ULTRA-COLD ATOMS ON OPTICAL LATTICES

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DISSERTATION

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Abstract

The field of ultra-cold atoms, since the achievement of Bose-Einstein Condensation (Anderson et al., 1995; Davis et al., 1995; Bradley et al., 1995), have seen an immensely growing interest over the past decade. With the creation of optical lattices, new possibilities of studying some of the widely used models in condensed matter have opened up. In this dissertation we shall study two such problems, one with two component attractive fermions on optical lattices, and the second one with a circular array of Josephson junctions made with independent BECs.

In the first part of the dissertation, we shall study fermions with an attractive interaction in an optical lattice with a single-band Hubbard model away from half-filling with on-site attraction $U$ and nearest neighbor hopping $t$. Our goal is to understand the crossover from BCS (Bardeen-Cooper-Schrieffer) superfluidity in the weak attraction limit to the BEC of molecules in the strong attraction limit, with particular emphasis on how this crossover in an optical lattice differs from the much better studied continuum problem. We use a large $N$ theory with $\text{Sp}(2N)$ symmetry to study the fluctuations beyond mean field theory. At $T = 0$, we calculate across the crossover various observables, including chemical potential, gap, ground state energy, speed of sound and compressibility. The superfluid density $n_s$ is found to have non-trivial $U/t$ dependence in this lattice system. We show that the transition temperature $T_c$ scales with the energy gap in the weak coupling limit but crosses over to a $t^2/U$ scaling in the BEC limit, where phase fluctuations controlled by $n_s$ determine $T_c$. We also find, quite contrary to our expectations, that in the strong coupling limit, the
large-$N$ theory gives qualitatively wrong trends for compressibility. A comparison with a simple Hartree shifted BCS theory, which takes into account both pairing and Hartree shifts, and correctly recovers the atomic limit and the right qualitative trend for compressibility, reveals that the large-$N$ theory on the lattice, although considers a larger number of diagrams, is in fact inferior to the simpler Hartree shifted BCS theory. The failure of the large-$N$ approach is explained by noting (i) the importance of Hartree shift in lattice problems, and (ii) inability of the large-$N$ approach to treat particle-particle and particle-hole channels at equal footing at the saddle point level.

In the second half of the dissertation, we investigate the problem of vortex trapping in cyclically coupled Bose-Josephson junctions. Starting with $N$ independent BECs we couple the condensates through Josephson links and allow the system to reach a stable circulation by adding a dissipative term in our semiclassical equations of motion. The central question we address is what is the probability to trap a vortex with winding number $m$. Our numerical simulations reveal that the final distribution of winding numbers is narrower than the initial distribution of total phases, indicating an increased probability for no-vortex configurations. Specifically, the final width of the distribution of winding numbers for $N$ sites scales as $\lambda N^\alpha$, where $\alpha = 0.47 \pm 0.01$ and $\lambda < 0.67$ (value predicted for the initial distribution). The actual value of $\lambda$ is found to depend on the strength of dissipation. The nonlinearity of the problem also manifests itself in the result that it is possible to obtain a non-zero circulation starting with zero total phase around the loop.
To my parents
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Chapter 1

