractive potential as in the BCS theory. In this context, we investigate the energetics of the system by computing the condensation energy as a function of temperature for different values of anisotropy.

The condensation energy is defined as the difference between the ground state energies of the superconducting and the normal state ($F_s - F_n$) where F_s is the energy of the superconducting state given by,

$$F_s = \frac{1}{N} \sum_k \frac{\Delta_k^2(1 - 2f(E_k))}{2E_k} + \frac{1}{N} \sum_k n_k^s \epsilon_k \quad (3.54)$$

Here the symbols carry the usual meaning. The normal state energy F_n is obtained by putting $\Delta_k \equiv 0$ and replacing superconducting density n_k^s , by the density in the normal phase, n_k^n . Even though the presence of pseudogap in unconventional superconductors makes the above definition of condensation energy questionable, still in the absence of any concrete theory, the above approach is likely to give important results.

The results (shown in Fig. 3.17) clearly point towards conventional potential energy driven superconductivity in the BEC limit as there is a reduction in the potential energy while the kinetic energy undergoes slight increment on entering the superconducting state. Thus the results extend its support to the picture of conventional pairing and disputes the recent claim of kinetic energy driven pairing in cuprates[240].

3.3 Summary

We have investigated the effect of random disorder on the evolution of a BCS superconductor to a BEC superfluid using BdG approximations on a two dimensional square lattice. The study includes both onsite (diagonal) and hopping (off-diagonal) disorder. While onsite disorder presents a case for inducing a crossover due to localisation effects, hopping disorder is shown to be *not* a catalyst for the crossover phenomenon, owing to delocalisation of the charge carriers. The existence (or non-existence) of the crossover scenario is confirmed by calculating the chemical potential, which when slips below the noninteracting band minimum, yields a crossover to a Bose phase. A third candidate of the crossover story is presented by the hopping anisotropy, yields a crossover in the extreme anisotropy limit, a possible artifact of the dimensional confinement of the charge carriers. The effect of carrier concentration on the crossover phenomena is also discussed and it is concluded that low density facilitates a crossover phenomena at moderate values of interparticle attraction. At higher densities, the overlap between the pairs increase substantially, thus denying an access to a phase comprising of local pairs, reminiscent of a BEC phase. We have also calculated two important length scales that characterise the superconducting condensate, viz the mean radius of the Cooper pairs and the penetration depth, for a two dimensional $t - J$ model with hopping anisotropies. It is observed that a BCS superconductor evolves smoothly into a phase with much shorter and fewer (although tightly bound) pairs, characteristics of a BE phase with increasing anisotropy. Further, we have investigated the condensation energy as a function of anisotropy which points

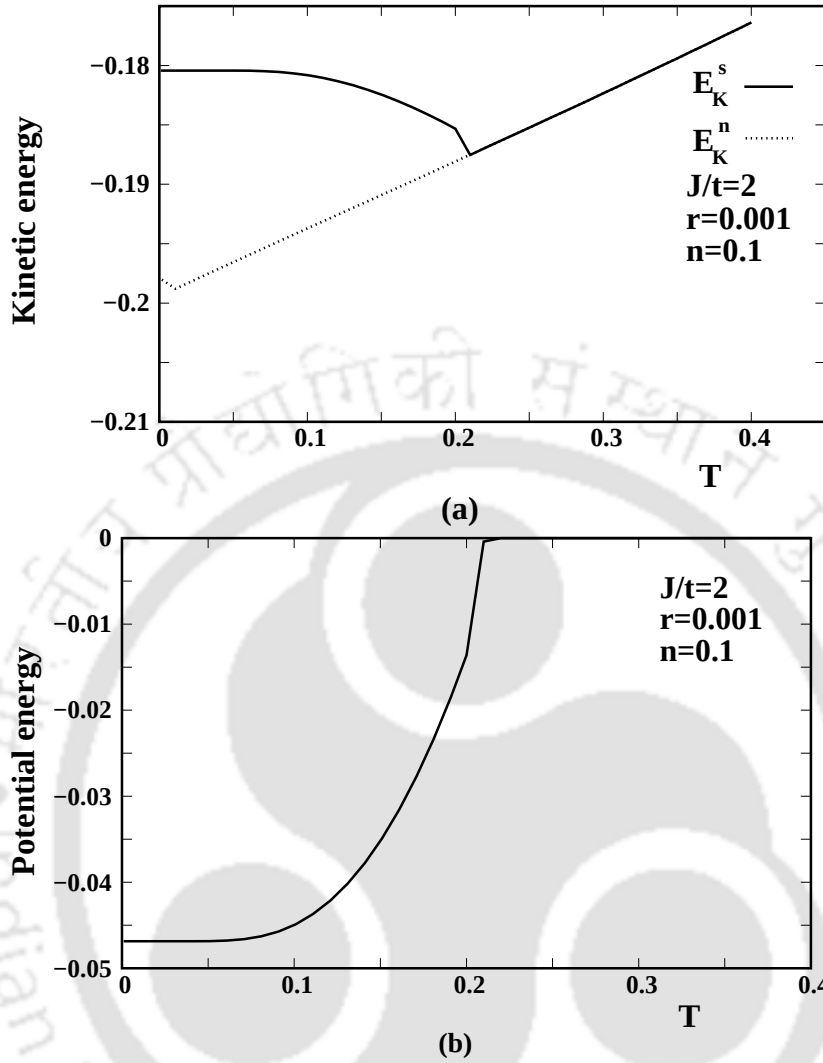


FIGURE 3.17: Kinetic energies (of the superconducting and normal states) and potential energy (of the superconducting state) are shown in Fig. 3.17(a) and Fig. 3.17(b) respectively, as a function of temperature T . Here $J/t = 2$, $r = 0.001$ and $n = 0.1$. The axes are in units of t .

towards conventional potential energy driven pairing in the BE phase (as in BCS case). A little introspection reveals that within a mean field formalism, the pairing mechanism should not switch loyalty from being potential energy driven to kinetic energy driven as a crossover-like phase emerges.

Improvements to our mean field (BdG) results is made by computing the phase fluctuations about the inhomogeneous BdG state via a *phase-only* model which provides a rough estimate of the actual transition temperature, obtained from the vanishing of the renormalised superfluid stiffness. The superfluid stiffness thus obtained, is then used in the NK relation

to obtain the transition temperature, T_{KT} . Interestingly, the variation of the mean field transition temperature and T_{KT} as a function of disorder strength, yields opening of a large region (between the two temperatures scales) where there is no phase coherence between the pairs, however amplitude correlations continue to exist, reminiscent of the pseudogap phase in cuprates.





Chapter 4

Real space toolbox for studying the crossover

4.1 Introduction

In the earlier chapter we have shown that a BCS-BEC crossover is achievable in a weakly coupled superconductor in presence of a random onsite disorder potential[193] with the crossover occurring at moderate values of disorder. At intermediate values of disorder, the system becomes unstable to the formation of bound pairs as the chemical potential falls below the noninteracting band minimum (Leggett criterion) as a function of disorder strength. In this chapter, we plan to boost the above crossover scenario by adopting concepts and techniques that are more widely used in other fields such as random matrix theory and quantum information and computation etc.

Due to lack of translational symmetry, it is wise to look at real space quantities. It may be important to look into the details of the BdG eigenfunctions as they are likely to hold clues to the crossover picture presented in the last chapter. The statistics of the eigenfunctions of a random matrix have been extensively reviewed by Guhr *et al.*[241] and Mirlin[242], where it is emphasized that the eigenfunctions show strong statistical fluctuations at the critical point of a quantum phase transition (QPT). Applications of this technique to study Anderson's metal insulator transition (MIT)[243–245] have provided vital clues to the critical behaviour observed in the vicinity of localization which is characterized by the vanishing of the spatial extent of

the electronic eigenstate. A measure of the latter is conveniently provided by the participation ratio (PR) (or its inverse, IPR) which efficiently distinguishes between the extended and localized states. Similar applications to plateau to plateau transitions in quantized hall systems and an associated fractal analysis from a scaling theory are available in literature[246–251]. Interesting usage of the participation ratio has been done to study transport properties of the complex systems such as DNA like molecules[252, 253]. Returning back to the focus of the current work, it is reasonable to state that a crossover between a BCS and a BEC regime should be characterized by an intermediate value of the PR that signifies persistence of the superfluid state with short ranged pairing correlations.

Another closely related quantity is the information entropy (also known as Von Neumann entropy) which provides a measure of randomness in the electronic charge density residing at a lattice site or equivalently signals the onset of a localized phase when the information entropy vanishes. The distinction between the information entropy and the thermodynamic entropy is a subtle one[254, 255], where the former depends on the fractal dimension, while the later holds no clue for it. For us, the crossover regime should have a low but finite entropy at intermediate disorder, which eventually becomes negligibly small at large values of disorder, signaling localization of states.

Another intriguing tool borrowed from quantum information theory is the overlap (scalar product) of two ground states corresponding to two slightly different values of the parameter that is responsible for inducing a QPT. Since QPT distinguishes between regions of the parameter space that are characterized by different order parameters, the overlap or as it is called the fidelity, undergoes a drop from its normalized value unity in the vicinity of a QPT. Zanardi *et al.*[256] reported a drop in ground state fidelity at the transition point in the Dicke and the XY models. It is also extensively studied in fermionic models[257–259], spin models[256, 260–262], Bose Hubbard models[263, 264] and in phase transitions which are not directly associated a microscopic order parameter[265, 266] such as topological phase transitions. More recently, the machinery is used in the context of studying BCS-BEC crossover in both continuum and lattice models where the interplay of density and interparticle interaction in the crossover issue is emphasized[267].

An elaborate discussion on the underlying model and formalism used has been earlier discussed in section 3.2 of chapter 3. We now proceed to discuss the results and their implications.

4.2 Results and Discussion

A number of useful quantities borrowed mostly from other fields such as chaos, quantum information and computation etc have been calculated to address the role of disorder in inducing a BCS-BEC crossover using the BdG eigenstates. They are the participation ratio (PR), localization length, information entropy, fidelity and fidelity susceptibility. A brief discussion on each of them will appear very helpful for later discussion.

We begin with the definition of participation ratio (PR). It is expressed as the inverse of fourth power of eigenfunctions and thus gives a measure of the number of lattice sites over which an eigenstate is extended[268]. The PR is defined as,

$$(PR)_\alpha = \frac{1}{\sum_{r_i} |\phi_\alpha(r_i)|^4} \quad (4.1)$$

where $\phi_\alpha(r_i)$ is the eigenstate obtained from the BdG analysis, α being the eigenvalue index. It distinguishes localized states ($PR \sim 1$) from the extended ones ($PR \sim N$, where N is total number of lattice sites). At large values of disorder, as done for the case of MIT, an investigation of the fractal dimensionality can be quite helpful. Suppose an electronic wavefunction is localized within a d -dimensional volume of average diameter ξ which can be roughly taken as a characteristic length for the asymptotic exponential decay, called the localization length[269], the PR behaves as ξ^d . For us, $d = 2$, so an estimate of the localization length can be obtained as

$$\xi = \sqrt{PR} \quad (4.2)$$

Another quantity which provides a measure of sites over which the eigenfunction is extended, is called the information entropy whose scaling properties in context of QPT are discussed at length[270], can be quite useful in the present situation. The information entropy can be defined as,

$$S(E) = \sum_{r_i=1}^N \phi_\alpha^2(r_i) \ln [\phi_\alpha^2(r_i)] \quad (4.3)$$

An estimate of the possible number of microstates, Ω can be obtained from,

$$\Omega(E) = \exp[S(E)] \quad (4.4)$$

with the Boltzmann constant $k_B = 1$, which as a function of disorder should vanish as the number of available microstates decrease or the eigenfunction extends over fewer sites as localization sets in.

As further elaborations to the ongoing endeavour of establishing the onset of the crossover scenario, we compute a quantity that is commonly used in quantum information theory, *viz.* fidelity that shows a sudden drop in the value of the wavefunction overlap for two close by values of the parameter that drives a QPT. Quite generally the fidelity is defined as[271],

$$F(\rho, \sigma) = \text{Tr} \left[\sqrt{\sqrt{\rho} \sigma \sqrt{\rho}} \right] \quad (4.5)$$

where ρ and σ are the density matrices for two slightly different parameters that parametrize the system. They are given by the outer product of the eigenstates of the system *viz.* $|\phi\rangle\langle\phi|$. It quantifies the difference between two different ground states. We specifically look for the overlap between two ground states (as the ground states are likely to be appreciably occupied, density being low) for two disorder strengths, differing only slightly and is given by,

$$F(\sigma + \delta\sigma, \sigma) = \langle \phi_0(\sigma + \delta\sigma) | \phi_0(\sigma) \rangle \quad (4.6)$$

where $\phi_0(\sigma)$ is the ground state wavefunction, which while computing we shall use the ground states obtained from our BdG calculations.

Another quantity called fidelity susceptibility, a close variant of the fidelity discussed above, measures the response of a state (say, ground state) to small changes in the driving parameter and is obtained from fidelity as follows. For an infinitesimal change in disorder strength, $d\sigma$, one can Taylor expand the ground state,

$$|\phi_0(\sigma + d\sigma)\rangle = |\phi_0(\sigma)\rangle + d\sigma \frac{d}{d\sigma} |\phi_0(\sigma)\rangle + \frac{1}{2!} (d\sigma)^2 \frac{d^2}{d\sigma^2} |\phi_0(\sigma)\rangle \quad (4.7)$$

Thus the fidelity, F takes the form,

$$F(\sigma + \delta\sigma, \sigma) = \left[\langle \phi_0(\sigma) | + d\sigma \frac{d}{d\sigma} \langle \phi_0(\sigma) | + \frac{1}{2!} (d\sigma)^2 \frac{d^2}{d\sigma^2} \langle \phi_0(\sigma) | \right] |\phi_0(\sigma)\rangle \quad (4.8)$$

The fidelity susceptibility, $\chi(\sigma)$ is represented in terms of F as[265, 267, 272]

$$\chi(\sigma) \equiv -\frac{1}{N} \lim_{\delta\sigma \rightarrow 0} \frac{4 \ln F(\sigma + \delta\sigma, \sigma)}{(\delta\sigma)^2} \quad (4.9)$$

where N is the number of sites of the system. $\chi(\sigma)$ should show a sharp peak at transition.

Next we comment on the choice of our parameters. We have chosen the interparticle interaction strength to be $|U| = 1.5t$ and density to be $n = 0.1$. Since our starting point is a weak coupled superconductor (BCS), we have chosen a small U . The rationale behind choosing small n is because of the following reason. We have earlier noted an absence of crossover for large values of n even for strong interaction strengths, *e.g.* U to be of the order of bandwidth or even more[230]. As discussed before, pairs overlap at higher densities which results in increase in correlation between the carriers. Thus the average pair size increases so as to minimize the total energy of the system and hence the condensate bears resemblance to BCS phase even for large U values. The size of the lattice for our numerical computation is chosen as 24×24 . Further, all the parameters are denoted in units of the hopping frequency, t which should be of the order of an eV.

To gain physical intuition on the crossover scenario, we present the plots of the local pairing amplitudes, $\Delta(r_i)$ (obtained from Eq. (3.7)) at different values of disorder strengths, *viz.* $\sigma = 0.5t, 1.2t, 2t$ and $3t$ on a 24×24 lattice in Fig. 4.1. One can notice formation of superconducting islands as σ is increased and at $\sigma = 3t$, the pairing amplitudes largely vanish, with the exception for a few sites. Let us concentrate on the plot for $\sigma = 1.2t$ which shows that the amplitudes are spread over fewer sites (than the one for $\sigma = 0.5t$), however long range order is still possible[193, 230].

We now plot the spatial distribution of electron occupancies, $\langle n_i \rangle (= 2 \sum_n v_n^2(\mathbf{r}_i))$ in Fig. 4.2 for different disorder strengths, *viz.* $\sigma/t = 0.5, 1.2, 2$ and 3 . It may be noted that the plot corresponding to stronger disorder shows localised electron occupancies and thus are supportive of a phase comprising of short and local pairs, reminiscent of a BEC phase. Such plots are also available for higher densities (not shown here), where the electron occupancies show considerable overlap.

Hence we analyze the behaviour of the participation ratio (PR) as a function of disorder strength. PR obtained from Eq. (4.1), is shown in table 4.1 for a few values of disorder strength. It may be noted that PR is of the order of few lattice sites for moderate disorder

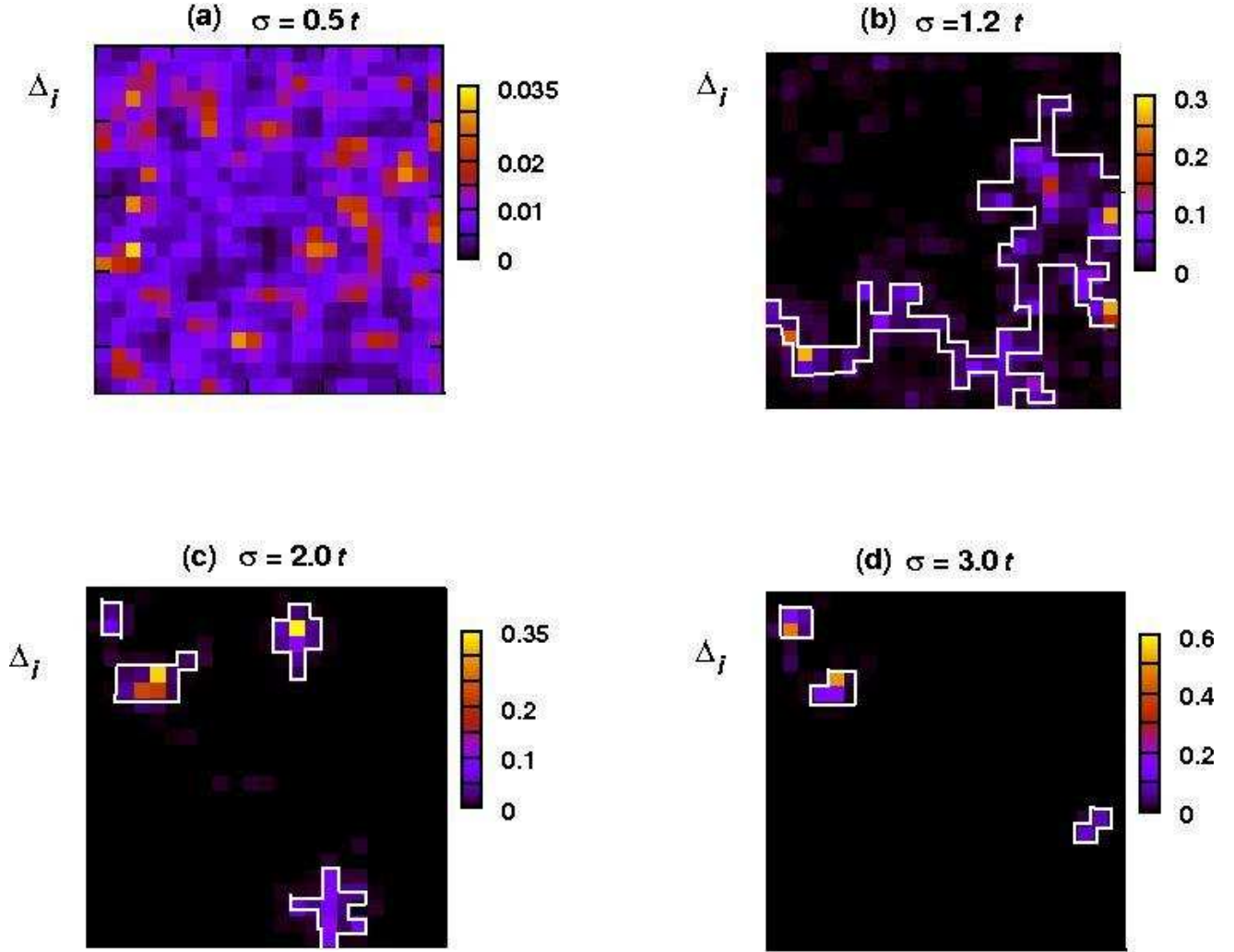


FIGURE 4.1: The real space profile of the local pairing amplitudes, $\Delta(r_i)$ (in units of t) is shown for four different values of disorder strengths, viz $\sigma = 0.5t$ (low), $1.2t$ (moderate), $2t$ (large) and $3t$ (very large). Note the formation of superconducting islands at (moderate to) large values σ .

strengths, which should account for the superfluid behaviour as the electronic wavefunction spreads out over some finite number of sites. At still higher values of disorder strength, the wavefunctions get localized and hence an insulating phase sets in.

The localization length, ξ ($\sim \sqrt{PR}$), which gives an idea about the spatial dimension over which the eigenfunction extends, is presented in Fig. 4.3. ξ is seen to drop by a factor of 5 from the corresponding value at $\sigma = 0$, while at large values of disorder, $\xi \simeq 1$, i.e. the amplitude of the wavefunction extends to exactly one site, signaling a complete localization.