Introduction

One of the most striking manifestations of many body collective effects in nature is the complex of phenomena called superfluidity. The modern day theory of superfluidity rests on the fundamental assumption that Bose systems like liquid He$^4$, under certain conditions, undergo a phase transition into a state where a finite fraction of the atoms occupy *one and only one* of the single particle states from an orthonormal basis, while the rest of the states maintain a population of the order 1 or less. This remarkable phase transition is known as Bose-Einstein condensation (for a detailed definition see (Leggett, 2001, 2006)) and its observation in trapped dilute alkali gases like Rb$^{87}$ in 2001 (Anderson et al., 1995; Davis et al., 1995; Bradley et al., 1995) has ushered in a new era of research in atomic and molecular physics. Although Bose-Einstein condensation had been observed in liquid He$^4$ more than sixty years earlier, the advantage that was gained with dilute alkali gases over liquid He$^4$ was a significant conceptual simplicity. While only about 10% of the atoms in He$^4$ are estimated to occupy the "condensate wavefunction" close to $T = 0$ because of strong interactions, the dilute alkali gases in the first generation Bose-Einstein condensates (BECs) were weakly interacting and hence made themselves amenable to studies using the macroscopic condensate wavefunction as a description of the whole system. Since then, over the past decade, experiments with ultracold gases have moved to whole new levels of complexities. With the realization of artificial lattice potentials created by laser light (Greiner et al., 2002), these systems are now increasingly being used to mimic several widely studied models in condensed matter physics (Jaksch and Zoller, 2005). While
the applicability of these models to real condensed matter systems is a completely different issue, and admittedly an important one, experiments with ultracold atoms could help us understand the physics contained in these models where a complete theoretical description might otherwise involve several sets of assumptions. Remarkably, not only have these experiments invited a huge amount of theoretical interest in their interpretations but have also inspired new research directions in theoretical physics. A major development further expanding the scope of research in the field was the achievement of Fermi degeneracy (DeMarco and Jin, 1999) and now fermions like K\(^{40}\) (Greiner et al., 2003; Zwierlein et al., 2003) and Li\(^{6}\) (Jochim et al., 2003) are being studied as much as their bosonic counterparts. A great deal of tunability of various parameters and in a time dependent way have encouraged theoretical research to explore, respectively, richer phase diagrams and far from equilibrium dynamics for various systems. A corner stone along the line has been the application of Feshbach resonances (Stoof et al., 1996; Stan et al., 2004) to independently tune the inter-particle interactions while keeping other parameters (like lattice depth) fixed. This new feature has led the research in ultracold atoms to a plethora of interesting problems in strongly correlated systems.

A second exciting research direction with ultracold gases lies in putting to test some of the fundamental tenets of quantum mechanics like measurement (Andrews et al., 1995) and decoherence (Leggett, 1998b). At the heart of this research lies the existence of a coherent, macroscopic matter wave upon which a measurement can be made either by making it interfere with itself or by looking at noise correlations. A good degree of isolation from its surroundings ensures that cold atomic systems have long lived coherence that can be studied in experimental time frames. This has further led to the intriguing possibility of realization of a qubit for quantum computing (Chu, 2002; Monroe, 2002; Jaksch et al., 1999). This dissertation will theoretically address two separate problems in the topic of ultracold atoms on optical lattices. We shall
begin with an overview.

1.1 BCS-BEC crossover - an overview

The problem that we shall discuss in the first half of the dissertation is the problem of crossover between a Bardeen-Cooper-Schrieffer (BCS) state of weakly bound cooper pairs to a BEC of tightly bound diatomic molecules in a system of two-component fermions on an optical lattice. Since its formulation in 1957, the BCS theory (Bardeen et al., 1957a,b) has arguably been the most widely used theories in condensed matter physics. According to the BCS theory, electrons in a metal with opposite spins and momenta and with phonon-mediated effectively attractive interactions, can Bose-condense into a spin-singlet state (s-wave) where the center of mass momentum of the pair is zero. One then has a macroscopic occupation of the zero center of mass momentum state (in technical terms, one of the eigenvalues of the two-particle reduced density matrix is of the order $N$, where $N$ is the total number of electrons, while the rest of the eigenvalues remain small). The ground state wavefunction is symmetric under the exchange of two pairs (here both the momentum and spin degrees of freedom of a pair need to be taken into account) and hence the BCS state can also alternatively be viewed as a “pseudo-BEC” giving rise to superconductivity or superfluidity of electron pairs commonly called Cooper pairs. In real space, two members of a Cooper pair are however widely separated - the Cooper pair radius $\xi_0$ at $T = 0$ in Al is $\approx 15,000 \, \text{Å}$ while the lattice spacing is $\approx 4 \, \text{Å}$. Now let us compare this situation to the earlier considered case of He$^4$. A He$^4$ atom is constituted of 6 fermions - 2 electrons, 2 protons and 2 neutrons. Nevertheless, He$^4$ atoms do Bose-condense as tightly bound composite bosons. One can therefore ask the hypothetical question: Starting from a BCS state of loosely bound Cooper pairs, if we increase the strength of attraction between the fermions, how does the system evolve to a BEC of tightly
bound pairs? This question was addressed by Eagles in 1969 and by Leggett in 1980, who used the BCS wavefunction as a “naive ansatz” for the wavefunction across the crossover and showed that the two limits interpolate smoothly (Leggett, 1980). In order to appreciate the non-triviality of this result, it is important to note that the two limits are qualitatively different. Firstly, pairing in the strong coupling regime is solely brought about by the strong attraction between two fermions of opposite spins. On the other hand, Cooper pairing relies heavily on the existence of a degenerate Fermi sea so that even an infinitesimally weak attraction can lead to pair formation in free space. Secondly, in the limit of strong coupling, which we shall term the “BEC limit”, the process of pair formation is quite different from Bose condensation. Indeed we shall see in Chapter 2, that the energy of dissociation of a pair in this regime would be orders of magnitude larger than the critical temperature $T_c$ for Bose condensation. On the other hand, in the weak coupling limit, which we shall call the “BCS limit”, the formation of Cooper pairs and the condensation of pairs are essentially the same phenomenon. In this limit, it would turn out to be thermodynamically unfavorable to have pairs formed and not condense. Quite naturally because of this difference, the relevant low energy excitations of the system would obey different statistics in the two limits - fermionic in the BCS limit and bosonic in the BEC limit.