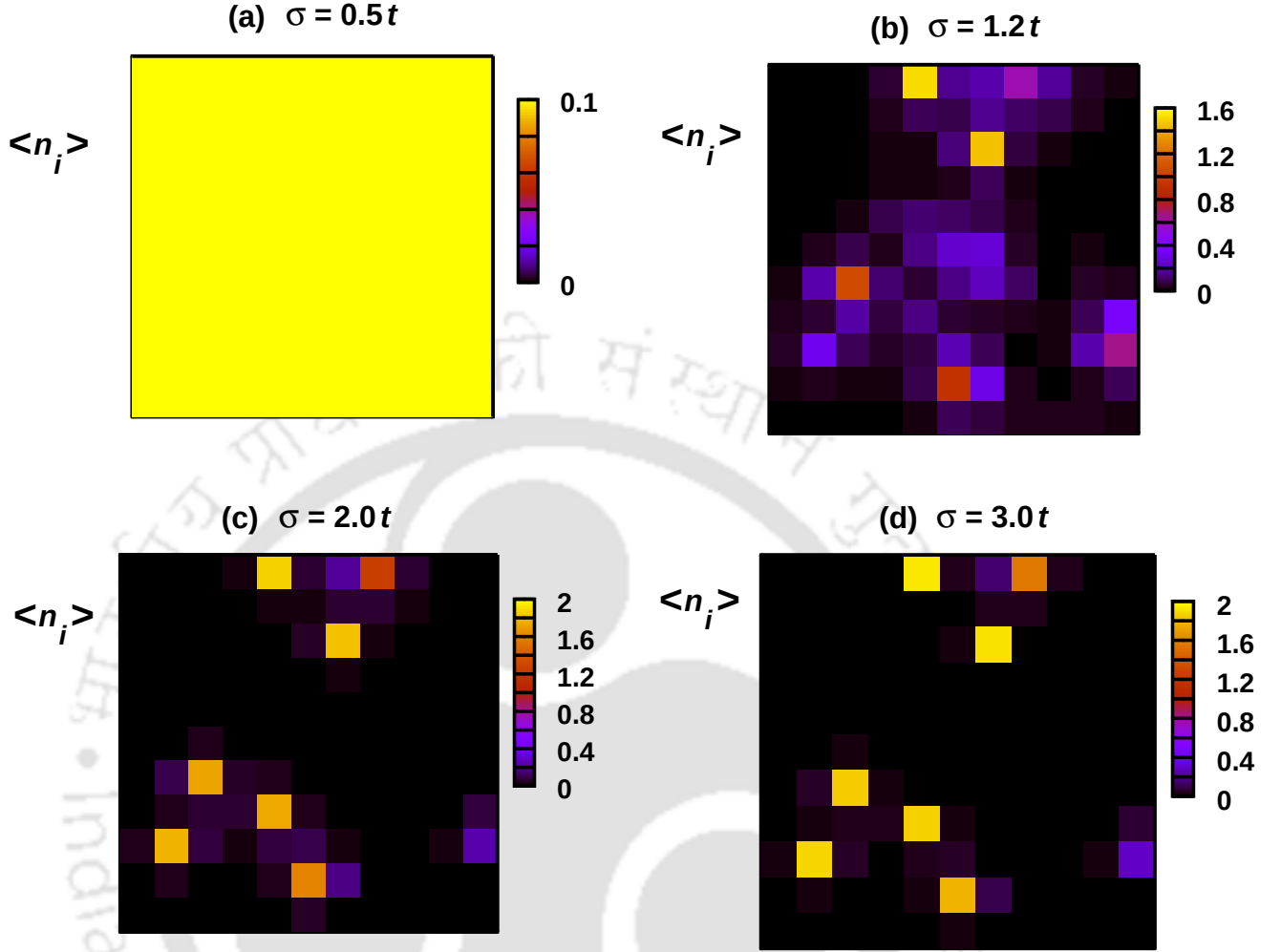


FIGURE 4.2: Spatial distribution of electron occupancies, $\langle n_i \rangle$ ($= 2 \sum_n v_n^2(\mathbf{r}_i)$) for disorder strengths viz $\sigma = 0.5t$ (low), $1.2t$ (moderate), $2t$ (large) and $3t$ (very large). The localised nature of the charge densities is to be noted for larger disorder. Here $\langle n_i \rangle$ is in units of t .

Hence we present results for the information entropy, or the exponential of it, $\Omega(E)$ defined in Eq. (4.4) in Fig. 4.4. $\Omega(E)$ is of the order of total number of lattice sites (N) for low values of disorder strength, drops to a value of a few lattice spacings for intermediate values and finally becomes of the order of unity in the limit of extreme disorder, implying complete localization of eigenfunctions and hence onset of an insulating phase. Thus all three of them, viz. PR, ξ and $\Omega(E)$ suggests of an insulating behaviour at large values of σ and importantly for us, before which a phase with finite superfluid properties exists for intermediate values of disorder, which is evident for the small but finite spread of the wavefunction.

We now focus on the ground state fidelity and the results obtained are shown in Fig. 4.5.

TABLE 4.1: Participation ratio, PR is shown for various values of σ . Note that PR reduces drastically with increasing disorder strength and approaches unity in the limit of extreme disorder.

Disorder strength (σ) (in units of t)	Participation ratio (PR)
0	575
0.25	313
0.75	43
1.0	24
1.2	5
1.5	4
3.0	1

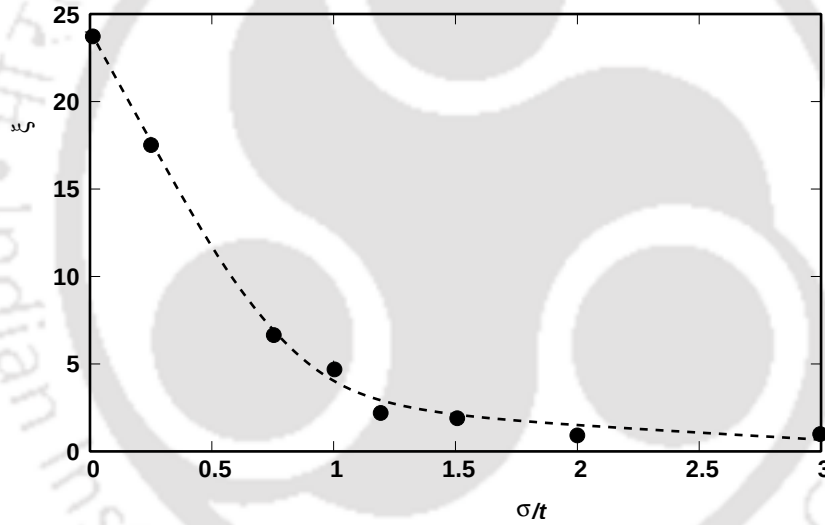


FIGURE 4.3: The localization length, ξ obtained from PR data via $\xi \sim \sqrt{PR}$ is shown as a function of disorder strength, σ . The dashed line is a guide to the eye. Same is true for the following figures in this chapter. Here ξ is in units of t .

Note the sudden drop in ground state fidelity in the near vicinity of $\sigma \simeq 1.2t$, which is referred to as onset of the crossover earlier. The sharp drop in fidelity suggests a significant change in the nature of the ground state for disorder values close to $\sigma \simeq 1.2t$, which results in a loss of overlap between the ground states corresponding to two slightly different disorder values near the crossover threshold. To provide evidence of how sharp the drop in fidelity is, we have taken sufficient amount of data around the crossover point. We indeed have observed the fall off in fidelity to be very sharp. The abrupt change in the ground state properties at

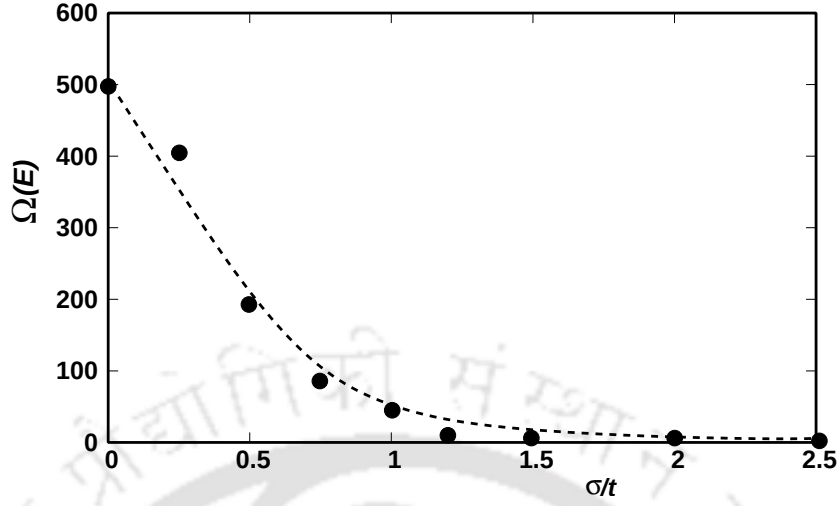


FIGURE 4.4: The information entropy, $\Omega(E)$ is shown as a function of disorder strength, σ . $\Omega(E)$ is moderate for intermediate values of disorder, while it vanishes at large σ . Here $\Omega(E)$ is in units of t .

intermediate values of disorder, is indicative of an onset of a different kind of phase which is characterized by the bound pairs of the constituent fermions.

As one enters the phase of bound pairs, the ground state overlap jumps to the normalized value unity. To us, this feature robustly demonstrates the emergence of a phase that resembles the crossover regime between a weakly coupled BCS superconductor and a BEC phase. Together with the Leggett criterion and the participation ratio analysis, the resemblance provides a compelling evidence for a disorder induced crossover scenario.

To ascertain the genuineness of the fidelity result and to rule out any correlation between the randomness in disorder potential (V_i in Eq. (3.1)) and the drop in ground state fidelity near $\sigma \simeq 1.2t$, we compute a quantity g defined as,

$$g = \sum_i [V_i(\sigma) - V_i(\sigma')]^2 \quad (4.10)$$

A plot of g vs. disorder strength, σ as shown in Fig. 4.6 is featureless and yields a constant value. Thus the drop in fidelity is uncorrelated with the random profile for disorder and is true for several different disorder configurations.

The fidelity susceptibility is presented in Fig. 4.7. It shows a sharp peak in the vicinity of the crossover threshold. The peak signifies the strong response of the ground state to small

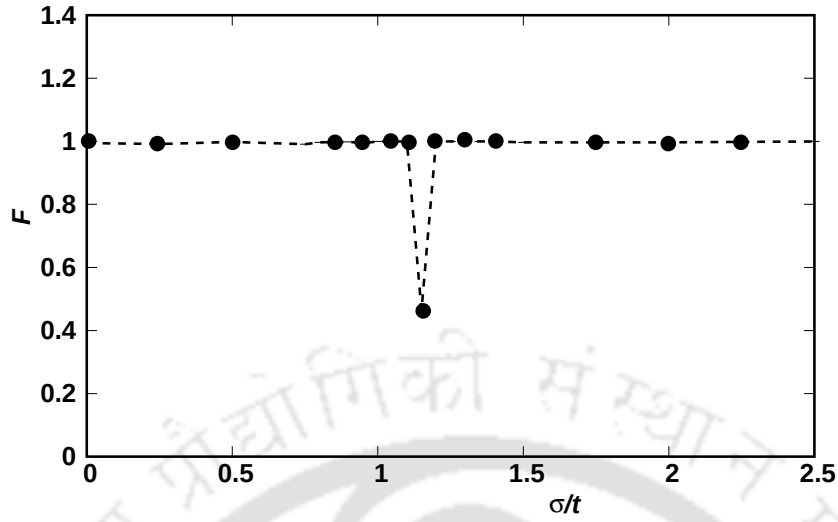


FIGURE 4.5: The ground state fidelity is shown as a function of σ . There is sudden drop in fidelity by a factor of 2-3 around the threshold value of disorder which marks the onset of a Bose-like phase, *i.e.* around $\sigma \sim 1.2t$. Note that the fidelity jumps to the normalized value unity as we cross the threshold. Here F is in units of t .

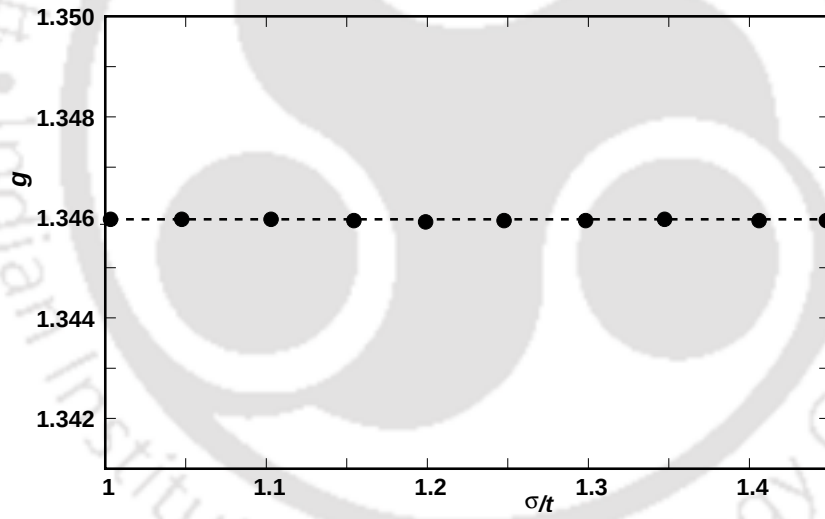


FIGURE 4.6: g (defined in text through Eq. (4.10)) is shown as a function of disorder strength, σ which is constant for disorder values near the crossover threshold, thereby ruling out any correlation between the randomness in the disorder profile and the drop in ground state fidelity (Fig. 4.5). Here g is in units of t .

changes in the driving parameter, *i.e.* σ in inducing a crossover.

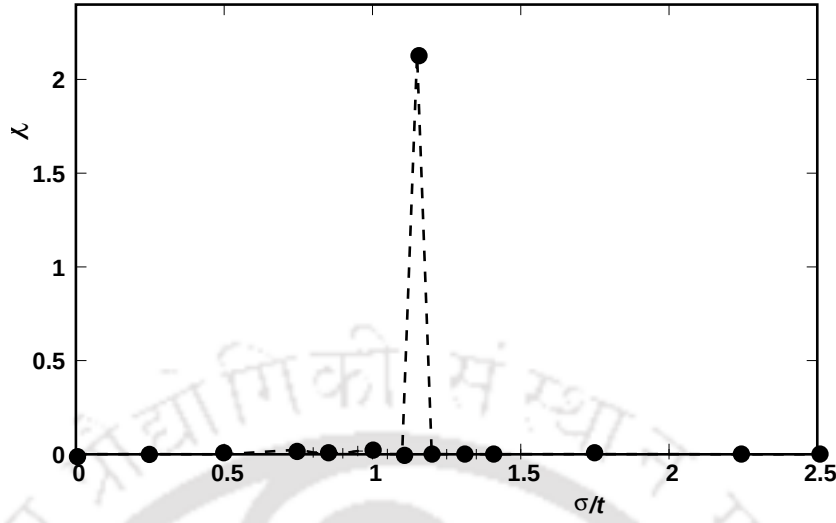


FIGURE 4.7: The fidelity susceptibility, χ is shown as a function of disorder strength, σ . It shows a sharp peak (where fidelity registers a drop), implying a strong response of the system to the onset of a ground state of 'different' nature. χ is in units of t .

4.3 Connection with the continuum model

Let us review for one final time the crossover from a BCS to a BEC phase that we have been engaged with in chapter 3 and this chapter. The crossover issue is mostly studied as a function of interparticle attraction strength. In our work, we have obtained a smooth evolution from a BCS ground state to a local pair phase whose properties bear much in common with BEC phase by tuning the strength of onsite disorder. The signature of the crossover is confirmed by calculating the chemical potential which slips below the band minimum for intermediate disorder strength thereby bearing signatures of onset of Bose phase (Leggett criterion). The local pairing amplitudes are obtained by solving the Bogoliubov equations self consistently as discussed earlier in this chapter.

To bring about a connection with the continuum picture, we need to establish the relation between the roles played by the random disorder and the interaction potential in inducing a crossover phenomena. The issue is more conveniently described by replacing the interaction term by a s -wave scattering length (valid for low energies), viz. a_s or a dimensionless variant of it i.e. $1/k_F a_s$. To remind ourselves, $a_s < 0$ in the BCS limit and $a_s > 0$ in the BEC. The threshold for the formation of the bound state occurs when a_s diverges, beyond which a_s represents the size of the bound state with binding energy, $E_b = 1/ma_s^2$ [63]. In the BCS limit, corresponding to $1/k_F a_s \rightarrow -\infty$ (k_F being the Fermi wavevector), the pairing amplitude is

given by[91],

$$\Delta = 8 e^{-2} \epsilon_F \exp\left(\frac{-\pi}{2k_F|a_s|}\right) \quad (4.11)$$

or equivalently,

$$\ln \Delta = -8 \pi \epsilon_F \frac{e^{-2}}{2k_F|a_s|} \quad (4.12)$$

which implies that $\ln \Delta$ decreases linearly as $1/k_F a_s$ increases. A re-look at our plots of the pairing amplitudes in real space for various values of the disorder strengths, σ (Fig. 4.1), suggests that average Δ ($= \frac{1}{N} \sum_i \Delta_i$) indeed grows at larger disorder strengths upto a certain intermediate value of disorder, which matches well with the crossover regime claimed in this thesis viz. $\sigma \sim 1.2t$. We show this in Fig. 4.8 which demonstrates $\ln \Delta$ diminishing as a function of $1/\sigma$, albeit not in a linear fashion and thereby suggesting of a more complicated relationship between the pairing amplitude and the disorder strength.

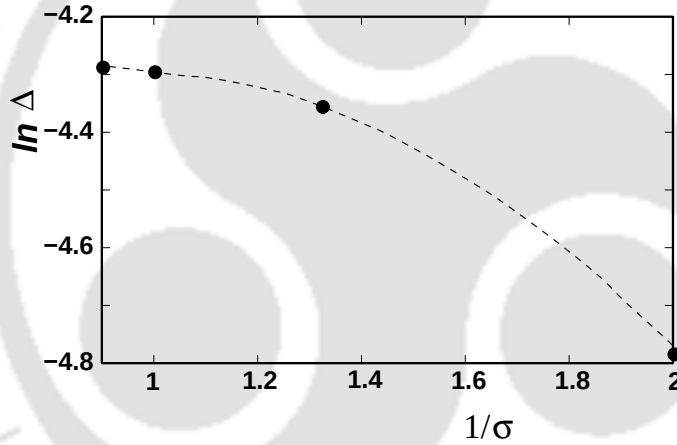


FIGURE 4.8: $\ln \Delta$ as a function of inverse of disorder strength, $1/\sigma$. Shown for small and intermediate values of disorder. The dashed line is a guide to the eye.

4.4 Summary

In this work we have studied the onset of a bosonic (paired) phase in a disordered weakly coupled superconductor using some real space quantities viz. local pairing amplitudes, electron occupancies, participation ratio, information entropy and the ground state fidelity. The crossover scenario is justified by the plots of the local pairing amplitudes which show formation of superconducting islands. At intermediate values of disorder, the islands shrink but still preserve long range order (see Fig. 4.1), which also is evident from the PR values obtained in

Table 4.1. The plots for electron occupancies are supportive of a phase comprising of short and local pairs, reminiscent of a BEC phase, as it shows localised electron occupancies corresponding to stronger disorder. Further investigation of quantities such as localization length and information entropy yield similar insights and supports our notion of crossover phenomena. Lastly, the ground state fidelity shows an abrupt drop at the onset of the Bose-like phase. This is an important result which endorses emergence of a significantly different ground state as the Leggett criterion is satisfied. The fidelity susceptibility, which can be thought of as the response of the ground state to small changes in the parameter values, signals onset of a significantly different phase through a sharp peak as a function of disorder.

From the above discussion, it is clear that the crossover picture portrayed by us at intermediate values of disorder is indeed an interesting topic to study. The role of moderate disorder is illustrated in the context of an inhomogeneous metallic phase[273] for a disordered Mott insulator described by a (repulsive) Hubbard model. Their observation were explained by screening of the random potential due to repulsive interaction thereby generating a weaker random potential. However at large values of disorder, screening is ineffective and an insulating phase emerges once again. A similar argument probably applies for our attractive interaction as well. However the attractive interaction, unlike the repulsive one, unscreens the random potential, thereby generating a stronger attractive interactions among the fermions (see Fig. 3.10(a)) leading to the emergence of a condensate of shorter but tightly bound pairs. At large values of the disorder potential, further enhancement of the effective potential leads to emergence of an insulating behaviour.



Chapter 5

The Fulde Ferrell Larkin Ovchinnikov phase

5.1 Introduction

In this chapter, we review the study of superconductivity in presence of magnetic field commenced nearly half a century ago with the works of Clogston and Chandrasekhar[103, 107]. Later more abounding implications of the presence of an external magnetic field is elucidated by Fulde and Ferrell[24] and by Larkin and Ovchinnikov[25] where a possibility of finite momentum pairing between the different participation species of electrons is explored. First experimental realization of a finite momentum pairing is obtained in a heavy Fermion compound (UPd_2Al_3) via thermal expansion of magnetostriction measurements[114]. Soon after many other heavy fermion compounds also reported FFLO phase[114–116]. Organic superconductors are the other candidates where occurrence of a FFLO phase is predicted[126–128]. However unambiguous realization of the phase in experiments is under scrutiny.

The factor aiding the heavy fermion compounds to be candidates for realizing Cooper pairing with a nonzero momentum can possibly be attributed to the extreme type-II behaviour, a high effective electron mass, m^* , with a large Ginzburg-Landau and Maki parameters and their availability in metallurgically clean state. All these qualities put together imply a very large upper critical field and thus underscore the ascendancy of paramagnetism over the orbital effect.

An alternative route to achieve the supremacy of paramagnetic effect is to use a layered structure in a strong magnetic field applied parallel to the layers, thereby undermining the orbital pair breaking effect further and augmenting the parameter space where FFLO can exist[175]. The organic superconductors strongly fit into these requirements and hence are considered as ideal candidates for FFLO phase[126–128]. Apart from these compounds, signatures of FFLO phases are also observed in other materials such as neutron stars[176] and ultracold atomic gases[274].

It is fairly evident from our previous discussion that the experimental signatures of the FFLO phase in real systems can still be questioned. This provides motivation for us to pursue the matter and look for the spatially modulated profile of the order parameter, a hallmark signature of the FFLO phase. At the same time, the stringency of a number of conditions to be met simultaneously that impede the scope of observing FFLO in experiments, are explored[131].

Starting with a weak coupling BCS superconductor in a magnetic field, we solve the mean field Bogoliubov de Gennes (BdG) equations for an attractive Hubbard model in two dimensions. The mean field order parameter thus obtained in real space shows periodic modulation, a signature of finite momentum Cooper pairing and hence a FFLO phase. The dependence of this modulated phase on the (attractive) Hubbard interaction, $|U|$ and band filling, μ (or particle densities, n) is investigated in details to comment on the possible difficulties in accessing this phase in experiments. Some of the characteristic properties of a superconductor are calculated such as coherence length (related to the wavefunction of modulation in the order parameter[118, 121]) to provide strong evidence in favour of observing FFLO phase. The relevance of our results to real materials, such as heavy fermion compounds are discussed.

5.2 Results and Discussion

We quickly review the underlying model which is a two-dimensional Hubbard model with $|U|$ as the magnitude of the onsite attractive interaction (refer to chapter 2 for details),

$$\mathcal{H} = -t \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) - |U| \sum_i \left(n_{i\uparrow} - \frac{1}{2} \right) \left(n_{i\downarrow} - \frac{1}{2} \right) + \sum_{i, \sigma} (\sigma h - \mu) n_{i\sigma} \quad (5.1)$$

$c_{i\sigma}^\dagger (c_{i\sigma})$ is the creation (destruction) operator for an electron with spin σ which can assume values ± 1 at a site $\mathbf{r}_i$, h is the magnetic field which couples with spin, σ of electrons via Zeeman coupling, $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ and μ denotes the chemical potential. Here t is the transfer integral. Other parameters such as, U , h and μ are expressed in units of t . t is typically of the order of 1eV .

Hartree Fock decomposition of the interaction term in Eq. (5.1) yields,

$$\mathcal{H}_{eff} = \sum_{ij\sigma} \mathcal{H}_{ij\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) + \sum_i [\Delta_i c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger - \Delta_i^* c_{i\uparrow} c_{i\downarrow}] \quad (5.2)$$

here $\mathcal{H}_{ij\sigma} = -t\delta_{i\pm 1j} - (\mu + U\delta n_{i\bar{\sigma}} - \sigma h)\delta_{ij}$ where $\delta n_{i\bar{\sigma}} = n_{i\bar{\sigma}} - 1/2$ with $\bar{\sigma} = -\sigma$. The local pairing amplitude, $\Delta_i = -|U|\langle c_{i\downarrow} c_{i\uparrow} \rangle$ is the order parameter.

The following transformations are used to diagonalize Eq. (5.2),

$$c_{i\sigma} = \sum_n [\gamma_{n\sigma} u_n(\mathbf{r}_i) - \sigma \gamma_{n\bar{\sigma}}^\dagger v_n^*(\mathbf{r}_i)] \quad (5.3)$$

where $\gamma_{n\sigma}$ and $\gamma_{n\bar{\sigma}}^\dagger$ are the quasiparticle operators, $u_n(\mathbf{r}_i)$ and $v_n(\mathbf{r}_i)$ are the BdG eigenvectors.

Applying the above transformations in Eq. (5.2), we get the BdG equations in a matrix form as,

$$\begin{pmatrix} \mathcal{H}_{ij\sigma} & \hat{\Delta}_i \\ \hat{\Delta}_i^* & -\mathcal{H}_{ij\bar{\sigma}}^* \end{pmatrix} \begin{pmatrix} u_n(\mathbf{r}_i) \\ v_n(\mathbf{r}_i) \end{pmatrix} = E_{n\uparrow} \begin{pmatrix} u_n(\mathbf{r}_i) \\ v_n(\mathbf{r}_i) \end{pmatrix} \quad (5.4)$$

where $E_{n\uparrow}$ are the eigenvalues. We start with initial guesses for the pairing amplitude, Δ_i and the density of up and down-spin electrons, $\langle n_{i\uparrow} \rangle$ and $\langle n_{i\downarrow} \rangle$ respectively. Subsequently, the eigenvalues, $E_{n\uparrow}$ and the eigenvectors ($u_n(\mathbf{r}_i), v_n(\mathbf{r}_i)$) are determined numerically from Eq. (5.4). The local pairing amplitudes at sites $\mathbf{r}_i$ and the density of up and down-spin electrons in terms of $u_n(\mathbf{r}_i)$ and $v_n(\mathbf{r}_i)$ are calculated from,

$$\Delta(\mathbf{r}_i) = -|U| \sum_n [u_n(\mathbf{r}_i) v_n^*(\mathbf{r}_i) f(E_{n\uparrow}) - u_n(\mathbf{r}_i) v_n^*(\mathbf{r}_i) f(-E_{n\downarrow})] \quad (5.5)$$

and

$$\langle n_{i\sigma} \rangle = \sum_n [|u_n(\mathbf{r}_i)|^2 f(E_{n\sigma}) + |v_n(\mathbf{r}_i)|^2 f(-E_{n\bar{\sigma}})] \quad (5.6)$$

where $f(E_{n\sigma})$ is the Fermi distribution function. We present results only at zero temperature where $f(E_{n\sigma})$ is unity. The entire process is iterated with new guesses for the above quantities until self-consistency is achieved for all of them simultaneously.

As discussed later, a number of self consistent solutions may exist for the pairing amplitude, $\Delta(\mathbf{r}_i)$ corresponding to one set of parameters. The winner among these will be decided by computing the free energies, $\mathcal{F}$ computed with respect to the free energy in vacuum (at zero temperature) and is given by[275]

$$\mathcal{F} = \sum_{n\sigma} E_{n\sigma} \left[f(E_{n\sigma}) - \sum_i |v_n(\mathbf{r}_i)|^2 \right] + |U| \sum_i \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle + \frac{1}{|U|} \sum_i \Delta_i^2 - \frac{|U|N}{4} \quad (5.7)$$

For example, consider one particular parameter set, $|U| = 2.5$, $\mu = -0.5$ and $h = 0.35$, all in units of t . The free energies are computed using Eq. (5.7) corresponding to BdG solutions that yield uniform, one period and two period modulations for the local pairing gap, Δ_i and are obtained as -1.2539 , -1.2543 and -1.2520 respectively (again in units of t) for a two dimensional lattice of size 32×16 (see discussion below). Since one period modulation for Δ_i yields the lowest energy, it is considered as a energetically favourable solution. We have carried out similar studies for all choices of U and μ corresponding to various values of h used in this work to pin down the stable solution.

Next we comment on the choice of parameters. We investigate the behaviour of the pairing amplitude for different values of μ corresponding to a few representative values of onsite interaction strengths, $|U| = 1, 2.5$ and 4 . The rationale behind the choice of U is to get an insight into the stability of FFLO phase at weak to moderate interparticle attraction strengths (mean field studies prohibit large U) for various densities. All our calculations are carried on a two-dimensional lattice of size 32×16 . The reason behind choosing a rectangular lattice instead of a square one, is as follows. The FFLO order parameter undergoes a *one dimensional modulation* with a period that is commensurate with the lattice size[173, 275]. Thus, the choice of rectangular lattice allows us to increase the lattice size along one direction such as to accommodate more periods of the pairing gap.

It is evident from our earlier discussions that magnetic field induces a nontrivial Cooper pairing and hence an unconventional superconductivity when all associated conditions are simultaneously satisfied. In an attempt to get a deeper understanding of this novel superconducting state, we compute few important length scales, viz coherence length, ξ and penetration

depth, λ that characterize a condensate, in the subsequent discussion. Since the modulation of the order parameter is suggestive of a FFLO phase, we first compute Δ_i for the parameter values discussed earlier. The self-consistent Δ_i thus obtained show interesting variations as magnetic field is increased, that is, starting with a uniform order at small h values, the order parameter shows periodic modulation at intermediate fields before vanishing at large fields. The modulating part between a lower and a upper threshold magnetic field values *viz* h_{c_1} and h_{c_2} respectively represents FFLO phase and is central to our discussion. The scenario is schematically shown in Fig. 5.1.

Before we proceed with the discussion on the effect of interparticle attraction, we note that the FFLO phase is not so sensitive to the carrier density. We are able to observe the existence of FFLO at almost all densities except for very low ones where superconductivity itself becomes very weak. To arrive at the above conclusion, we have scanned a large $U - \mu$ parameter space. Thus we have fixed μ at $\mu = -0.5$ such that the density is fixed at a value around quarter filling.

The interaction effects are invoked via a comparison between $|U| = 2.5$ and 4 which yields a broader FFLO phase for the larger $|U|$. For $|U| = 4$, the region intervening two critical fields (h_{c_1} and h_{c_2}) is wider than that for $|U| = 2.5$, thereby establishing the fact that FFLO state is stable for strong interaction strengths. To quote some values for extending support to the above argument, h_{c_1} and h_{c_2} are obtained as 0.35 and 0.55 respectively for $|U| = 2.5$ whereas the same for $|U| = 4$ are 0.9 and 1.88. The periodic modulation of the pairing amplitude presented in Fig. 5.2, suggests that Δ_i has a larger amplitude for stronger U . Also note that with increasing h , the amplitude decreases and along with that more periods are accommodated. The latter can be understood as follows. The rise in the number of broken Cooper pairs ($\Delta_i = 0$) results in increase in the number of nodes in the spatial profile of the order parameter. At still lower values of U , *e.g.* $|U| = 1$, a direct transition from superconducting to normal phase is obtained mainly because of weak superconducting correlations.

A subtle point needs mention in the preceding discussion. The fully self consistent solutions for the BdG equations demand simultaneous self consistencies of Δ_i , $\langle n_{i\uparrow} \rangle$ and $\langle n_{i\downarrow} \rangle$ and thus require more computational time in the vicinities of h_{c_1} and h_{c_2} owing to the existence of different competing solutions. The difficulty can only be partially taken care of by clever choices of the initial guesses for the above quantities.

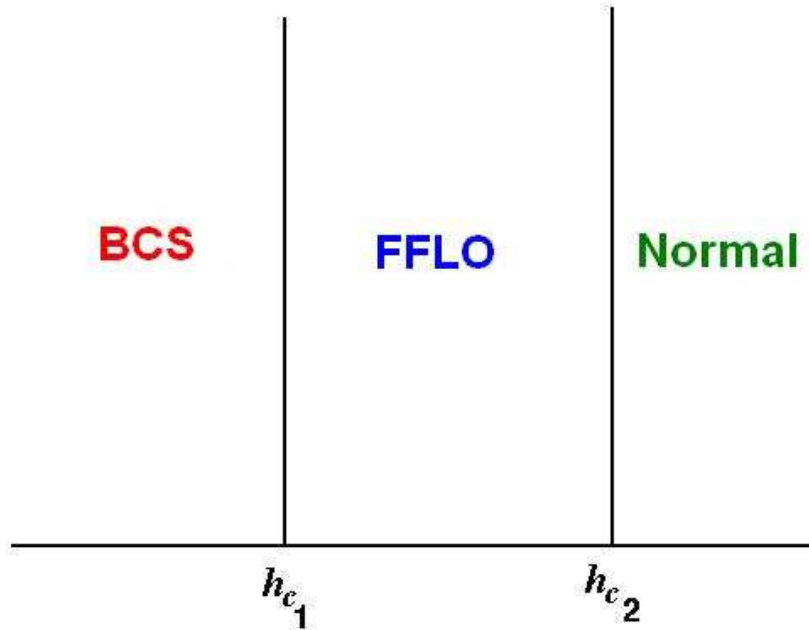


FIGURE 5.1: A schematic representation of the FFLO phase is shown as a function of the magnetic field. This phase, obtained via minimization of the corresponding free energy, is intermediate to a BCS superconductor (homogeneous Δ_i) and a normal phase ($\Delta_i = 0$). The boundaries of the FFLO phase are marked by h_{c1} and h_{c2} , the lower and upper critical magnetic fields respectively. The diagram is valid over a large regime of U - μ parameter space, except at low U and densities where the intermediate space is vanishingly small.

We now focus on the coherence length, ξ which is the separation between the Bloch walls of broken Cooper pairs ($\Delta_i = 0$)[118]. More concretely, ξ is of the order of the wavelength of the order parameter and can be computed from the modulation seen in Δ_i presented in Fig. 5.2. It is seen that ξ undergoes appreciable reduction from a large value (practically infinite corresponding to homogeneous Δ_i in the BCS phase) to a few lattice spacings at the onset of FFLO phase. This result is elucidated in Fig. 5.3 which also shows ξ reducing further within the FFLO phase. We note that the reduction in the magnitude of ξ as h increases is more pronounced for $|U| = 4$ (than for $|U| = 2.5$) which accommodates more periods of the order parameter and hence is characterised by even shorter ξ . A short coherence length makes it easy for the condition, $l \gg \xi$ (l being the electron mean free path) to be met, a requirement laid out for realizing FFLO phase.

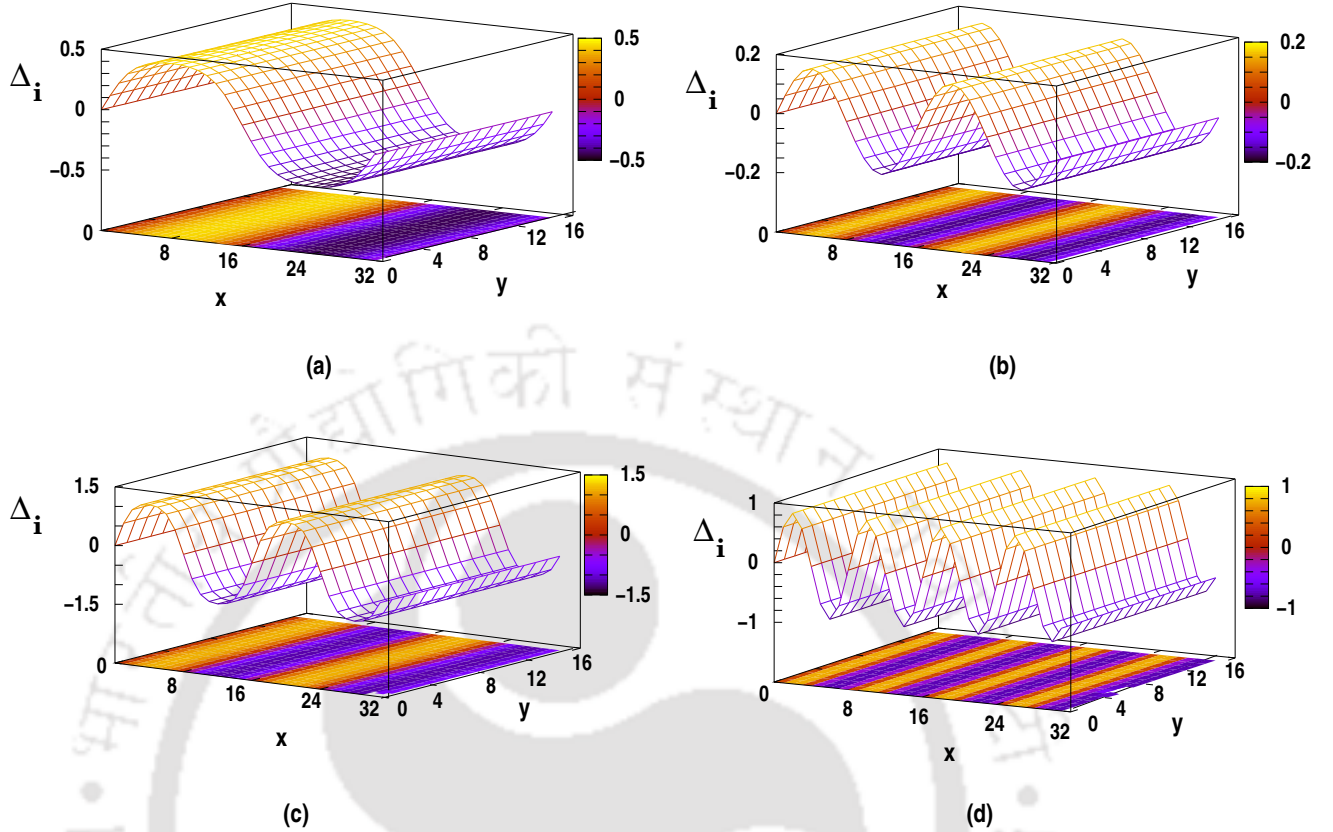
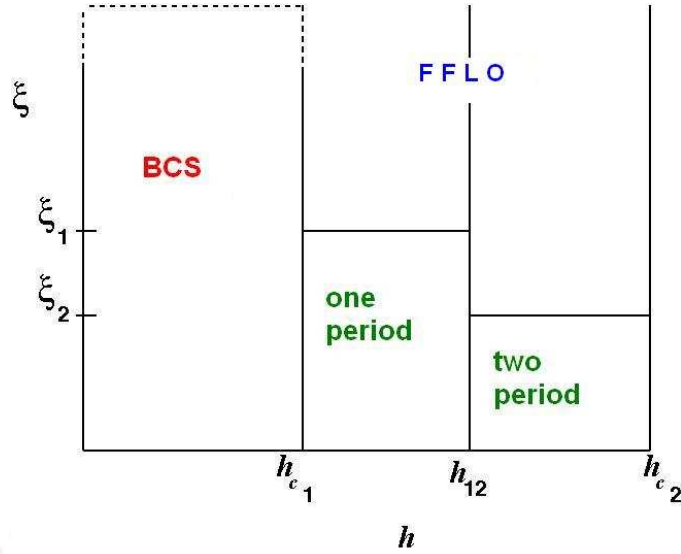


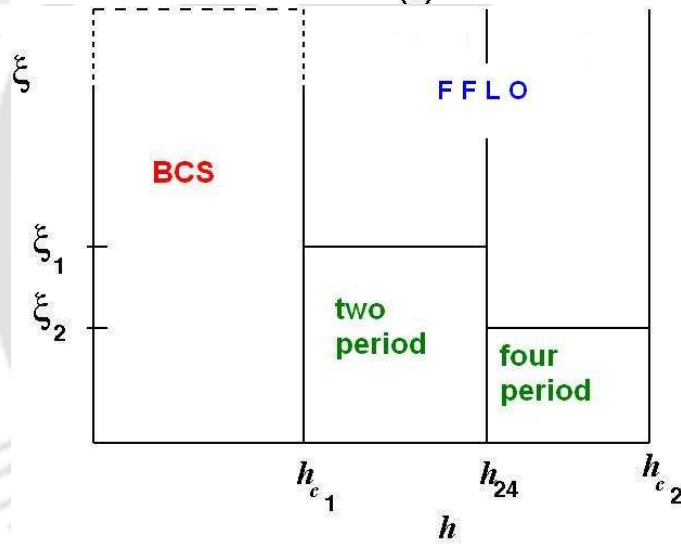
FIGURE 5.2: Local pairing amplitude (in units of t) modulation is shown for $|U| = 2.5$ ((a) and (b)) and $|U| = 4$ ((c) and (d)) for magnetic field values between h_{c1} and h_{c2} . The four figures correspond to $h = 0.35$ (a), 0.5 (b), 0.9 (c) and 1.2 (d). The band filling is chosen to be $\mu = -0.5$ and the system size is $L_x \times L_y = 32 \times 16$ and the same are considered for other figures. All the parameters are in units of t (true for all other figures) and our calculations are done at $T = 0$.

5.3 Summary

We summarize the important results obtained here. The presence of FFLO phase is investigated in the context of a two dimensional superconductor in presence of a magnetic field. The existence of a phase characterised by modulated local pairing amplitude (FFLO) for a number of parameter values, i.e., electronic interaction, $|U|$ and band filling, μ (or particle density) is convincingly demonstrated. Weak to moderate values of U , such as $|U| = 1, 2.5$ and 4 are considered and except for $|U| = 1$, we obtained FFLO phase for the other two representative values with the larger one among them showing brisk modulation (more periods) in the spatial profile of the pairing amplitudes as magnetic field is increased. Thus larger values of the interaction parameter facilitates a realization of the FFLO phase. All of these features are present



(a)



(b)

FIGURE 5.3: The coherence length, ξ (in units of t) measured from the modulation profile of Δ_i (Fig.5.2) is schematically shown for $|U| = 2.5$ (a) and $|U| = 4$ (b) as a function of the magnetic field. In (a), $h_{c1} = 0.35$ marks the onset of a one period modulation (FFLO) with $\xi_1 = 32$. At $h_{12} = 0.4$, a transition from a one period to a two period modulation ($\xi_2 = 16$) is obtained which persists till $h_{c2} = 0.55$. In (b), the FFLO regime commences with a two period modulation at $h_{c1} = 0.9$ with $\xi_1 = 16$ (one period solution does not exist), then crossing over to a four period solution (with $\xi_2 = 8$) at $h_{24} = 1.2$ and continuing till $h_{c2} = 1.88$. Note that ξ is infinitely large (shown by broken line) corresponding to homogeneous Δ_i in the BCS phase.

for a large range of band filling, excepting the ones for which the particle density becomes very small.