The hallmark of Leggett’s “naive ansatz”, in retrospect, is that it captures the correct qualitative picture at $T = 0$ and all subsequent corrections to this picture have mostly been quantitative. In 1985, Nozières and Schmitt-Rink (NSR) calculated the transition temperature $T_c$ at which condensation takes place by looking for pairing instabilities in a normal gas (Nozières and Schmitt-Rink, 1985). NSR also extended Leggett’s analysis at $T = 0$ for the continuum, to a lattice system. One year later, Bednorz and Müller (1986) discovered high temperature superconductors with critical temperatures greater than the boiling point of liquid Nitrogen (77K) in

\footnote{name borrowed from Leggett (2006)}
copper-oxide based compounds. These compounds are highly anisotropic with the Copper and Oxygen atoms arranged in a two-dimensional plane. To a first approximation, the structure of a CuO₂ plane is that of a simple square lattice with a lattice constant \( \approx 3.84 \) Å. If one applied BCS theory to these compounds one would find that the approximate Cooper pair size at \( T = 0 \) is \( \xi_0 \approx 15 \) Å, which is only 5 times larger than the lattice spacing and significantly smaller than the pair size of the conventional superconductors. This observation led to a resurgence of interest in the crossover problem and attempts were made to explain the several features of high \( T_c \) superconductors as a strong coupling limit of the conventional BCS theory. Randeria and co-workers studied the problem in two dimensions (Randeria et al., 1989, 1990), which has some special features, and also analyzed the collective modes at \( T = 0 \) within a random phase approximation (RPA). They addressed the problem on a lattice (by considering the attractive Hubbard model) and confirmed that the crossover was indeed a smooth one; the collective mode evolved from the Anderson mode in the weak coupling to the Bogoliubov sound mode in the strong coupling limit (Belkhir and Randeria, 1992). The plasmon, which was reminiscent of the Anderson mode in charged systems, was shown to have a similarly smooth crossover (Belkhir and Randeria, 1994). In 1993, Sa de Melo, Engelbrecht and Randeria reformulated the NSR calculation and determined the width of the Ginzburg-Landau regime (Sa de Melo et al., 1993). The phase diagram of the system revealed a region of "pre-formed pairs" in strong coupling regime, which had striking similarities with the proposed pseudo-gap phase in the cuprates. Note that the wavefunction symmetry in cuprates was at that time a contentious issue and it was not settled until 1993 when it was conclusively shown by van Harlingen and co-workers to be \( d \)-wave (Wollman et al., 1993) unlike the \( s \)-wave symmetry in BCS theory.

On the computational side, Scalapino and co-workers had been using Quantum Monte Carlo (QMC) to study the two-dimensional attractive Hubbard model since
the late 80's (Scalettar et al., 1986). Unlike the repulsive case, QMC with attractive fermions did not suffer the sign problem (Hirsch, 1983) that came from the antisymmetry of wavefunctions under the exchange of two fermions (Loh Jr et al., 1990). The QMC results are still widely accepted as the closest to being accurate in the crossover problem, both in the continuum and on the lattice. It was shown that the lattice system was unstable to a new order, namely a Charge Density Wave (CDW) order at half-filling (filling is defined as the number of fermions divided by the number of lattice sites). As a function of filling, the pairing-field correlations became more dominant and CDW ordering was suppressed. No phase separation was observed (Scalettar et al., 1989).

QMC also helped to extend the study of the crossover problem to non-zero temperatures where an RPA was shown to fail. The normal state spin susceptibility for intermediate coupling was shown to be strongly dependent on temperature, while the charge susceptibility in normal state showed almost no temperature dependence. This “spin-charge separation” was pitched as an explanation to the spin-gap behavior observed in NMR experiments in some of the cuprates (Randeria et al., 1992; Trivedi and Randeria, 1995). These authors argued that the normal state of a superconductor with a pair size of the order of interparticle spacing naturally show a pairing pseudogap for a range of $T$ above their $T_c$, despite being in a degenerate Fermi regime.

The pseudogap phase in the underdoped high $T_c$ superconductors is however a much more complicated phenomena than the pairing pseudogap in the attractive Hubbard model. The latter is merely a simple model which captures one feature of the cuprates: pairing above $T_c$. The high $T_c$ cuprate pseudogap, in addition to sharing this feature, has several other characteristics: $d$-wave pairing (Wollman et al., 1993) with low energy fermionic excitations, the proximity to a Mott insulating state and the existence of order parameters like antiferromagnetism that compete with superconductivity. It was therefore generally agreed that although the attractive Hubbard
model could give qualitative insight into many features shown by the cuprates, the true mechanism of superconductivity in these compounds lied elsewhere.

It would not be until a decade later that interest in the crossover problem would revive due to experiments with ultracold atomic gases. The first major development in realizing the crossover phenomenon in ultracold atoms was the achievement of Fermi degeneracy by DeMarco and Jin (1999) and later by others. In 1996 Stoof et al. had proposed that Feshbach resonances in a degenerate Fermi gas like Li\(^6\) could be used to tune the attractive interaction between two hyperfine states and hence there was a possibility to study the crossover phenomenon in these systems. These ideas had earlier been proposed by Modawi (1981) to induce Cooper pairing in spin-polarized deuterium. After Stoof's proposal it was further established that weakly bound fermion pair states could be stable near Feshbach resonances. The achievement of Fermi degeneracy along with the application of Feshbach resonances (Stan et al., 2004) to tune the interactions finally led to the formation of molecular condensates (Greiner et al. (2003); Jochim et al. (2003); Zwierlein et al. (2003)) and finally allowed one to study the crossover phenomenon with ultracold atoms. Radiofrequency (rf) measurements were used to probe the presence of pairing (Gupta et al., 2003) and superfluidity in these systems was established by the observation of quantized vorticity (Zwierlein et al., 2005). Recently, these studies have been extended to include unequal populations of "spin up" and "spin down" atoms in presence of the trap, and the suppression of pairing due to a mismatch of Fermi surfaces has been studied.

On the theory side, several analytical techniques like functional integral formalism (Diener et al., 2008), self-consistent approximations (Haussmann et al., 2007), large \(N\) expansion (Veillette et al., 2007; Nikolic and Sachdev, 2007) and numerical techniques like QMC (Carlson et al., 2003; Burovski et al., 2006) and Dynamical Mean Field Theory (DMFT) (Garg et al., 2005; Toschi et al., 2005) have been used to reformulate the crossover problem in the continuum. One of the few exact results that
were reported was the calculation of the dimer-dimer scattering length in the BEC regime by (Petrov et al., 2004). Their value for the dimer-dimer scattering length has become one of the standard figures along with QMC results (Carlson et al., 2003) for testing quantitative accuracies for crossover theories in the BEC limit.