The implications of these results to real materials are elucidated in the following manner. The sharp drop of the coherence length, ξ at h_{c1} , marked by the onset of a modulated local pairing amplitude underscores the cleanliness of the sample where the condition $l \gg \xi$, a requirement for FFLO can easily be met. Moreover, ξ further reduces between h_{c1} and h_{c2} , owing to a more dramatic change in the period of modulation making room for the above condition to be satisfied with a greater ease.

The condition mentioned above seems to be satisfied to a large extent in heavy fermion compounds and organic superconductors and thus are considered as suitable candidates to achieve a modulated phase, a theoretical prediction that was made nearly five decades ago. In a simple model for a two dimensional superconductor, we have demonstrated that how some of these conditions are met in presence of a magnetic field rendering support to the candidature of heavy fermion and other systems where FFLO phase may be realized experimentally. Possibly in ultracold atomic superfluids, some of these requirements are met easily and hence demonstrate signatures of the FFLO phase in experiments more convincingly than their fermionic counterparts[274].



Chapter 6

Correlation studies of the FFLO phase in a harmonic trap

6.1 Introduction

Ultracold Fermi gases in optical lattices provide unprecedented advantage of controlled tuning of the interatomic attractive interaction using Feshbach resonance[40, 190]. Superfluidity of attractive fermions is achieved for a wide range of interaction strengths thus a smooth crossover from Bardeen-Cooper-Schreiffer (BCS) phase to the Bose-Einstein condensation (BEC) of bosonic molecules[276, 277] is made accessible. Another noteworthy development in this field, is the achievement of a quantum phase transition from a superfluid to a Mott-insulating (SIT) phase mainly in bosonic systems[194, 195], though there are evidences of SIT in fermionic systems as well[197]. The superfluid phase, where phase coherent atomic wavefunctions spread over entire lattice for low lattice potential strengths, transforms to an insulating phase with exact number of atoms at individual sites, thereby losing phase coherence for higher values of lattice potential. The loss of phase coherence with increasing potential strength is studied in experiments by sudden turn off of the lattice potential thereby allowing free expansion of the atomic wavefunctions[194], where a high contrast interference pattern is obtained in the superfluid regime owing to maximum interference between the delocalized atomic wavefunctions possessing definite relative phases between different lattice sites. As the lattice potential is made larger, the interference maxima is completely lost due

to the complete localization of atomic wavefunctions at a single lattice site and hence giving rise to an insulating phase.

Further, recent experiments have opened up intriguing directions for studying many-body phenomena in the cold atom systems by analyzing some crucial correlations in the strongly correlated gases. For example, the density-density correlations which are the correlations between densities at different lattice positions, are given by the time of flight measurements. It provides important information about the pairing correlations in the Fermi gas and are also very useful in characterizing different phases in optical lattices[278–280]. Other crucial probes are the noise correlation technique which detects pairing correlations in deeply bound molecules[279], the phase-contrast imaging which reveals local correlations between different spin states, imaging of the vortex lattice by stirring which gives information about the macroscopic phase coherence[143] and radio frequency spectroscopy[281, 282] which probes the binding energy of the fermion pairs.

The cold atoms in optical lattices also offers the possibility to explore the novel superfluid phase of imbalanced fermions[141–143, 178]. The imbalance between the different hyperfine states is created by radio-frequency sweeps in experiments. Numerous proposals for the paired state have been suggested for the spin polarized gas. For example, the spatially modulating Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase[24, 25], breached pairing[27], Sarma superfluidity[26] and phase separated phase in which BCS superfluid coexists with an unpaired normal phase[28–30]. The theoretical consensus on the true ground state of a spin polarized Fermi system is yet to be reached[155–157, 283]. However, the oscillations in the density difference between majority and minority spins obtained in experiments, are considered as a potential indication of the FFLO state[284].

Several theoretical studies have been performed to underscore the effect of dimensionality on the exotic FFLO phase. In one dimensions, it was argued that the ground state of the homogeneous attractive Fermi gases with unequal spin populations is the one dimensional analogue of the FFLO phase[161]. In trapped environment, the one dimensional gas separates in a two-shell structure, with a FFLO superfluid core surrounded by either a fully paired or a fully polarized phase depending upon the value of the spin polarization[91]. An elaborate study of the scenario in two dimensional systems has yielded many intriguing results[162, 163]. In particular, a quasiclassical analysis in[164] using a Ginzburg-Landau expansion of the free energy in Fourier components of the superconducting order parameter, had shown that the

FFLO transition in two dimensions is continuous at low temperatures. In a separate study of a two dimensional two-component atomic Fermi gas with population and mass imbalance, it was argued that the normal and homogeneous balanced superfluid phases are separated by an inhomogeneous FFLO-like phase[165]. The study of FFLO phase in three dimensional systems[156, 166], have predicted a narrow region of FFLO phase in the phase diagram as compared to one and two dimensional cases. In another work by Nandini *et al.*[285], the stability of the LO phase in a three dimensional lattice system has been compared and contrasted with the continuum case in presence of a harmonic confinement.

The FFLO is an exotic superfluid characterized by a finite momentum Cooper pairing that yields a spatially modulating order parameter. The search for the FFLO state in different crystal lattices spans over more than five decades now since its discovery. The elusive nature of the phase is attributed to several necessary conditions which needs to be satisfied simultaneously for it to be realized in experiments. One of the conditions being that system should be ultra-clean since the FFLO state is readily destroyed by impurities. Since in atomic systems, the 'cleanliness' condition is readily achieved, they are considered as potential candidates for realization of the FFLO phase. Thus the issue demands a thorough study as the evidences supporting the phase is only cursory.

In this work, we study the occurrence of FFLO phase in a two dimensional spin polarized *s*-wave superconductor with underlying harmonic confinement using Bogoliubov de Gennes method. The superconducting order parameter thus obtained undergoes sign change along the radial direction for moderate values of spin imbalance (small imbalance yields a unpolarized phase and a fully polarized state stabilizes at larger imbalance). The core of the trapped gas is an inhomogeneous superfluid arising due to pairing between equal spin species, while the FFLO phase exists only in the edges of the trapped Fermi gas. Signatures of such **radial FFLO** in presence of confinement, has been observed earlier[179, 180, 186–189]. An interesting situation emerges upon switching off the external confinement when the spatially modulating superconducting order parameter with one dimensional periodic modulation extends over the entire lattice with the periodicity wave vector proportional to density imbalance of the participating species. We call this **extended FFLO** as opposed to a **radial FFLO** for the trapped case. Other correlations e.g. the pair-pair, density-density correlations and the fluctuation in the local number density are computed to highlight the contrast between the trapped case and when the trap is released.

6.2 Results and Discussion

As discussed in chapter 2, we resort to an attractive version of the two-dimensional Hubbard model in presence of a constant Zeeman field, h and a harmonic trapping potential at site r_i , V_i written as,

$$\mathcal{H} = -t \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) - |U| \sum_i (n_{i\uparrow} - \frac{1}{2}) (n_{i\downarrow} - \frac{1}{2}) + \sum_{i, \sigma} (V_i - \mu + \sigma h) n_{i\sigma} \quad (6.1)$$

μ denotes the chemical potential, t is the hopping matrix element between the nearest neighbours of a two dimensional square lattice. The creation (annihilation) operator for fermionic electrons corresponding to spin σ is $c_{i\sigma}^\dagger$ ($c_{i\sigma}$). The excess of one species of electrons (say with spin- $\uparrow$) over another is controlled by the magnetic field h (or equivalently an effective chemical potential, $\mu' = \sigma h - \mu$). V_i is assumed to be of the form,

$$V_i = V_0 (r_i - r_0)^2 \quad (6.2)$$

where V_0 is the strength of the trapping potential and r_0 is the position where the center of the trap lies and is located at the center of the lattice. Thus the potential is minimum (deepest) at the center of the lattice and is maximum (shallow) at the edges. All of U , h , μ and V_0 are expressed in units of hopping strength, t whose scale is set by the lattice recoil energy in ultracold atomic gas experiments and has typically a value of about 3 kHz or 10^{-11} eV. A mean field decoupling of the interaction term in Eq. (6.1) yields the effective Hamiltonian of the form,

$$\mathcal{H}_{eff} = \sum_{ij, \sigma} \mathcal{H}_{ij\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) + \sum_i [\Delta_i c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger - \Delta_i^* c_{i\uparrow} c_{i\downarrow}] \quad (6.3)$$

here $\Delta_i = -|U| \langle c_{i\downarrow} c_{i\uparrow} \rangle$ is the gap parameter for the fermionic superfluid. $\mathcal{H}_{ij\sigma} = -t \delta_{i\pm 1j} + (V_i - \mu - U \delta n_{i\bar{\sigma}} + \sigma h) \delta_{ij}$ where $\delta n_{i\bar{\sigma}} = n_{i\bar{\sigma}} - 1/2$ with $\langle n_{i\sigma} \rangle = \langle c_{i\sigma}^\dagger c_{i\sigma} \rangle$ and $\bar{\sigma} = -\sigma$.

Eq. (6.3) is hence diagonalized using Bogoliubov transformation which yields,

$$\begin{pmatrix} \mathcal{H}_{ij\sigma} & \hat{\Delta}_i \\ \hat{\Delta}_i^* & -\mathcal{H}_{ij\bar{\sigma}}^* \end{pmatrix} \begin{pmatrix} u_n(\mathbf{r}_i) \\ v_n(\mathbf{r}_i) \end{pmatrix} = E_n \begin{pmatrix} u_n(\mathbf{r}_i) \\ v_n(\mathbf{r}_i) \end{pmatrix} \quad (6.4)$$

where $u_n(\mathbf{r}_i)$ and $v_n(\mathbf{r}_i)$ are the BdG eigenvectors satisfying $\sum_n [u_n^2(\mathbf{r}_i) + v_n^2(\mathbf{r}_i)] = 1$ for all $\mathbf{r}_i$ and E_n are the eigenvalues.

The gap parameter and density are obtained self-consistently from Eqns. (5.5) and (5.6) at each lattice site. It may be noted that a number of self-consistent solutions may exist for the gap parameter, Δ_i corresponding to one set of parameters with different initial guesses. The winner among these will be decided by computing the free energies, $\mathcal{F}$ (with respect to the free energy of vacuum at zero temperature) as discussed earlier.

We perform our studies for an inter-particle attraction strength $|U| = 2.5t$ which may be considered to be weak, and hence suitable as we propose a BCS superfluid as a starting point. It should be noted that further lower values of $|U|$ yield a vanishing gap parameter for any reasonable value of density. All quantities are calculated at zero temperature and for two values of polarization, $P (= \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow})$, viz. $P = 0, 0.10$ (with trap) and $P = 0, 0.13$ (without trap) corresponding to the magnetic field values, $h = 0.1t$ and $h = 0.4t$ for each of the cases. It is important to note that, since the spin imbalance is created by the Zeeman field, h (see Eq. (6.1)), we compute different quantities for fixed h values, viz the ones mentioned above. However, when results are quoted, the unpolarized and the polarized cases are distinguished by P , a quantity that can be controlled experimentally. Further, the value of polarization is different for the trapped case than the one corresponding to no trap, which is obvious as the trap has an additional effect on the imbalance between different spin species at a fixed value of h . We have chosen density n to be 0.66 and the strength of confining potential V_0 is $0.016t$. We have considered other values for density, ranging from moderate to large (very small densities do not yield a stable superfluid phase) and different interaction strengths, U . However, we have not noted any qualitative change in behaviour of the correlation functions for these choices of density and interaction strength. We have also studied the correlations for other choices of trapping strength, V_0 . For trapping strengths below $V_0 = 0.016t$, the correlations are unaffected by the trapping because of its small magnitude whereas for stronger trapping strengths, the correlations rapidly decay because of strong localization of the electrons. Without trap, we have considered a two dimensional lattice of size 32×16 with periodic boundary condition. The reason for considering a rectangular lattice ($L_x \neq L_y$) is the one-dimensional nature of the modulation of gap parameter[173] (so a larger lattice length in the direction of modulation) and together with economizing the computational time. With trap, the dimension of the lattice is chosen to be 24×24 with open boundary conditions and the trap center is located at the center of the lattice.

To investigate the effect of harmonic confinement on a spin polarized gas, we compute various correlation functions in real space. The correlations investigated here are the gap parameter, magnetization, pair-pair and density-density correlations for two different values of population imbalance but fixed trap depth ($V_0 = 0.016t$). The external trapping is then switched off and the nature of the spin polarized phase (FFLO) in a free (no trap) environment is analyzed in details.

We begin our discussion with the results on gap parameter, Δ_i as shown in Fig. 6.1. It may be noted that for $P = 0$ and $V_0 = 0.016t$, Δ_i dips close to the trap center which is attributed to an insulating state arising because of (almost) complete occupancy of the sites near trap center at high filling ($n = 0.66$ here, see Fig. 6.1(a)). Δ_i attains a maximum value at intermediate distances from the trap center in an annular ring around the trap center and vanishes at large distances where atomic density is expected to be negligibly small. We call this phase as 'unpolarized' ($P = 0, V_0 = 0.016t$) phase. When the external trapping is turned off, a homogeneous Δ_i (as expected for a BCS superconductor with $P = 0, V_0 = 0$) is obtained as shown in Fig. 6.1(b).

In order to feed the contrast between free and trapped cases with regard to population imbalance being zero and finite, we analyze the behaviour of the local magnetization, m_i ($= \langle n_{i\uparrow} \rangle - \langle n_{i\downarrow} \rangle$) shown in Fig. 6.2. m_i for the BCS phase, is zero understandably (being non-magnetic due to lack of unpaired particles) across the lattice (see Fig. 6.2(a) and (b)). The magnetization profile in the presence of trap shows a minimum at the center of trap and attains finite value around the ring like nodal line where gap parameter undergoes a sign change (see Fig. 6.2(c)). The behaviour is more clearly captured in the two dimensional projection of m_i where the value of m_i is maximum around a ring corresponding to the nodal line in case of Δ_i . Trapping effects thus lead to phase separation, in which a small number of particles are squeezed into the inner core of the harmonic trap due to pair formation while the excess unpaired (majority) carriers are pushed to outside of the core. This explains the existence of the FFLO phase only at the edges of the trap. When the trap is released, m_i modulates across the entire lattice thereby confirming the onset of **extended FFLO** correlations (Fig. 6.2(d)). Large values of magnetization are obtained at nodal lines with broken pairs, whereas lattice sites with finite Δ_i correspond to weak magnetization.

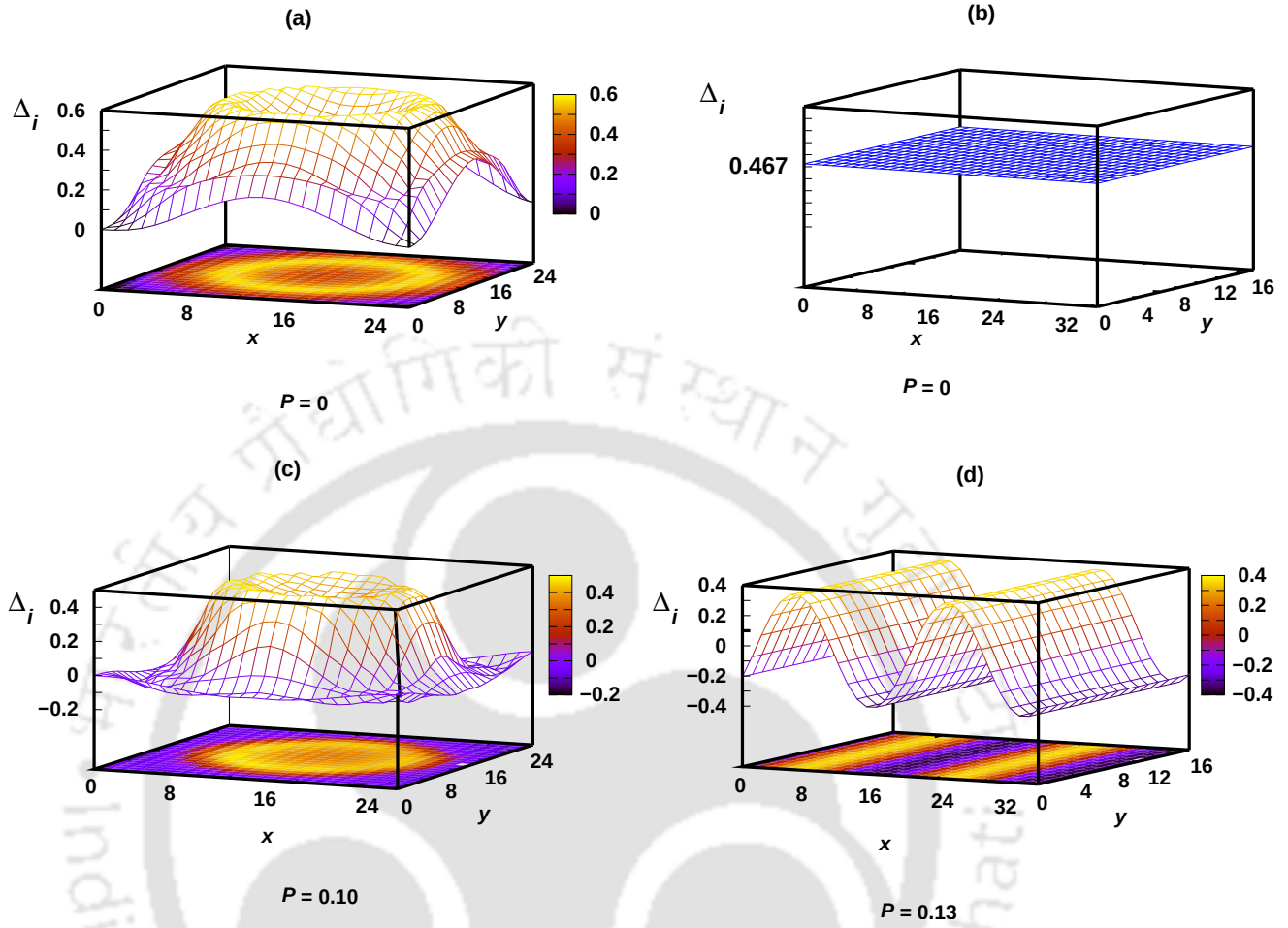


FIGURE 6.1: Gap parameter, Δ_i (in units of t) in unpolarized (a), BCS (b), **radial FFLO** (c) and **extended FFLO** (d) phases are shown for $|U| = 2.5t$ and $n = 0.66$. Figs. (a) and (c) are for cases in presence of trap with trapping strength $V_0 = 0.016t$ while (b) and (d) are for no trap. The system size is 32×16 in the absence of trap and 24×24 when the trapping potential is present and are same for all our results. To understand why the polarization values are different i.e. $P = 0.1$ for (c) and $P = 0.13$ for (d), see discussion in text. Same is true for rest of the figures in this chapter.

We now focus on the pair-pair and density-density correlation functions. The pair-pair correlation function is defined as,

$$\begin{aligned} C_{ij} &= \langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_{j\uparrow} c_{j\downarrow} \rangle \\ &= \langle \Delta_i^\dagger \Delta_j \rangle \end{aligned} \quad (6.5)$$

where the angular bracket denotes expectation value taken over the BdG eigenstates and symbols having usual meaning. Since it quantifies the correlation between two distinct onsite

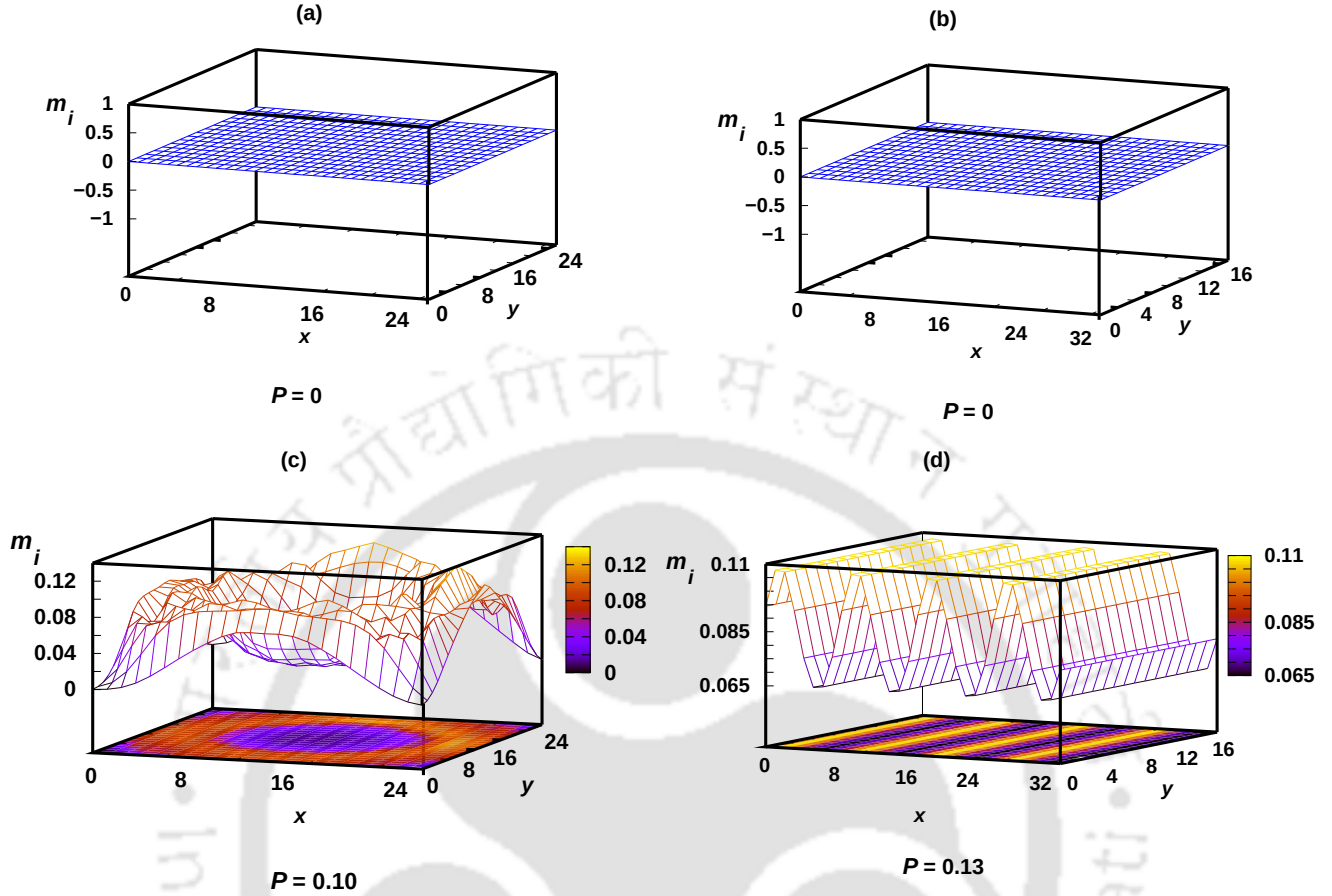


FIGURE 6.2: Local magnetization, m_i (in units of t) is shown in unpolarized (a), BCS (b), **radial FFLO** (c) and **extended FFLO** (d) phases both in the absence and presence of the confining potential for $|U| = 2.5t$ and $n = 0.66$. Figs. (a) and (c) are for cases in presence of trap with trapping strength $V_0 = 0.016t$ while (b) and (d) are for no trap.

(s-wave) pairs at different positions, it bears information about the nature of the condensate.

The real space scan of C_{ij} taken along the length of the lattice is presented in Fig. 6.3(a) and (b). Note that C_{ij} (also K_{ij} , d_i and $(\langle \delta n_i \rangle)^2$ discussed later) has been shown across the entire length for the trapped case where open boundary condition is used, whereas because of the presence of periodic boundary condition in absence of trap, they are presented upto half the length of the lattice. C_{ij} in the unpolarized phase ($P = 0$) is higher than the value in the FFLO phase both in the absence ($P = 0.13$) and presence ($P = 0.10$) of trap. This supports weakening of the superconducting correlations as spin imbalance is enhanced which is also evident from Fig. 6.1. The qualitative behaviour of C_{ij} is more or less same for both unpolarized and **radial FFLO** in presence of harmonic confinement. C_{ij} attains maximum at distances far away from the center and drops at the center which is in agreement with the

behaviour of Δ_i presented in Figs. 6.1(a) and (c). This conveys that trapping effects suppresses the distinction between zero and finite values of spin polarization. A close observation of the behaviour of C_{ij} however reveals few important differences between the two cases. For example, the drop in C_{ij} is more in the case of the unpolarized phase than the **radial FFLO** since the insulating phase (at the trap center) is stabilized in the presence of equal number of the participating species which forms a pair. Also, note the *dip* in C_{ij} at the trap edges in the **radial FFLO** phase which occurs because of the presence of the ring-like nodal line in Δ_i and is absent in the unpolarized phase. The **extended FFLO** phase can be readily distinguished from the BCS phase in the absence of trap by a spatially varying C_{ij} which arises because of the unequal distribution of pairs separated by array of Bloch type magnetic walls formed by broken Cooper pairs with polarized spins. We thus observe that the trap suppresses the distinction between the unpolarized and FFLO.

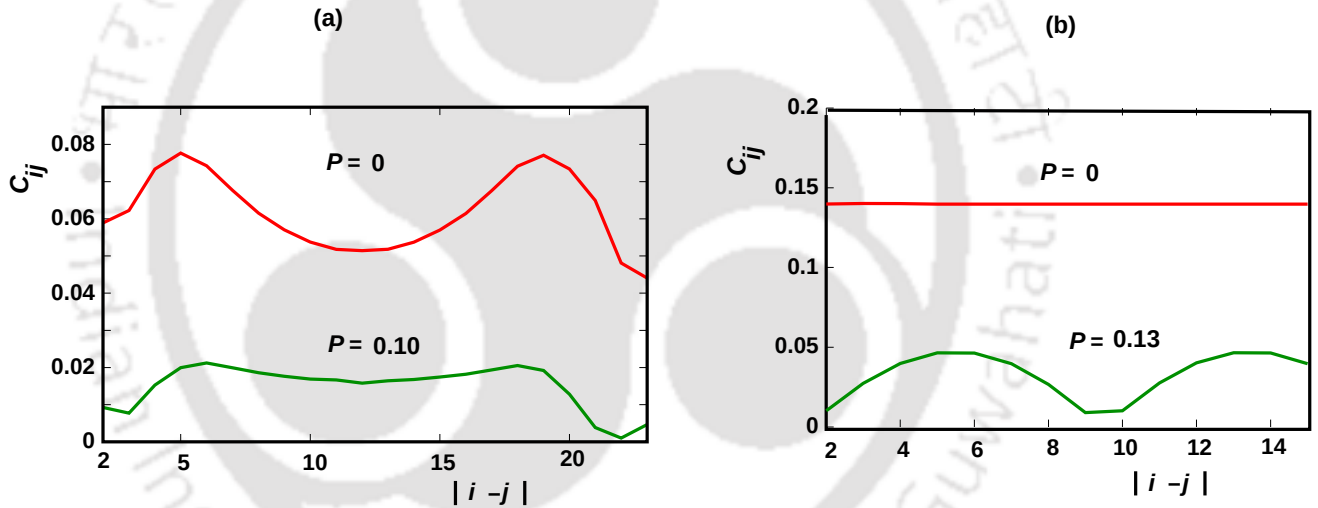


FIGURE 6.3: Pair-pair correlation function, C_{ij} (in units of t) is shown across the lattice for zero and finite spin polarization values with trap (a) and compared with the case when the trapping effects are turned off (b). C_{ij} is plotted across entire length for the trapped case where open boundary condition is invoked whereas in the no trap case, it is shown till half the lattice length because of periodic boundary condition. Here $|U| = 2.5t$ and $n = 0.66$.

We now analyze the density-density correlations. We begin with the off-diagonal density-density correlations given by,

$$\begin{aligned}
 K_{ij} &= \langle (n_{i\uparrow} + n_{i\downarrow})(n_{j\uparrow} + n_{j\downarrow}) \rangle \\
 &= \langle n_{i\uparrow}n_{j\uparrow} \rangle + \langle n_{i\uparrow}n_{j\downarrow} \rangle + \langle n_{i\downarrow}n_{j\uparrow} \rangle + \langle n_{i\downarrow}n_{j\downarrow} \rangle
 \end{aligned}
 \tag{6.6}$$

In presence of the trap, there is no significant difference between the behaviour of K_{ij} in the unpolarized and **radial FFLO** phases (see Fig. 6.4(a)). The reason behind K_{ij} showing a hump-like behaviour irrespective of the phase being unpolarized or **radial FFLO**, is as follows. The occupancy of the sites is maximum at the center of the trap as the underlying trapping potential is minimum (deep) at the center. However, it drops at the edges where the trapping potential is high (shallow), thereby confirming the domination of the trapping potential which washes away any distinction between the cases of zero and finite polarization. Upon switching off the external trapping, the **extended FFLO** correlations get enhanced and thus can be clearly distinguished from the BCS as shown in Fig. 6.4(b). While K_{ij} remains constant across the lattice in BCS, it undergoes modulation for the **extended FFLO** phase. The spatial inhomogeneity in K_{ij} for the FFLO is attributed to the unequal distribution of density across the lattice.

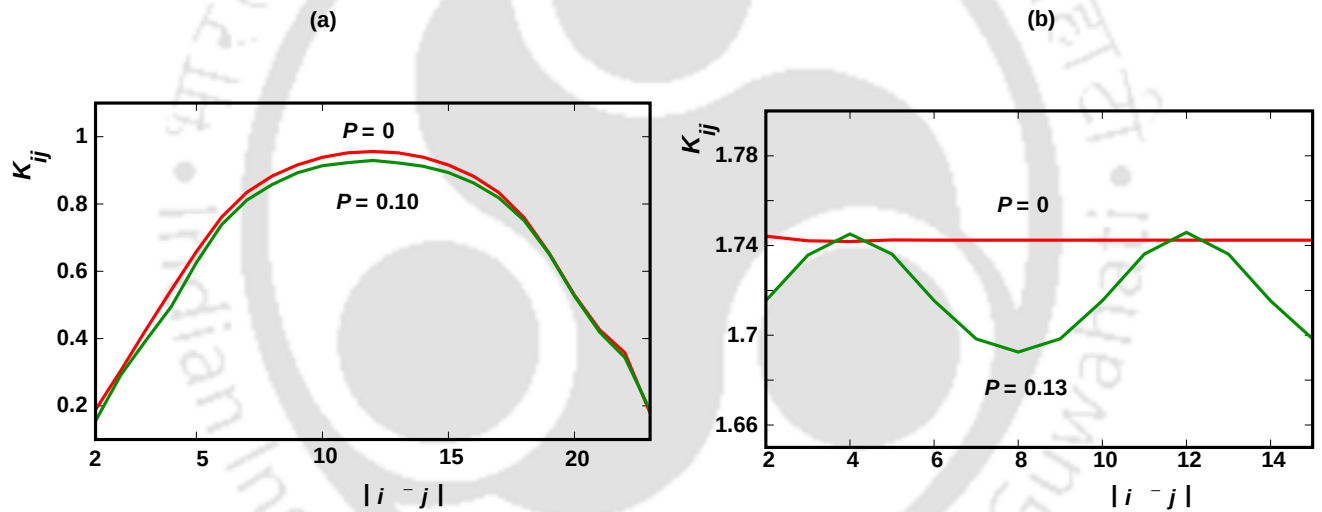


FIGURE 6.4: Off diagonal density-density correlation function K_{ij} (in units of t) is shown across the lattice for zero and finite spin polarization values with trap (a) and without trap (b). The trap suppresses the distinction in (a) while it is significant in (b). K_{ij} is plotted across entire length for the trapped case where open boundary condition is invoked whereas in the no trap case, it is shown till half the lattice length because of periodic boundary condition.

Here $|U| = 2.5t$ and $n = 0.66$.

The onsite density-density correlations which provide information about the correlations between electrons at the same site and hence the local double occupancy, is given by,

$$d_i = \langle n_{i\uparrow} n_{i\downarrow} \rangle \quad (6.7)$$

This is infact the expectation value of the interaction energy term (scaled by $|U|$). d_i for the unpolarized and **radial FFLO** phases exhibits similar hump-like behaviour arising because of the trap (as in Fig. 6.4(a)) and hence not included here. In the absence of trap, the uniform distribution of the pairs yields a constant d_i in the BCS regime whereas coexistence of pairs with unpaired electrons result in a spatially modulating d_i in the **extended FFLO** phase (see Fig. 6.5).

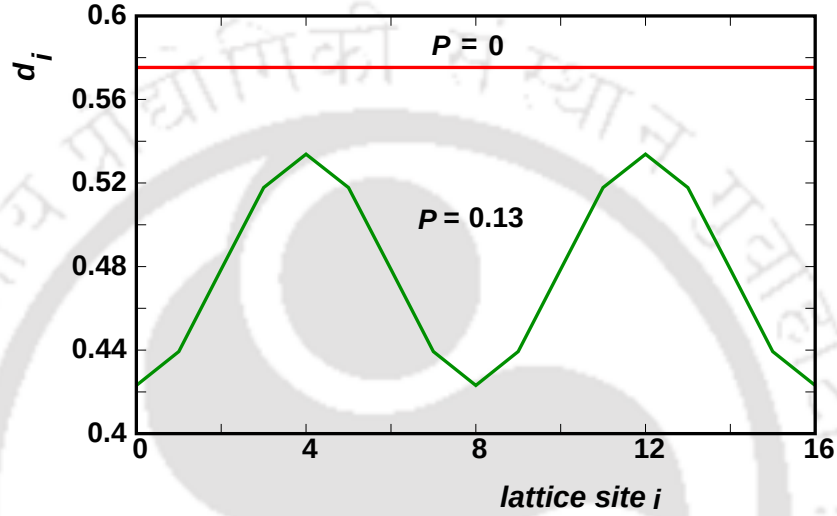


FIGURE 6.5: Onsite density-density correlation function (in units of t) d_i is shown across the lattice in BCS and **extended FFLO** phases without trap. Here $|U| = 2.5t$ and $n = 0.66$.

Finally, we investigate the effect of trapping on the fluctuation in local number density defined as,

$$(\delta n_i)^2 = \langle n_i^2 \rangle - \langle n_i \rangle^2 \quad (6.8)$$

where $n_i = (n_{i\uparrow} + n_{i\downarrow})$. It is clear from Fig. 6.6 that trapping reduces the fluctuation in local number density. The low $(\delta n_i)^2$ in presence of trap is attributed to the confinement of the atomic density near trap center which results in fixed number of particles and hence definite occupancy of lattice sites. The scenario is different in the absence of trap where all sites are equally probable to be unoccupied, double occupied, singly occupied with a up-spin or singly occupied with a down-spin, thereby resulting in a rise in density fluctuations.

We now analyze the fluctuation in local density in unpolarized and **radial FFLO** phases in presence of trap (see Fig. 6.6(a)). It may be noted that the fluctuations are maximum at the trap center for both the phases. The trap center being mostly occupied by pairs results in

higher values of onsite density correlations between different spin states. The onsite correlations between identical spin states are also large because of Pauli's exclusion principle. Both these quantities together contribute significantly to $\langle n_i^2 \rangle$ (in Eq. (6.8)) leading to large density fluctuations. The fluctuations in the **radial FFLO** phase (near trap center) are however slightly smaller compared to the unpolarized phase which is mainly caused by the population imbalance which results in lower onsite density correlations. Further, the unpaired (majority) electrons which are pushed outwards by the trap, cause larger density fluctuations at the trap edges for **radial FFLO** than the unpolarized phase. As the trapping potential is switched off, the density fluctuation becomes homogeneous in the BCS phase since all sites are equally probable to be singly occupied, doubly occupied or unoccupied (Fig. 6.6(b)). The scenario changes in the presence of population imbalance where $(\delta n_i)^2$ undergoes spatial modulation owing to the presence of sites (corresponding to the nodal points) which are no more doubly occupied thereby resulting in drop in density fluctuations at those sites.

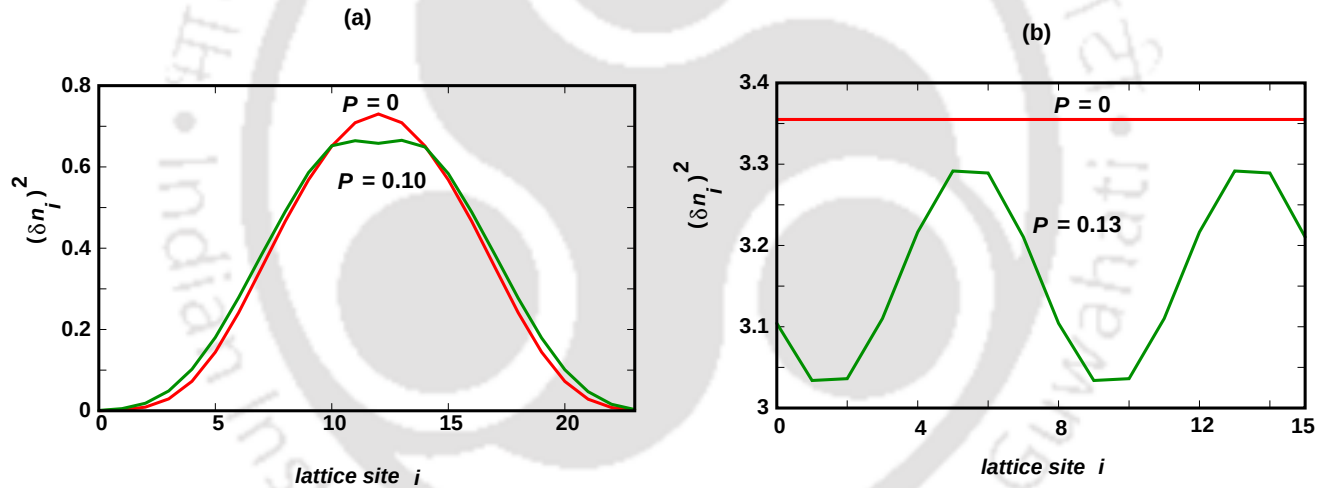


FIGURE 6.6: Local density fluctuations, $(\delta n_i)^2$ (in units of t) is shown with trap (a) and without trap (b). Again trap almost washes away the distinction between different polarization values.

Here $|U| = 2.5t$ and $n = 0.66$.

It is important to realize that fluctuations in a particular quantity (here density) is related to the temperature and susceptibility or response (here isothermal compressibility) of the system via fluctuation dissipation theorem[286]. Thus the density fluctuations provide useful knowledge on response of the system to driving parameters, *e.g.* polarization and trapping potential, but more crucially, yield measurement of temperature, which is usually a difficult quantity to compute for degenerate Fermi gases.

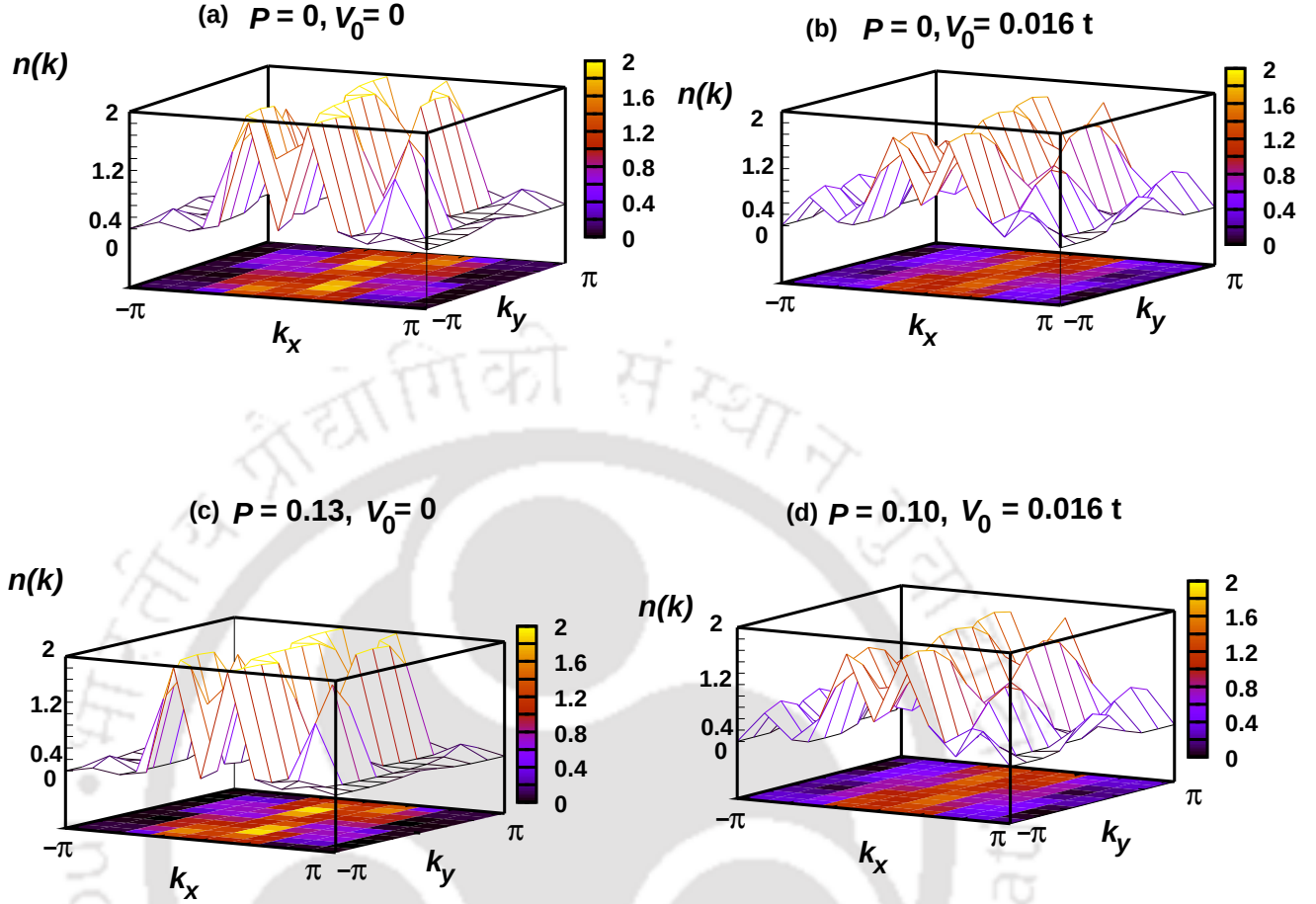


FIGURE 6.7: Momentum distribution, $n_{\mathbf{k}}$ (in units of t) is shown for (a) $P = 0, V_0 = 0$, (b) $P = 0, V_0 = 0.016t$, (c) $P = 0.13, V_0 = 0$ and (d) $P = 0.1, V_0 = 0.016t$. Note that the population imbalance has (nearly) no effect on $n_{\mathbf{k}}$, i.e. as one compares (a) with (c) and (b) with (d). However, spectral weights are suppressed as trapping effects are invoked, keeping the value of P same (compare between (a) and (b) ($P = 0$) and between (c) and (d) ($P \neq 0$)).