More recently, fermi gases like Li$^6$ (Stöferle et al., 2006) and K$^{40}$ (Chin et al., 2006) have been loaded onto optical lattices. Experiments with fermions on optical lattices have so far only looked for some basic properties of degenerate Fermi gas like the existence of a Fermi surface and presence of a band insulator at half-filling. While cooling a degenerate Fermi gas to temperatures below the band gap in deep optical lattices poses a technical challenge in experiments, it is quite likely to be overcome in near future. The lattice problem in the light of ultracold experiments has already attracted a lot of theoretical interest. The critical temperature has been calculated across the crossover and at unitarity (a concept introduced in Chapter 2) using self-consistent methods (Haussmann et al., 2007) and diagrammatic QMC (Burovski et al., 2006) respectively. DMFT has been used to study the phase diagram of the attractive Hubbard model in presence of a mass imbalance between the two species (Dao et al., 2007). Dynamical instabilities close to half-filling have been studied and a possibility of supersolid phase has recently been reported (Burkov and Paramekanti, 2008).

We had several motivations for understanding better the BCS-BEC crossover in an optical lattice. The lattice crossover problem is different from the extensively studied continuum problem in that the lack of Galilean invariance on a lattice means that the superfluid density at $T = 0$ is no longer the total density, and is a nontrivial function of the interaction strength. This is likely to have an important effect on the phase diagram based on the following argument (Emery and Kivelson, 1995). The transition temperature $T_c$ is determined by those excitations which can most easily destroy the condensate. In the BCS limit it is quasiparticle excitations corresponding to breaking pairs which dominate the thermodynamics and thus the gap energy scale determines
However if one has a superconductor where the phase stiffness, closely related to the superfluid density $\rho_s$, which has an energy scale much smaller than the energy gap, then $T_c$ is determined by $\rho_s$. One of our goals was to see if this is realized in the BEC limit of the crossover. In addition the lattice problem also has several other features different from the continuum case, such as a particle-hole constraint on the thermodynamics and the importance of Hartree shifts, and we wanted to investigate how these are properly taken into account in the crossover analysis. This work was done in collaboration with Roberto Diener and Mohit Randeria (Ghosh et al., in preparation).

1.2 Statistics of vortex trapping in quenched systems - motivation and overview

In this section we give a general overview of the second part of the dissertation that studies a far from equilibrium situation in Josephson junction arrays. Our analysis is motivated by the Kibble-Zurek scenario for the formation of topological defects in systems undergoing a quench through a second order phase transition. It has long been believed that the vacuum immediately following the Big Bang possessed a higher symmetry than what we observe today. The subsequent expansion and cooling of the universe led to a series of symmetry-breaking phase transitions that split apart the four fundamental forces as we know them now. In 1976 Kibble proposed that if the above scenario was correct, then these rapid symmetry-breaking phase transitions in the early universe could leave behind (meta)stable topological defects (e.g. cosmic strings, magnetic monopoles etc.) (Kibble, 1976) and these defects could be responsible for seeding large-scale structures, for anisotropy of the microwave background radiation, and predominance of matter over antimatter. The conceptual idea behind the proposed mechanism for the formation of topological defects is quite a simple
one. The scenario proposes that during the rapid expansion of the early universe, causally disconnected regions of space, called “domains” were formed. When some continuous gauge symmetry like electroweak symmetry was broken in each of these regions, local order parameters, with indefinite relative phases were formed. Eventually, when these regions got connected causally, a random relative phase was established between the local order parameters. This opened up the possibility to incorporate topological defects in the resulting global order parameter where the overall phase around a loop could wind by an integer multiple of $2\pi$. This later condition not only ensures the single-valuedness property of the order parameter but any integer multiple other than zero would result in a topological defect. Zurek generalized Kibble’s ideas in 1985 to all phase transitions that broke continuous symmetry and applied them to He$^4$ undergoing a quench from a normal state to a superfluid phase through the $\lambda$-transition (Zurek, 1985). This general scenario for the formation of topological defects, which is now called the Kibble-Zurek (KZ) scenario, derives from the fact that the response time of the system to any change in parameters (like temperature or pressure) that drives the system through the transition, diverges at the transition. Consequently, any phase transition that is not accomplished infinitesimally slowly, would go through a non-adiabatic phase, passing through which, the system would emerge with independent domains. The rest of the argument follows from Kibble’s original scenario.