To elucidate a comprehensive role of the trap, we have computed the momentum distribution function given by, $n_{\mathbf{k}} = \sum_{\sigma} \langle c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} \rangle$ (fourier transform of $\langle c_{i\sigma}^{\dagger} c_{i\sigma} \rangle$) for the homogeneous (BCS) and spin polarized (FFLO) cases in presence and absence of trap effects. In time of flight experiments, the residual velocity (or equivalently momentum) distribution of the constituent particles are examined after long interval of time, which yield transport properties of the condensate. We present $n_{\mathbf{k}}$ plots for $P = 0$ and $P \neq 0$ for both $V_0 = 0$ and $V_0 = 0.016t$ (see Fig. 6.7). One may note nearly identical features for both zero and finite polarization values when the trapping potential is zero. Even for nonzero trapping effects, the corresponding plots have very similar features. Thus the population imbalance (caused by the magnetic field h) does not affect the momentum distribution profile. However, suppressed spectral weights are

noted when trapping effects are introduced, keeping the spin polarization same (true for both $P = 0$ and $P \neq 0$). This implies that the trap has larger influence on the superfluid properties as is also evident from the study of correlation functions discussed above.

6.3 Summary

We have investigated a spin imbalanced s-wave superconductor described by an attractive Hubbard model on a two-dimensional lattice in presence of a harmonic confinement. The main aim of this work was centered around understanding the nature of the superfluid state when the trap is released, a tool usually employed in spectroscopic studies. We observe that the nature of the superconducting order parameter and magnetization change both in equal spin and spin imbalanced cases as the trap effects are switched off. Interestingly for a finite spin polarization, the superconducting gap from being radially modulated (we call it **radial FFLO**) in presence of the trap, changes to a modulation profile that extends throughout the lattice (**extended FFLO**). Further, we propose that in order to distinguish between the states characterized by zero and finite spin polarization values, it is important to have the trap effects to be minimum, as the physical and experimentally accessible quantities, such as pair-pair, density-density (double occupancy) correlations and local number density fluctuations comprehensively show that trap effects suppress the distinction, while the free case (no trap) demonstrates a significant difference in the nature of above correlations that should be detected in experiments.

Chapter 7

Signatures of SIT in presence of confinement

7.1 Introduction

In the previous chapter, we discussed that the ultracold atoms in optical lattices can be employed to study models of strongly correlated fermions in which the strength of the collisional interaction between the spin-up and spin-down atomic states are controlled using Feshbach resonance[40, 190]. The periodic potential to which the atoms are exposed in an optical lattice, is created by superimposing mutually perpendicular laser standing waves. The controlled tuning of the interaction has been used to study fermionic superfluidity in the strongly interacting regime. The interest in this field is further intensified by various studies which have established superfluidity in ultracold fermionic atoms with imbalanced spin state populations. Further, starting with a superfluid state, it is possible to go over to an insulating phase continuously which has been an intensely studied problem in condensed matter physics.

The signatures of superfluidity are obtained in the form of fermionic pairs and vortices in rotating atomic clouds over a broad range of population imbalances[141]. Partridge *et al.*[142] have reported quantum phase transition in a strongly interacting Fermi gas with imbalanced spin populations. The study claims evidence for a homogeneous superfluid state with unequal densities below a critical population imbalance and a phase separated state with a core of superfluid pairs surrounded by a shell of excess spin-up atoms above a critical population

imbalance. The transition from the superfluid to the normal state in an imbalanced Fermi gas has been also seen by Zwierlein *et al.*[143] where the fermion pair condensates and the normal state were detected through sudden changes in the shape of clouds of fermionic atoms as seen by lowering the trap depth below a critical value in time of flight measurements.

Various exotic phases emerge in spin-imbalanced gases because of Fermi energy mismatch between different participating species of atoms *e.g.* Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase[24, 25], the Sarma[26], breached pair phase[27] and a mixed phase in which BCS superfluid coexists with an unpaired normal phase[28–30]. However, the experimental realization of these phases is still inconclusive because of the difficulty in creating magnetized superconductors. Of special importance among the above are the FFLO phases which are characterized by pairing between two spin-split Fermi surfaces, with the Cooper pairs having a finite center-of-mass momentum and the superconducting order parameter exhibiting spatial modulation. Serious attempts have been made in different crystal lattice systems to realize FFLO phase in experiments. Even theoretical studies reveal that the spatial extent of the FFLO phase in the phase diagram (defined by temperature and magnetic field) is extremely narrow as this phase stabilizes only when the orbital pair breaking effects are suppressed as compared to the Pauli paramagnetic effects, while at stronger fields, the former starts dominating [287], thereby making it difficult to observe such a phase.

Keeping the preceding discussion in mind, we wish to examine a transition from a superconductor to an insulator in a trapped spin-imbalanced Fermi gas in two dimensions described by an attractive Hubbard model. The trapping potential is taken to be harmonic with a minimum at the center of the lattice, which gradually becomes shallow at the edges and is characterized by a single parameter V_0 (> 0). Though V_0 can be expressed in terms of parameters of the optical lattice potential and other parameters such as energy scales of the Hamiltonian and s-wave scattering length etc[288, 289], we have not made any such specific attempts and V_0 is considered as an independent tuning parameter in our work. Our objective is to examine how the imbalanced gas of Fermions respond to the confining potential as the trap depth is tuned.

In this work, the signature of a transition from a superfluid to an insulator is seen via a non-monotonic behaviour of the spectral gap, which initially shows a decrease with increasing V_0 , while beyond a certain value, it starts increasing. The order parameter that characterizes the superfluid phase however vanishes with increasing V_0 . The two results collectively indicate

onset of a gaped phase that has no long range order. The transition to an insulating state scenario is further nourished by an increase in average onsite potential energy and a decrease in average kinetic energy which are suggestive of localization effects. Additional support of the confinement effects are provided via real space profiles of density and double occupancy, and finally a drastic drop in participation ratio confirms the localization of the trapped eigenstates to individual lattice sites.

7.2 Results and Discussion

In crystal lattices, where electrons are the main carriers that contribute to transport properties of materials, obtaining a model Hamiltonian that describes the physical properties satisfactorily is a difficult task owing to a highly complicated band structure. However a gaseous system of fermionic atoms in a confining potential is a much neater realization of the simplest model that incorporates strong correlations between atoms at short distances. We use an attractive version of the two-dimensional Hubbard model subjected to an external trapping potential as discussed in the previous chapter. The mean field decoupling of the Hamiltonian yields the effective Hamiltonian which is then diagonalized using Bogoliubov transformation to obtain the eigensolutions.

The gap parameter and density in terms of the eigenvectors $u_n(\mathbf{r}_i)$ and $v_n(\mathbf{r}_i)$ at a temperature T are obtained self-consistently from Eq. (5.5) and Eq. (5.6) at each lattice site.

We comment on the choice of parameters. The occurrence of SIT has been investigated for various values for density, ranging from moderate to large (very small densities do not yield a stable superfluid phase) and different interaction strengths, U . We observe that the results are qualitatively unaltered for these different choices. As our starting point is a weak coupling superfluid, we choose an (attractive) interparticle interaction that is moderately weak, viz. $|U| = 2.5t$ and density, n (defined as the ratio between number of electrons and the total number of sites) to be $2/3$ or 0.66 . Further, the Zeeman field that creates the imbalance between the up- and down-spins is maintained at a value $h = 0.4t$. The rationale behind using such a value is that to have a spin polarization $P \left(= \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow} \right)$ where $N_\uparrow$ and $N_\downarrow$ are the densities of up- and down-spin particles respectively) that corresponds to FFLO phase for $V_0 = 0$. All quantities are calculated at zero temperature, and hence the Fermi function has been taken as

unity. The dimension of the lattice is chosen to be 24×24 with open boundary conditions and the trap center is located at the center of the lattice.

To establish our claim of SIT as a function of V_0 , we have computed various physical quantities e.g. the spectral gap, mobility of the carriers, onsite interaction energy, local density distribution, double occupancy and the participation ratio. In the subsequent discussion, we present results in the above order.

Before we proceed with the issue of SIT, we wish to brief on the nature of the superconducting state which subsequently undergoes a transition to an insulating state at large trap depths. Thus we compute the gap parameter, Δ_i by solving Eq. (5.5) and Eq. (5.6) self-consistently, for a spin imbalanced gas where the difference in the population of spin up- and down-species is caused by h ($= 0.4t$). Δ_i thus obtained (Fig. 7.1(a)) undergoes modulation along one direction (x -axis) of the lattice and hence confirms the phase to be the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase which is characterized by a spatially modulating gap parameter.

A subtle point needs mention in the preceding discussion. The fully self consistent solutions for the BdG equations demand simultaneous self consistencies of Δ_i , $\langle n_{i\uparrow} \rangle$ and $\langle n_{i\downarrow} \rangle$ and thus require more computational time in the vicinities of the lower and upper values of critical magnetic fields, h_{c1} and h_{c2} respectively owing to the existence of different competing solutions. The difficulty can only be partially taken care of by clever choices of the initial guesses for the above quantities. We have used both uniform and modulating solutions as initial guesses for solving Eqns. Eq. (5.5) and Eq. (5.6) numerically for a given set of parameters defined by U , n and h . For some parameter values, both the initial guesses converge to the same self consistent solution i.e. to uniform (for BCS) or modulating (for FFLO). However at other values of the parameters, different guesses yield different solutions, and the favoured solution is the one that corresponds to lower free energy.

To comment on the effect of trapping on such a phase, we present Δ_i for the same value of h but in the presence of a harmonic trap of strength $V_0 = 0.016t$ in Fig. 7.1(b). It may be noted that Δ_i is maximum around the core of the trap but undergoes a sign change from the trap center thereby confirming the presence of the FFLO phase around the edges. As the trapping strength is made stronger, Δ_i vanishes because of extreme confinement leading to loss of phase coherence between the electrons (the corresponding plots are not shown here).

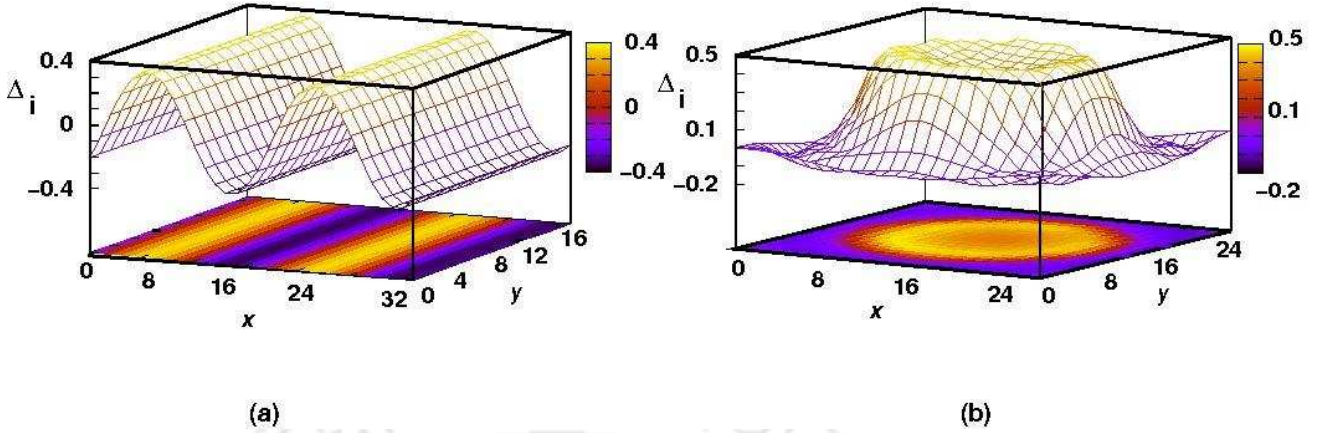


FIGURE 7.1: Gap parameter, Δ_i (in units of t) in the absence (a) and presence (b) of harmonic confinement of strength $V_0 = 0.016t$. Here $|U| = 2.5t$, density $n = 0.66$ and $h = 0.4t$. The system size is 32×16 in the absence of trap where periodic boundary condition is used and 24×24 when the trapping potential is present and we have used open boundary condition.

An important quantity which provides an estimate of how superconductivity is affected is the spectral gap, E_{gap} which is the difference between the ground state and the lowest lying state of the excitation spectrum obtained from the BdG eigenvalues. E_{gap} thus obtained is plotted in Fig. 7.2 as a function of increasing trapping strength along with the superconducting order parameter, Δ_{op} defined by the long distance behaviour of the correlation $\langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_{j\downarrow} c_{j\uparrow} \rangle \rightarrow \Delta_{op}^2 / |U|^2$ for $|\mathbf{r}_i - \mathbf{r}_j| \rightarrow \infty$ [290]. While E_{gap} shows a non-monotonic behaviour with increasing trapping strength, Δ_{op} rapidly drops to zero. A finite E_{gap} along with a vanishing Δ_{op} for larger values of trapping potential clearly point towards the emergence of an insulating state in the limit of large confinement[98].

Next we compute the average kinetic energy of the carriers across the lattice, $\langle KE \rangle$ ($= \langle t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} \rangle$) which is a measure of mobility[291] and the onsite potential energy, $\langle U \rangle$ illustrated in Fig. 7.3. While the mobility of the carriers reduces significantly with increasing trapping strength, the onsite potential energy grows, thereby resulting in greater confinement of carriers to individual sites.

Let us analyze the energy issues of the trapped system more closely. An attractive Hubbard model has two critical end points viz. $U = 0$ (metal to superconductor transition) and $U = \infty$ (superconductor to localized insulator transition)[292] at zero temperature. Thus a larger $\langle U \rangle$ in presence of stronger confinement demands a careful analysis of the behaviour of the eigenstates that plays an important role. The eigenstates must be strongly affected

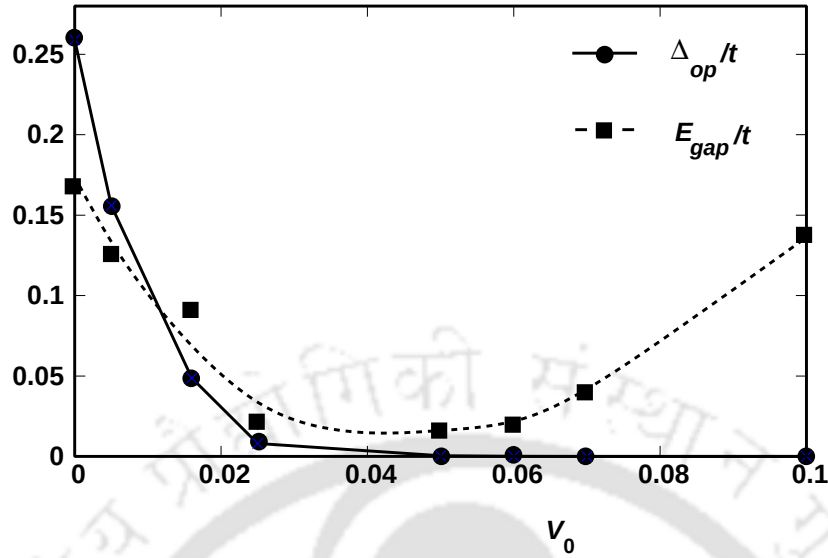


FIGURE 7.2: The spectral gap, E_{gap} and the superconducting order parameter, Δ_{op} (defined in text) are shown as a function of increasing trapping potential V_0 . Here $|U| = 2.5t$, density $n = 0.66$ and $h = 0.4t$. Note that E_{gap} depends on V_0 in a non-monotonic fashion while Δ_{op} vanishes monotonically as V_0 is increased. The dotted line to E_{gap} data is a guide to the eye. Both the axes are in units of t .

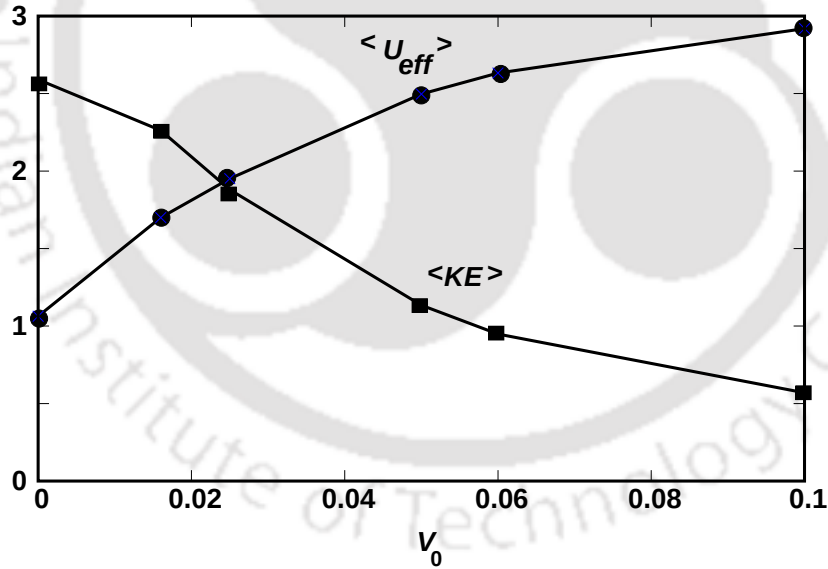


FIGURE 7.3: The average kinetic energy of the charge carriers, $\langle KE \rangle$ and the onsite potential energy, $\langle U \rangle$ is plotted as a function of V_0 . Here $|U| = 2.5t$, density $n = 0.66$ and $h = 0.4t$. Both the axes are in units of t .

i.e. transform from being extended to localized, is seen via computing the participation ratio, defined and discussed later.

TABLE 7.1: The polarization, $P \left(= \frac{N_{\uparrow} - N_{\downarrow}}{N_{\uparrow} + N_{\downarrow}} \right)$ is shown as a function of increasing trapping strength, V_0 (in units of t) for $h = 0.4t$. P drops significantly as the trapping strength is made larger.

Trapping strength (V_0) (in units of t)	Polarization (P)
0.0	0.130
0.016	0.100
0.025	0.097
0.05	0.060
0.06	0.049
0.1	0.030

Let us concentrate on the confinement effects on the spin polarization, P . As the trap depth is increased, P decreases leading to disappearance of the spin polarized (FFLO) phase (table 7.1). This phase can in principle be a homogeneous BCS superconductor or an insulating phase as both of them can be characterized by equal number of up- and down-spin particles. However, our earlier signatures of an increasing spectral gap along with a decaying superconducting order parameter (see Fig. 7.1) confirms the phase to be an insulator.

We now probe into the behaviour of various local quantities *e.g.* total density, and the double occupancy for various strengths of trapping. The local occupation number $\langle n_i \rangle$ presented in Fig. 7.4, shows distinct rise in the occupancy of sites near the trap center with increasing V_0 such that a plateau of constant density $\langle n_i \rangle$ equal to 2 is eventually obtained for the case of extreme confinement of particles with $V_0 = 0.1t$. Thus, the atomic gas separates into a phase that comprises of localized bound pairs without phase coherence at the core surrounded by a 'conducting' ring of excess unpaired electrons. The constant occupation number at large trap depths bears signatures of a *localized* insulator as also noted in Ref. [293], which is in agreement with experiments where similar density profiles are obtained using *in situ* imaging of the trapped atomic gas[294]. We now plot the real space profile of double occupancy in Fig. 7.5 which again attains a maximum value (equal to 4) at the trap center and becomes very flat with increasing trapping strength.