Zurek applied this scenario to the case of He$^4$ undergoing a normal-superfluid transition that has been associated to the breaking of global $U(1)$ gauge symmetry. He proposed that He$^4$ contained in an annular geometry with a radius much larger than the cross-sectional radius, can be quenched through the $\lambda$-point by reducing the pressure rapidly. He then argued that the resulting superfluid should, à la Kibble, consist of independent domains along the circumference of the annulus. Adjacent domains would eventually establish a relative phase, such that the sum total of the
relative phases around the annulus is an integral multiple of \(2\pi\). Since, the relative phases are chosen randomly, the resulting phase mismatch around the loop would have, from the Central Limit Theorem, a dispersion proportional to the number of such independent domains. The net result would be a metastable superflow, the direction and magnitude of which would vary from run to run. Zurek's estimate of the resulting superfluid velocity (discussed at length in Chapter 2) suggests that such superflows could be detected in experiments.

Zurek's proposal prompted a series of experiments, the first of which was by Dodd et al. (1999) at the University of Lancaster. The set-up of the Lancaster experiments involved \(\text{He}^4\) in a cylindrical container and yielded no vorticity, although their first set of experiments in 1994 had *prima facie* supported the KZ scenario. Further, their experimental setup would suggest that even if one had observed vortices, other mechanisms for their production (e.g. fluid rubbing against the walls of the container) could not be ruled out. Following the Lancaster experiments, an alternative experimental situation that also mimics the "primordial fireball" was conceived in \(\text{He}^3\) by Bäuerle et al. (1996) and Ruutu et al. (1996). These experiments relied on the following neutron-induced nuclear reaction: \(\text{n} + \text{He}^3 \rightarrow \text{p} + \text{He}^3 + 0.76\,\text{Mev}\), to create local "hot-spots" with temperature greater than \(T_c\) in bulk superfluid \(\text{He}^3\). The idea is that, as quasiparticles rapidly diffuse away from these hot-spots, they would leave behind a normal fluid below \(T_c\). These bubbles of normal fluid would then be quenched through \(T_c\) thereby creating the possibility of formation of a random network of vortices via the Kibble mechanism. The advantage these experiments had over the Lancaster experiments was that a much higher quench rate could be achieved in the later experiments compared to mechanical expansion. The first set of experiments by the Grenoble group relied on a calorimetric technique by which they found an energy deficit of \(\sim 50\,\text{KeV}\) from the total energy of \(0.76\,\text{MeV}\) released by the above nuclear reaction and ascribed this energy deficit to vortex formation.
The obvious weakness of this interpretation is that it precludes all alternative energy sinks. Indeed, Leggett (1998b) pointed out that one such energy sink could be the so-called molecular excimers which consist of two quasibound He₃ atoms, one of them being in an excited state. The lifetime of these excimers are estimated around 10-15s, and could possibly account for the energy deficit. The second set of experiments at Helsinki, involved a rotating cryostat and used NMR to measure vorticity directly. In the rest frame of the normal liquid, the superfluid would have a counterflow through the vortex loops. One can then derive from Zurek’s scenario a scaling of the total number of vortex lines with the velocity of the counterflow and the Helsinki data seem to fit this scaling well. More recent efforts to test this scenario have involved Josephson tunnel junctions in high Tc superconductors like YBCO (Carmi et al., 2000) and ordinary superconductors like Nb (Monaco et al., 2002, 2009). The most recent of these experiments using thin Nb loops have confirmed spontaneous fluxoid formation during rapid normal-superconducting phase transitions; however the probability of vortex formation scales with the quench time with an exponent that is two times the value predicted by Zurek. Finally, Scherer et al. (2006) have investigated vortex formation when multiple Rb⁸⁷ BECs are merged in a confining potential. They find when three BECs, initially separated by a trapping potential are merged to form one BEC, by either lowering of the barrier or during the final stages of evaporative cooling for low barrier energies, vortices are formed in the final BEC. Scherer et al. interpret their results along the arguments of Zurek: The three independent BECs have arbitrary relative phases between them. When they are merged their relative phases get established and on some runs of the experiment the total phase winding around a loop ends up being ±2π and a superflow is established.

The motivation of the current thesis is to revisit Zurek’s assumption that the initial distribution of sum total of relative phases around a loop correctly reflects the distribution of stable winding numbers, a vital difference between the two stemming
from the fact that unequal relative phases and hence unequal currents in the individual junctions is a situation far from equilibrium. We shall address this point about stability by considering an analogous situation where $N$ independent BECs arranged on a ring are suddenly connected through weak Josephson links. We shall study the dynamics in presence of a phenomenological Ohmic damping of individual Josephson currents and phase slips between adjacent BECs. We shall show that if the system has time to settle to a stable or metastable fixed point, then the final distribution of stable winding numbers is much narrower than the initial distribution of relative phases around the loop. The width of the final distribution is shown to be dependent on the strength of the phenomenological damping characterized by $\gamma$ and for some range of $\gamma$, stronger damping is shown to enhance the probability for no-vortex configuration. Finally, it will be shown that due to the non-linearity of the equations of motion, it is even possible to end up with a finite circulation starting with a zero sum total of relative phases around the loop. This work was done in collaboration with Fernando Sols (Ghosh and Sols, 2008).
Chapter 2

BCS-BEC crossover in optical lattice

2.1 Introduction

The problem of the BCS-BEC crossover of strongly interacting fermions has been well studied in the continuum both theoretically (Leggett, 1980; Eagles, 1969; Nozieres and Schmitt-Rink, 1985; Randeria, 1995; Sa de Melo et al., 1993; Diener et al., 2008; Engelbrecht et al., 1997; Haussmann et al., 2007; Veillette et al., 2007; Nikolic and Sachdev, 2007; Carlson et al., 2003; Pieri et al., 2005; Chen et al., 2005) and experimentally (Greiner et al., 2003; Zwierlein et al., 2003). The system smoothly interpolates between a BCS state of loosely bound Cooper pairs to a Bose-Einstein condensate of tightly bound diatomic molecules. The Leggett-BCS mean field theory gives qualitatively correct physics at $T = 0$ across the crossover and methods like functional integral formalism (Sa de Melo et al., 1993; Diener et al., 2008; Engelbrecht et al., 1997), self-consistent approximations (Haussmann et al., 2007), large $N$ expansions (Veillette et al., 2007; Nikolic and Sachdev, 2007) and quantum Monte Carlo (Carlson et al., 2003; Pieri et al., 2005) have been used to find quantitative corrections. Experiments have demonstrated the condensation of molecules in the BEC limit (Greiner et al., 2003) and the superfluidity of the system across resonance has been observed (Zwierlein et al., 2003).

The inclusion of a lattice in the system leads to several qualitative differences with the continuum which are listed as follows:

(i) One of the key features distinguishing a lattice system from the continuum is the
dependence on interaction strength and filling fraction of the superfluid stiffness of the gas even at $T = 0$. This is in contrast to the continuum case, where the $T = 0$ superfluid stiffness is fixed by the particle mass and density due to Galilean invariance. Consequently, when phase fluctuations play a dominant role in the loss of phase coherence and the superfluid stiffness sets the scale for transition temperature (Emery and Kivelson, 1995), the above mentioned difference between the lattice and the continuum becomes explicit.

(ii) A second difference, which is not entirely unrelated to point (i), that arises between the continuum and the lattice is regarding the effective mass of the bound pairs in the BEC limit. In the continuum, the mass of the bound pair in the BEC limit is simply twice the mass of the fermions and hence does not scale with the coupling strength. In contrast, the effective mass of the bosons on the lattice becomes increasing larger with the strength of the coupling. This is due to the fact that the bosons on the lattice can only move around by virtual ionization, and hence the corresponding hopping matrix element for the bosons, calculated within a simple perturbation theory, has an energy denominator equal to the coupling strength. Consequently, the boson mass which is inversely proportional to the hopping becomes larger with the strength of coupling.