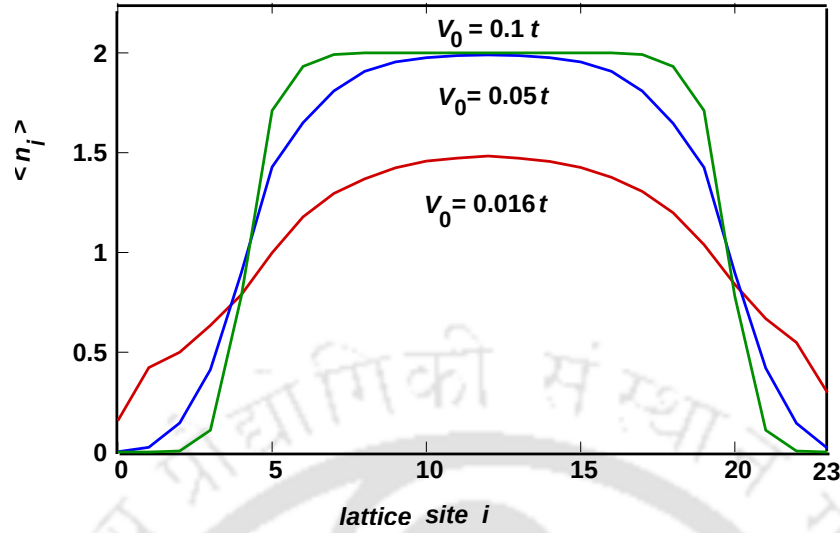


FIGURE 7.4: Occupation number, $\langle n_i \rangle$ ($= \langle n_{i\uparrow} \rangle + \langle n_{i\downarrow} \rangle$) is shown as a function of site i on a 24×24 lattice. Note that the sites near trap center are fully occupied by pairs ($\langle n_i \rangle = 2$) at large trap depths indicating onset of an insulating phase. The lattice sites are numbered from $0 \rightarrow 23$. Here $|U| = 2.5t$, density $n = 0.66$ and $h = 0.4t$. $\langle n_i \rangle$ is in units of t .

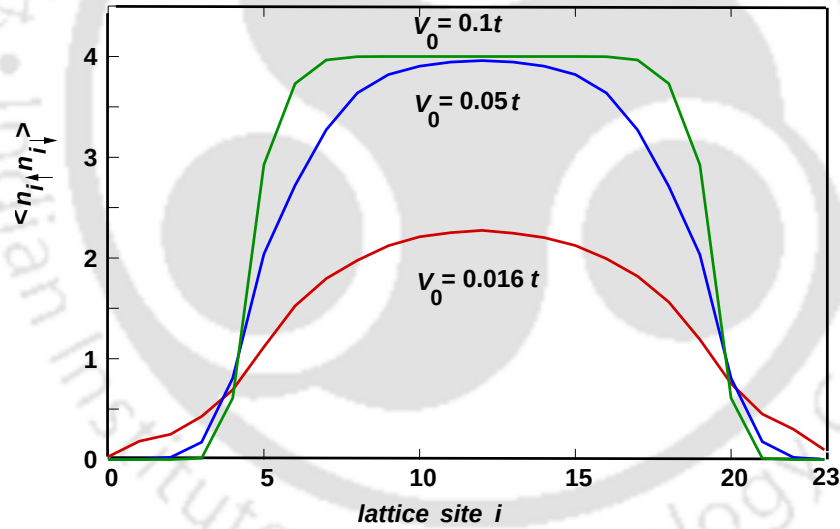


FIGURE 7.5: Double occupancy, $\langle n_{i\uparrow} n_{i\downarrow} \rangle$ (in units of t) is shown as a function of site i on a 24×24 lattice. The lattice sites are numbered from $0 \rightarrow 23$. Here $|U| = 2.5t$, density $n = 0.66$ and $h = 0.4t$.

Next, we generalize Anderson's idea of pairing of time reversed energy eigenstates[191] of the non-interacting Hamiltonian given by,

$$\mathcal{H}_0 = -t \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) + \sum_{i, \sigma} (V_i - \mu + \sigma h) n_{i\sigma} \quad (7.1)$$

All the quantities appearing in Eq. (7.1) are defined above. We then construct a matrix whose elements are defined by $M_{\alpha\beta} = \sum_{r_i} |\phi_\alpha^0(r_i)|^2 |\phi_\beta^0(r_i)|^2$ where $\phi_\alpha^0(r_i)$ is the eigenstate of $\mathcal{H}_0$ [98]. $M_{\alpha\beta}$ for various values of V_0 are shown in Fig. 7.6. At small values of trapping potential ($V_0 = 0.016t$), different eigenstates ($\alpha \neq \beta$) of the non-interacting Hamiltonian have finite overlap which results in persistence of superconducting correlations. As the trapping reaches intermediate values ($V_0 = 0.05t$), the contribution from the diagonal elements of $M_{\alpha\beta}$ starts dominating and the overlap between different eigenstates decreases. Finally, at strong confinement (say, $V_0 = 0.6t$ as shown in Fig. 7.6), different exact eigenstates hardly overlap as evident from vanishing off-diagonal elements of the matrix and the diagonal elements reach maximum value. Thus at such large trap depths, eigenstates are completely localized to individual sites with no overlap between different states, thereby suggestive of onset of an insulating phase.

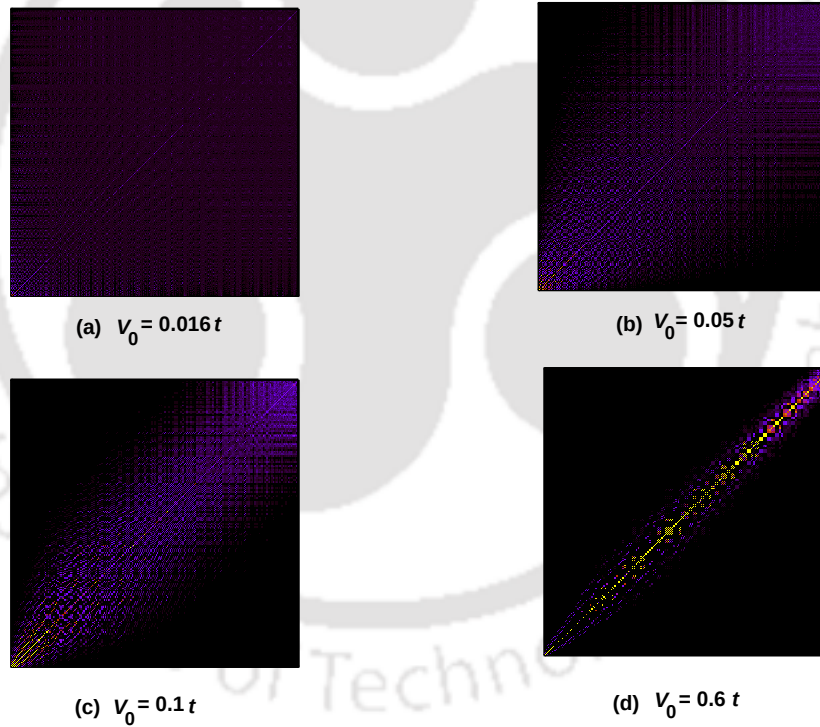


FIGURE 7.6: $M_{\alpha\beta} = \sum_{r_i} |\phi_\alpha^0(r_i)|^2 |\phi_\beta^0(r_i)|^2$ is presented for various values of V_0 . The overlap between different eigenstates decreases as V_0 is increased. Note that the diagonal matrix elements are largest for $V_0 = 0.6t$ implying vanishing overlap between different eigenstates and hence strong localization. Here $|U| = 0$, density $n = 0.66$ and $h = 0.4t$.

Further, we analyze the behaviour of the participation ratio (PR) as a function of confining potential in order to strengthen our claim of SIT. PR gives a measure of the number of lattice

sites over which an eigenstate is extended[268]. It distinguishes localized states ($PR \sim 1$) from the extended ones ($PR \sim N$, where N is total number of lattice sites) and hence can be used to predict localization of atomic states. The PR is defined as,

$$PR = \frac{1}{\sum_{r_i} |\phi_\alpha(r_i)|^4} \quad (7.2)$$

where $\phi_\alpha(r_i)$ is the eigenstate obtained from the BdG analysis and α is the eigenvalue index. Using Eq. (7.2), PR is computed as a function of increasing trapping strength (see table 7.2). It may be noted that PR is of the order of a few lattice sites for low trapping strengths which makes superconductivity still feasible as the electronic wavefunction spreads out over some finite number of sites and long range order persists. But as the trapping is made stronger, PR drops to a value equal to one, implying a particular number of electrons confined at individual sites. The localization of the eigenstates in the limit of extreme confinement, is also evident from the reduction in the localization length, ξ . Suppose an electronic wavefunction is localized within a d -dimensional volume of average diameter ξ which can be roughly taken as a characteristic length for the asymptotic exponential decay, called the localization length[269], the PR behaves as ξ^d . For us, $d = 2$, so an estimate of the correlation length can be obtained as

$$\xi = \sqrt{PR} \quad (7.3)$$

It is clear from table 7.2 that ξ drops from a value of about 22 lattice spacings for $V_0 = 0$ to $\xi \simeq 1$ at $V_0 = 0.1t$, indicating emergence of an extremely localized insulating phase.

For the kind of attractive interaction strength used in our work i.e. $|U| = 2.5t$, one would not expect a transition to an insulating state, except for infinitely large values of V_0 . However, the drastic drop in the PR and hence ξ for small V_0 values as obtained here, conclusively show the effectiveness of the trapping potential in inducing localization effects in a spin-imbalanced superfluid Fermi gas.

TABLE 7.2: Participation ratio, PR is shown for various values of V_0 . Note that it reduces drastically with increasing confinement and approaches unity at the limit of extreme confinement.

Trapping strength (V_0) (in units of t)	Participation ratio (PR)
0	498
0.001	127
0.005	22
0.016	11
0.025	8
0.06	3
0.1	1

7.3 Summary

In this work, we have made an attempt to investigate the response of a spin-imbalanced Fermi gas to a harmonic confinement. The confinement signals SIT as the strength of the trapping potential is tuned since strong confining effects leads to an effective increase in the on-site (attractive) interaction between fermions which is known to yield a localized insulating phase[292]. To support our claim, we have computed relevant physical quantities *e.g.* the gap in the excitation spectrum, superconducting order parameter, local density distribution, double occupancy, mobility of the carriers and the participation ratio. The spectral gap thus obtained shows a non-monotonic behaviour while the superconducting order parameter decreases with increasing confinement and finally vanishes, thereby pointing towards emergence of an insulating phase. Further, a constant density (with a value 2) around the core of the harmonic potential, rise in the double occupancy, reduction in the mobility of the charge carriers along with increase in onsite interaction energy at large trap depths, strengthen our claim of SIT. The emergence of the insulating phase at strong confinement, is attributed to localization of eigenstates which is confirmed by computing the overlap between different (exact) eigenstates given by the participation ratio which reduces significantly with increasing trapping strength. It becomes unity at large trapping strengths indicating that the eigenstates have been confined to exactly *one* lattice site leading to complete localization.

Finally it is worth mentioning that we have also examined the effect of spin imbalance in the context of SIT by computing various physical quantities discussed in this work. While

switching off the trap effects, one obtains a number of interesting differences for zero and finite spin imbalanced cases, the existence of the trap (as small as $V_0 = 0.016t$) nearly washes away such differences in the balanced and imbalanced cases and the spin imbalance does not have any perceivable influence on SIT.



Chapter 8

Conclusions

In this thesis, we have performed an elaborate study of two different exotic phases of a s -wave superconductor. The first one deals with a BCS-BEC crossover. The second one explores a fascinating superconducting phase which is induced by spin imbalance known as the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase. In doing so, we have studied the ground state properties of an attractive Hubbard model as a model for two dimensional s wave superconductor which has been investigated as a function of disorder for the first problem and for various values of magnetic field that causes a spin imbalance for the second problem. The behaviors of the quasiparticles are described by the Bogoliubov de Gennes (BdG) equations for both the problems.

We have performed a detailed study of the effect of random disorder on the evolution of a BCS superconductor to a BEC superfluid. The various kinds of disorder that are studied include onsite disorder, hopping disorder and hopping anisotropy. Among them, the onsite disorder and hopping anisotropy are found to be capable of inducing a crossover from a BCS to a BEC phase due to localization effects. Hopping disorder on the other hand, fails to catalyze the crossover phenomenon, owing to delocalization of charge carriers. The first claim for the existence of a crossover in the disordered model is made on the basis of behaviour of the chemical potential as a function of disorder, which slips below the band minimum (Leggett criterion) at the onset of Bose phase. The investigation of the effect of density on the crossover phenomenon bears interesting results of the crossover being feasible only at low densities. The reason being at higher densities, the overlap between the pairs increases substantially thereby denying access to a BEC-like phase at intermediate values of disorder.

The emergence of a Bose phase at intermediate values of disorder is further confirmed by computing various physical quantities viz. off diagonal long range order, spectral gap and superfluid stiffness as a function of disorder strength which confirm persistence of long range order in the system. The reduction in the pair size with increasing disorder strength results in substantial rise in fluctuation effects of the order parameter and hence play crucial role in the strong disorder limit. We thus incorporate the effect of fluctuations within a harmonic approximation about the inhomogeneous BdG state using a phase-only model. The results thus obtained are intriguing as it yields opening of a large region between the mean field transition temperature and the actual transition temperature (obtained from the vanishing of the renormalized superfluid stiffness), which is characterized by the presence of pairs with no phase coherence thereby bearing resemblance to the pseudogap phase that is observed in the context of underdoped cuprates. All the above mentioned results form the content of chapter 3.

In chapter 4, we present various real space quantities e.g. the pairing amplitude, electron occupancy, participation ratio and fidelity in order to strengthen our claim for disorder driven BCS-BEC crossover. The spatial distribution of the pairing amplitude shows clear signatures of appearance of spatially correlated cluster of sites possessing large pairing amplitudes (termed as 'superconducting islands') which are separated by an insulating sea characterised by vanishing pairing amplitude in the limit of strong disorder. The result of spatial distribution of electron occupancy for strong disorder shows localized electron occupancies and thus is supportive of a phase comprising of short and local pairs, reminiscent of a BEC phase at intermediate values of disorder. Our results for the participation ratio are insightful, as it is of the order of few lattice sites for intermediate values of disorder, thereby implying long range order persisting due to the presence of short ranged pairs which resemble a Bose phase. We hence use fidelity to characterize the crossover phenomena which undergoes an abrupt and sharp drop near the crossover point obtained from chemical potential data. Thus, there is drastic change in the ground state for disorder values close to the crossover point which results in a reduction in overlap between the ground states (corresponding to two slightly different disorder values near the crossover point) thereby implying transition to a different kind of phase.

A detailed analysis of the spin imbalance induced FFLO phase is presented in chapter 5. The spin imbalance between the two different spin states is created by an externally applied magnetic field. We have computed the local pairing amplitudes and magnetization for various

values of interaction strengths and band filling via solving BdG equations. Both the quantities undergo spatial modulation with the modulation wavevector being a function of the effective momentum of the Cooper pair. Since a short coherence length is one of the necessary requirements for the realization of the FFLO phase, we have computed the superconducting coherence length which shows appreciable reduction from a large value (practically infinite corresponding to homogeneous pairing amplitude in the BCS phase) to a few lattice spacings at the onset of FFLO phase.

In chapter 6, we have investigated a spin imbalanced s -wave superconductor in presence of a harmonic confinement. The nature of the superconducting order parameter and magnetization are observed both in equal spin and spin imbalanced cases in the presence of trap and then when the trap effects are switched off. The superconducting order parameter modulates in a radial direction at the trap edges for finite spin polarization values whereas it extends over the entire lattice as soon as the trapping potential is turned off. Other physical quantities which are computed include pair-pair, density-density correlations and local number density fluctuations for two different values of population imbalance but fixed trap depth. The external trapping is then switched off, thereby allowing the condensed phase to expand and the nature of the correlations in the absence of trap is analyzed in details. Our results show that the distinction between the zero and finite spin polarization values is significantly suppressed in the presence of trap and hence the trapping potential should be switched off in order to distinguish between the states.

One of the greatest achievement in the study of cold atoms has been the observation of superfluid to insulator transition (SIT) in a controlled environment. In chapter 7, we have investigated SIT in a spin-imbalanced gas of fermionic atoms with increasing strength of the trapping potential using a two-dimensional attractive Hubbard model. In order to investigate this, we have computed relevant physical quantities *e.g.* the gap in the excitation spectrum, local density distribution, double occupancy, mobility of the carriers, effective on-site interaction energy and the participation ratio. All these quantities indicate emergence of an insulating phase at a small value of trapping strength.

A possible extension of our problems is to investigate the scenario in superconductors with d -wave, p -wave and other more complicated symmetries of the order parameter such as a combination of d and s -wave etc. Another interesting prospect is to investigate the relevance of our studies in the context of cold atomic systems. Some of the issues are settled in bosonic

systems, however experiments are now being done on fermionic gases as well. An interesting extension may include the investigation of the scenario in Bose-Fermi mixtures. Further, extending the results to finite temperatures for both these problems, can also be potentially interesting. Besides these, random disorder effects on the FFLO physics may demand renewed attention.



Appendix A

Renormalized superfluid stiffness at finite temperatures

The phase only Hamiltonian as in Eq. (2.46) of chapter 2 is given by,

$$\begin{aligned} H_\theta &= \frac{U}{2} \sum_i \hat{n}_i^2 + J \sum_{\langle ij \rangle} [1 - \cos(\theta_i - \theta_j)], \\ &= E_c + E_J. \end{aligned} \quad (\text{A.1})$$

Here $\hat{n}_i$ is the number operator for Cooper pairs on the i -th grain and U is related to the inverse of the capacitance of the assembly of superconducting islands. The second term is specified by the Josephson coupling strength J , with θ_i being the phase angle on the i th grain. It may be noted that the charging energy, E_c favors insulating behaviour as it arises due to the fact that it costs energy to transfer a Cooper pair from one superconducting island to another. However, the Josephson coupling energy, E_J establishes a (global) phase coherence among the islands and thus gives rise to a superconducting ground state.

The harmonic approximation of the cosine term in Eq. (A.1) gives the trial Hamiltonian as,

$$H_0 = \frac{U}{2} \sum_i \hat{n}_i^2 + \sum_{\langle ij \rangle} \frac{K}{2} (\theta_i - \theta_j)^2. \quad (\text{A.2})$$

where $K = \frac{D_s}{4}$ with D_s as the renormalized superfluid stiffness.

The expectation value of $(H_\theta - H_0)$ in the trial basis is,

$$\langle H_\theta - H_0 \rangle_0 = \langle J \sum_{\langle ij \rangle} [1 - \cos(\theta_{ij})] - \frac{D_s}{8} (\theta_{ij})^2 \rangle_0 \quad (\text{A.3})$$

where $(\theta_i - \theta_j) = \theta_{ij}$. It may be noted that the charging term cancels out.

Feynman theorem (Gibbs-Bogoliubov inequality) yields a relation between the free energies corresponding to H_0 and H_θ given by [220],

$$F_\theta \leq F_0 + \langle H_\theta - H_0 \rangle_0, \quad (\text{A.4})$$

where F_0 is the free energy of the system described by the trial Hamiltonian given in Eq. (A.2).

Now,

$$\begin{aligned} \langle H_\theta - H_0 \rangle_0 &= \sum_{\langle ij \rangle} \left[J - J \langle \cos \theta_{ij} \rangle_0 - \frac{D_s}{8} \langle \theta_{ij}^2 \rangle_0 \right], \\ &= \sum_{\langle ij \rangle} \left[J - J e^{-\frac{\langle \theta_{ij}^2 \rangle_0}{2}} - \frac{D_s}{8} \langle \theta_{ij}^2 \rangle_0 \right] \end{aligned} \quad (\text{A.5})$$

The above equation is valid for small θ_{ij} .

We then obtain D_s using a variational approach. For this, we determine $\frac{\partial F_0}{\partial D_s}$ using partition function given by,

$$\mathcal{Z}_0 = \int \mathcal{D}\theta \exp \left(-\frac{1}{\hbar} S_0 [\theta] \right) \quad (\text{A.6})$$

where the action, $S_0 [\theta]$ is defined as,

$$\begin{aligned} S_0 [\theta] &= \int_0^{\hbar\beta} d\tau H_0 [\theta], \\ &= \int_0^{\hbar\beta} d\tau \left[\frac{U}{2} \sum_i \hat{n}_i^2 + \sum_{\langle ij \rangle} \frac{D_s}{8} \theta_{ij}^2 \right] \end{aligned} \quad (\text{A.7})$$

Using $\hat{n}_i = \left(\frac{\hbar}{2U} \right) \frac{\partial \theta_i}{\partial \tau}$, the first term of the Hamiltonian (the charging term) is written as,

$$H_{CE} = \frac{\hbar^2}{8U} \sum_i \left(\frac{\partial \theta_i}{\partial \tau} \right)^2 \quad (\text{A.8})$$

Using Eq. (A.8) in Eq. (A.7) we get,

$$S_0[\theta] = \int_0^{\hbar\beta} d\tau \left[\frac{\hbar^2}{8U} \sum_i \left(\frac{\partial\theta_i}{\partial\tau} \right)^2 + \sum_{\langle ij \rangle} \frac{D_s}{8} \theta_{ij}^2 \right] \quad (\text{A.9})$$

So,

$$\mathcal{Z}_0 = \int \mathcal{D}\theta \exp \left[-\frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \left(\frac{\hbar^2}{8U} \sum_i \left(\frac{\partial\theta_i}{\partial\tau} \right)^2 + \sum_{\langle ij \rangle} \frac{D_s}{8} \theta_{ij}^2 \right) \right] \quad (\text{A.10})$$

and the corresponding free energy is,

$$F_0 = -\frac{1}{\beta} \ln \int \mathcal{D}\theta \exp \left[-\frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \left(\frac{\hbar^2}{8U} \sum_i \left(\frac{\partial\theta_i}{\partial\tau} \right)^2 + \sum_{\langle ij \rangle} \frac{D_s}{8} \theta_{ij}^2 \right) \right] \quad (\text{A.11})$$

Hence taking derivative with respect to D_s , we get,

$$\begin{aligned} \frac{\partial F_0}{\partial D_s} &= -\frac{1}{\beta} \frac{1}{\mathcal{Z}_0} \int \mathcal{D}\theta \exp \left[-\frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \left(\frac{\hbar^2}{8U} \sum_i \left(\frac{\partial\theta_i}{\partial\tau} \right)^2 + \sum_{\langle ij \rangle} \frac{D_s}{8} \theta_{ij}^2 \right) \right] \left(-\frac{1}{8\hbar} \right) \int_0^{\hbar\beta} d\tau \sum_{\langle ij \rangle} \langle \theta_{ij}^2 \rangle_0, \\ &= \frac{1}{8\hbar\beta} \int_0^{\hbar\beta} d\tau \sum_{\langle ij \rangle} \langle \theta_{ij}^2 \rangle_0 \end{aligned} \quad (\text{A.12})$$

Eq. (A.4) can be also written as,

$$\begin{aligned} F_\theta &\leq F_0 + \frac{1}{\hbar\beta\mathcal{Z}_0} \int \mathcal{D}\theta \exp \left(-\frac{1}{\hbar} S_0 \right) (S_\theta - S_0), \\ &= F_0 + \frac{1}{\hbar\beta} \langle S_\theta - S_0 \rangle_0 = \tilde{F} \end{aligned} \quad (\text{A.13})$$

where

$$\frac{1}{\hbar\beta} \langle S_\theta - S_0 \rangle_0 = \frac{1}{\hbar\beta} \int_0^{\hbar\beta} d\tau \sum_{\langle ij \rangle} \left[J - J e^{-\frac{\langle \theta_{ij}^2 \rangle_0}{2}} - \frac{D_s}{8} \langle \theta_{ij}^2 \rangle_0 \right] \quad (\text{A.14})$$

The free energy is minimized by considering the infinitesimal variation in $\tilde{F}$,

$$\delta\tilde{F} = \delta \left(F_0 + \frac{1}{\hbar\beta} \langle S_\theta - S_0 \rangle_0 \right) = 0 \quad (\text{A.15})$$

Since $\langle \theta_{ij}^2 \rangle$ is also a function of D_s , the above condition becomes,

$$\left(\frac{\partial \tilde{F}}{\partial D_s} \right)_{\langle \theta_{ij}^2 \rangle_0} + \left(\frac{\partial \tilde{F}}{\partial \langle \theta_{ij}^2 \rangle_0} \right)_{D_s} \left(\frac{\partial \langle \theta_{ij}^2 \rangle_0}{\partial D_s} \right) = 0 \quad (\text{A.16})$$

Next we calculate the partial derivative,

$$\frac{1}{\hbar\beta} \left(\frac{\partial \langle S_\theta - S_0 \rangle_0}{\partial D_s} \right)_{\langle \theta_{ij}^2 \rangle_0} = -\frac{1}{8\hbar\beta} \int_0^{\hbar\beta} d\tau \sum_{\langle ij \rangle} \langle \theta_{ij}^2 \rangle_0 \quad (\text{A.17})$$

Using Eq. (A.12) and Eq. (A.17), we get,

$$\left(\frac{\partial \tilde{F}}{\partial D_s} \right)_{\langle \theta_{ij}^2 \rangle_0} = \frac{\partial F_0}{\partial D_s} + \frac{1}{\hbar\beta} \left(\frac{\partial \langle S_\theta - S_0 \rangle_0}{\partial D_s} \right)_{\langle \theta_{ij}^2 \rangle_0} = 0 \quad (\text{A.18})$$

Thus the second term in Eq. (A.16) yields a nonzero contribution. Now, F_0 is not an explicit function of $\langle \theta_{ij}^2 \rangle_0$, so we are left with the second term in Eq. (A.16) which is calculated in the following as,

$$\begin{aligned} \left(\frac{\partial \tilde{F}}{\partial \langle \theta_{ij}^2 \rangle_0} \right)_{D_s} &= \frac{1}{\hbar\beta} \left(\frac{\partial \langle S_\theta - S_0 \rangle_0}{\partial \langle \theta_{ij}^2 \rangle_0} \right)_{D_s} \\ &= \frac{1}{2\hbar\beta} \int_0^{\hbar\beta} d\tau \sum_{\langle ij \rangle} \left[J e^{-\frac{\langle \theta_{ij}^2 \rangle_0}{2}} - \frac{D_s}{8} \right] \end{aligned} \quad (\text{A.19})$$

Inserting Eq. (A.18) and Eq. (A.19) in Eq. (A.16), we get,

$$\frac{1}{2\hbar\beta} \int_0^{\hbar\beta} d\tau \sum_{\langle ij \rangle} \left[J e^{-\frac{\langle \theta_{ij}^2 \rangle_0}{2}} - \frac{D_s}{4} \right] \left(\frac{\partial \langle \theta_{ij}^2 \rangle_0}{\partial D_s} \right) = 0 \quad (\text{A.20})$$

The value of D_s is thus obtained as,

$$D_s = D_{s0} e^{-\frac{\langle \theta_{ij}^2 \rangle_0}{2}} \quad (\text{A.21})$$

where $J = \frac{D_{s0}}{4}$.

We now derive an expression for $\langle \theta_{ij}^2 \rangle_0$. Expanding $\theta_i(\tau)$ into a Fourier series,

$$\theta_i(\tau) = \frac{1}{N} \sum_k \theta_k(\tau) e^{i\vec{k} \cdot \vec{R}_i} \quad (\text{A.22})$$

where $\vec{R}_i$ refer to position of lattice sites. We can write,

$$\langle \theta_{ij}^2 \rangle_0 = \frac{1}{N^2} \sum_{kk'} \left(e^{i\vec{k} \cdot \vec{R}_i} - e^{i\vec{k} \cdot \vec{R}_j} \right) \left(e^{i\vec{k}' \cdot \vec{R}_i} - e^{i\vec{k}' \cdot \vec{R}_j} \right) \langle \theta_k \theta_{k'} \rangle_0 \quad (\text{A.23})$$

Translational invariance of the array implies,

$$\langle \theta_k \theta_{k'} \rangle_0 = \langle \theta_k \theta_{-k} \rangle_0 \delta_{k, -k'} \quad (\text{A.24})$$

Using this result in Eq. (A.23), we get,

$$\langle \theta_{ij}^2 \rangle_0 = \frac{2}{N^2} \sum_k \left[1 - \cos(\vec{k} \cdot \vec{R}_{ij}) \right] \langle \theta_k \theta_{-k} \rangle_0 \quad (\text{A.25})$$

where $\vec{R}_{ij} = \vec{R}_i - \vec{R}_j$. Next we calculate the equal time correlation function $\langle \theta_k \theta_{-k} \rangle_0$. We express the trial action $S_0[\theta]$ in terms of the Fourier components, $\theta_{k,n}$ given by,

$$\theta_k(\tau) = \sum_{n=-\infty}^{\infty} \theta_{k,n} e^{-i\omega_n \tau} \quad (\text{A.26})$$

where $\omega_n = \left(\frac{2\pi n}{\hbar\beta} \right)$ are the Matsubara frequencies and assume integral values (an being both positive and negative, including zero).

Introducing Eq. (A.22) and Eq. (A.26) in the charging part of $S_0[\theta]$, we obtain

$$S_{CE}[\theta] = \frac{\hbar^3 \beta}{8UN} \sum_k \sum_n \theta_{k,n} \theta_{-k,-n} \omega_n^2 \quad (\text{A.27})$$

Now, making similar substitutions in the Josephson coupling term, we get

$$\begin{aligned} S_{JE} &= \frac{D_s}{8} \int_0^{\hbar\beta} d\tau \sum_{\langle ij \rangle} \frac{D_s}{8} \theta_{ij}^2 \\ &= \frac{D_s}{8N^2} \int_0^{\hbar\beta} d\tau \sum_{\langle ij \rangle} \sum_{kk'} e^{i(\vec{k}+\vec{k}') \cdot \vec{R}_i} \left(1 - e^{i\vec{k} \cdot \vec{R}_{ij}}\right) \left(1 - e^{i\vec{k}' \cdot \vec{R}_{ij}}\right) \theta_k(\tau) \theta_{k'}(\tau) \end{aligned} \quad (\text{A.28})$$

The subscripts *CE* and *JE* refer to charging energy and Josephson coupling energy terms.

We perform the summation over R_i using the identity,

$$\sum_i e^{i(\vec{k}+\vec{k}') \cdot \vec{R}_i} = N \delta_{\vec{k}, -\vec{k}'} \quad (\text{A.29})$$

Using Eq. (A.26) in S_{JE} , we get,

$$S_{JE} = \frac{\hbar\beta D_s}{8N} \sum_k \sum_n \sum_{j(i)} \left[1 - \cos(\vec{k} \cdot \vec{R}_{ij})\right] \theta_{k,n} \theta_{-k,-n} \quad (\text{A.30})$$

The summation over nearest neighbours, j of a grain site i , defines structure factor of the lattice as,

$$f(k) = \sum_{j(i)} \left[1 - \cos(\vec{k} \cdot \vec{R}_{ij})\right] = z - 2 \sum_{j=1}^d \cos(k_j a) \quad (\text{A.31})$$

where z and d are the coordination number and the dimensionality of the lattice respectively.

We obtain the trial action in a Fourier transformed form as,

$$\begin{aligned} S_0[\theta] &= S_{CE} + S_{JE} \\ &= \frac{\hbar\beta}{N} \sum_k \sum_n \left(\frac{\hbar^2}{8U} \omega_n^2 + \frac{D_s}{8} f(k) \right) |\theta_{k,n}|^2 \end{aligned} \quad (\text{A.32})$$

where we have used,

$$\theta_{k,n}^* = \theta_{-k,-n} \quad (\text{A.33})$$

Note that

$$\theta_{k,n} = \theta_{k,n}^r + i\theta_{k,n}^i \quad (\text{A.34})$$

Using Eq. (A.26), we get,

$$\langle \theta_k \theta_{-k} \rangle_0 = \sum_n \langle \theta_{k,n} \theta_{-k,-n} \rangle_0 \quad (\text{A.35})$$

Because of Eq. (A.33), $(k, n) > 0$, say k_0 and n_0 . We obtain,

$$\langle \theta_{k_0, n_0} \theta_{-k_0, -n_0} \rangle_0 = \frac{1}{\mathcal{Z}_0} \int \mathcal{D}\theta \exp\left(-\frac{S_0[\theta]}{\hbar}\right) (\theta_{k_0, n_0} \theta_{-k_0, -n_0}) \quad (\text{A.36})$$

Here,

$$\begin{aligned} (\theta_{k_0, n_0} \theta_{-k_0, -n_0}) &= (\theta_{k_0, n_0} \theta_{k_0, n_0}^*) \\ &= (\theta_{k_0, n_0}^r)^2 + (\theta_{k_0, n_0}^i)^2 \end{aligned} \quad (\text{A.37})$$

Using Eq. (A.37) in Eq. (A.36), we get,

$$\begin{aligned} \langle \theta_{k_0, n_0} \theta_{-k_0, -n_0} \rangle_0 &= \frac{1}{\mathcal{Z}_0} \prod_{k>0, n>0} \int_{-\infty}^{\infty} d\theta_{k,n}^r \int_{-\infty}^{\infty} d\theta_{k,n}^i \left[(\theta_{k_0, n_0}^r)^2 + (\theta_{k_0, n_0}^i)^2 \right] \\ &\times \exp\left[-\frac{2\beta}{N} \left(\frac{\hbar^2}{8U} \omega_n^2 + \frac{D_s}{8} f(k) \right) \left[(\theta_{k,n}^r)^2 + (\theta_{k,n}^i)^2 \right]\right] \end{aligned} \quad (\text{A.38})$$

Note that the integrals over Fourier components with $k \neq k_0$ and $n \neq n_0$ get cancelled with $\mathcal{Z}_0$. So, only one integral is left, which is,

$$\begin{aligned} \langle \theta_{k_0, n_0} \theta_{-k_0, -n_0} \rangle_0 &= 2 \langle (\theta_{k_0, n_0}^r)^2 \rangle_0 \\ &= 2 \frac{\int_{-\infty}^{\infty} d\theta_{k_0, n_0}^r (\theta_{k_0, n_0}^r)^2 \exp\left[-\frac{2\beta}{N} \left(\frac{\hbar^2}{8U} \omega_n^2 + \frac{D_s}{8} f(k) \right) (\theta_{k_0, n_0}^r)^2\right]}{\int_{-\infty}^{\infty} d\theta_{k_0, n_0}^r \exp\left[-\frac{2\beta}{N} \left(\frac{\hbar^2}{8U} \omega_n^2 + \frac{D_s}{8} f(k) \right) (\theta_{k_0, n_0}^r)^2\right]} \end{aligned} \quad (\text{A.39})$$

Using standard integrals,

$$\begin{aligned} \int_{-\infty}^{\infty} dx e^{-\alpha x^2} &= \sqrt{\frac{\pi}{\alpha}} \\ \int_{-\infty}^{\infty} dx x^2 e^{-\alpha x^2} &= \frac{1}{2\alpha} \sqrt{\frac{\pi}{\alpha}} \end{aligned} \quad (\text{A.40})$$

We get

$$\langle \theta_{k_0, n_0} \theta_{-k_0, -n_0} \rangle_0 = \frac{N}{2\beta} \left[\frac{\hbar^2}{8U} \omega_n^2 + \frac{D_s}{8} f(k) \right]^{-1} \quad (\text{A.41})$$

Introducing this result in Eq. (A.35), we obtain,

$$\langle \theta_k \theta_{-k} \rangle_0 = \sum_n \frac{N}{2\beta} \left[\frac{\hbar^2}{8U} \omega_n^2 + \frac{D_s}{8} f(k) \right]^{-1} \quad (\text{A.42})$$

Thus Eq. (A.25) gives,

$$\begin{aligned} \langle \theta_{ij}^2 \rangle_0 &= \frac{2}{N^2} \sum_k \sum_n \left[1 - \cos(k \cdot R_{ij}) \right] \frac{N}{2\beta} \left[\frac{\hbar^2}{8U} \omega_n^2 + \frac{D_s}{8} f(k) \right]^{-1} \\ &= \frac{1}{N\beta} \sum_k \sum_n \frac{\left[1 - \cos(k \cdot R_{ij}) \right]}{\left[\frac{\hbar^2}{8U} \omega_n^2 + \frac{D_s}{8} f(k) \right]} \end{aligned} \quad (\text{A.43})$$

We now introduce a bond averaged $\langle \theta_{ij}^2 \rangle_0$ defined as,

$$\begin{aligned} \langle \bar{\theta}_{ij}^2 \rangle_0 &= \frac{1}{z} \sum_{j(i)} \langle \theta_{ij}^2 \rangle_0 \\ &= \frac{1}{N\beta z} \sum_k \sum_n \frac{f(k)}{\frac{\hbar^2}{8U} \left(\omega_n^2 + \frac{UD_s f(k)}{\hbar^2} \right)} \end{aligned} \quad (\text{A.44})$$

The structure factor for a two dimensional square lattice ($d = 2, z = 4$) and in the long wavelength limit yields,

$$\begin{aligned} f(k) &= 4 - 2 \left[\cos(k_x a) + \cos(k_y a) \right] \\ &= k_x^2 a^2 + k_y^2 a^2 \\ &\approx k^2 a^2 \end{aligned} \quad (\text{A.45})$$

Now, let us evaluate Eq. (A.44) at zero temperature and at finite temperatures.

Zero temperature

As $T \rightarrow 0$, the Matsubara sum in Eq. (A.44) is evaluated using[220],

$$\sum_{n=-\infty}^{\infty} \frac{1}{\omega_n^2 + \omega_\alpha^2} = \frac{\hbar\beta}{2\omega_\alpha} \quad (\text{A.46})$$

In the present case $\omega_\alpha = \sqrt{\frac{U f(k) D_s}{\hbar^2}}$. So,

$$\sum_{n=-\infty}^{\infty} \frac{1}{\omega_n^2 + \omega_\alpha^2} = \frac{\hbar^2\beta}{2\sqrt{U f(k) D_s}} \quad (\text{A.47})$$

Using Eq. (A.47) in Eq. (A.44), we get,

$$\begin{aligned} \langle \bar{\theta}_{ij}^2 \rangle_0 &= \frac{1}{N} \sum_k \left[\frac{f(k) U}{D_s} \right]^{1/2} \\ &= \frac{1}{N\xi} \sum_k \left[\frac{f(k)}{D_s \kappa} \right]^{1/2} \end{aligned} \quad (\text{A.48})$$

where $U = \left(\frac{1}{\kappa \xi^2} \right)$.

Finite temperatures

The summation over frequency can be performed by introducing a contour integral given by[295],

$$\sum_{n=-\infty}^{\infty} \frac{1}{\omega_n^2 + \omega_\alpha^2} = \frac{\beta}{2\pi i} \int_{C_1} \frac{dz}{(e^{\beta z} - 1)(-z^2 + \omega_\alpha^2)} \quad (\text{A.49})$$

where $z = i\omega_n$.

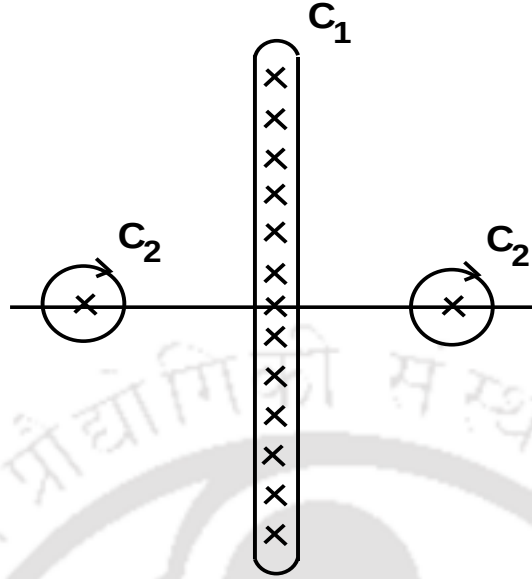


FIGURE A.1: Contours C_1 and C_2 for solving the integral in Eq. (A.49). C_1 is the contour in the imaginary axis enclosing the poles at $z = i\omega_n$. C_2 enclose the poles at $z = \omega_\alpha$ and $z = -\omega_\alpha$.

The contributions of the two poles which lie inside C_2 is obtained using residue theorem which gives,

$$\begin{aligned} \frac{\beta}{2\pi i} \oint_{C_2} \frac{dz}{(e^{\beta z} - 1)(-z^2 + \omega_\alpha^2)} &= \frac{\beta}{2\omega_\alpha} \left[\frac{1}{e^{\beta\omega_\alpha} - 1} + \frac{1}{1 - e^{-\beta\omega_\alpha}} \right] \\ &= \frac{\beta}{2\omega_\alpha} \coth\left(\frac{\beta\omega_\alpha}{2}\right) \end{aligned} \quad (\text{A.50})$$

Using Eq. (A.50) in Eq. (A.44), we get,

$$\langle \bar{\theta}_{ij}^2 \rangle_0 = \frac{1}{N\xi} \sum_k \left[\frac{f(k)}{D_s k} \right]^{1/2} \coth \left[\frac{1}{2T\xi} \left(\frac{f(k)}{D_s k} \right)^{1/2} \right] \quad (\text{A.51})$$

where $\hbar = 1$ is taken.

Note that the above expression reduces to Eq. (A.48) when T is substituted to be zero (since $\coth(x) = 1$ when $x \rightarrow \infty$).

We now substitute Eq. (A.51) in Eq. (A.21) and obtain,

$$\begin{aligned} D_s &= D_{s0} \exp \left[-\frac{1}{N\xi} \sum_k \left[\frac{f(k)}{\kappa D_s} \right]^{1/2} \coth \left(\frac{1}{2T\xi} \left[\frac{f(k) D_s}{\kappa} \right]^{1/2} \right) \right] \\ &= D_{s0} \exp \left[\frac{-\phi(\kappa, \xi, T)}{\xi \sqrt{\kappa D_s}} \right] \end{aligned} \quad (\text{A.52})$$

Here κ is the compressibility ($= \frac{dn}{d\mu}$) and ξ is the coherence length. ϕ in the above expression is given by,

$$\phi = \frac{1}{N} \left[\sum_k \left(\sqrt{f(k)} \coth \left(\frac{\beta}{2\xi} \sqrt{\left(\frac{D_s f(k)}{\kappa} \right)} \right) \right) \right] \quad (\text{A.53})$$

as noted in Eq. (2.50).



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1. Poulumi Dey and Saurabh Basu, *Signatures of superconductor to insulator transition in spin imbalanced superfluid fermi gas in a harmonic confinement*

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