(iii) Further, as we shall see, there is a particle-hole transformation on the lattice that puts additional constraints on thermodynamics. On a bipartite lattice one can derive relations between various thermodynamic quantities on the particle and the hole sides. Any physical theory for the lattice should therefore respect these additional constraints.

(iv) Finally, on a lattice, there is an emergence of a new density order (Charge Density Wave) at half-filling (number of fermions equal to the number of lattice sites) that competes with the superfluid (pairing) order. This new order arises because at half-filling the lattice Hamiltonian has a higher symmetry (SU(2)) in the spin space that is spontaneously broken.
Our primary objective for studying attractive fermionic atoms on a lattice is therefore to understand how the broken continuous translational invariance affects various physical quantities across the crossover. Moreover, there is a growing interest in performing experiments with ultra-cold fermionic clouds of both $^{40}$K (Stöferle et al., 2006) and $^6$Li (Chin et al., 2006) atoms in optical lattices, and in future these experiments should be able to test the findings of our current work.

In this chapter we shall study the BCS-BEC crossover in a gas of spin 1/2 fermions on a three-dimensional cubic lattice away from half-filling (we shall therefore not be concerned with the CDW order). It was mentioned in Chapter 1 that Leggett’s “naive ansatz” for the wavefunction across the crossover, which was simply applying the BCS mean field theory across the crossover, together with self-consistent calculation of the chemical potential, captured all the correct qualitative trends at $T = 0$. However, this simple mean field theory neglects all pairing fluctuations and hence all subsequent corrections to the BCS mean field theory are aimed at capturing these effects. For example, a functional integral approach (Diener et al., 2008) in the continuum, includes pairing fluctuations up to Gaussian order and is able to inter alia capture the Fermi liquid corrections in the BCS limit, give a quantitatively better estimate of the dimer-dimer scattering length in the BEC limit, and account for $\sim 35\%$ reduction of energy density at unitarity (unitarity is explained below).

However, it is easy to check that the BCS mean field theory, which is the saddle point of the functional integral method, when applied to the lattice does not respect the particle-hole constraints. A remedy to the problem is to include a Hartree shift (which is expected to come at the Gaussian order in a functional integral formalism) at the mean field level. At this point one encounters a technical difficulty (explained below) with the functional integral method. All this necessitates a different approach that starts with a Hartree shifted mean field theory and then takes into account the Gaussian fluctuations. We shall see that this theory has a major drawback: it predicts,
in the strong coupling regime, an unphysical negative compressibility indicative of a phase separation when there exists none (see Appendix A). We suspect that a possible reason for this could be an overestimation of the feedback of the Gaussian fluctuations in the number and gap equations.

With this caveat, we next turn to a large-$N$ approach on the lattice where we generalize the problem to include $N$ arbitrary flavors for each spin species. In this approach, we shall use an expansion of various physical quantities in orders of $1/N$ assuming $N$ is large. The mean field theory with this Hamiltonian, which is essentially the BCS mean field theory, will respect the new set of particle-hole constraints imposed by the large-$N$ Hamiltonian and will be exact in the limit $N \to \infty$. In the other limit $N = 1$, the large $N$ model will correctly describe the physical problem of two-component fermions on a lattice. The virtue of doing this is Gaussian fluctuations will come at $O(1/N)$ and accordingly their feedback will be linearized to $O(1/N)$ in the number and gap equations. Indeed, as we had anticipated, the compressibility comes out to be positive in the strong coupling limit. Our goal therefore is to develop, using (in principle) a systematic expansion in $1/N$, a mean field theory that is zeroth order in $1/N$ and fluctuations upto $O(1/N)$, and calculate various physical quantities across the crossover for the large-$N$ model. We shall then set $N = 1$ and check if the qualitative and quantitative trends match with what we expect physically.

It will be shown, that the large-$N$ results compare well with the standard BCS results in the weak coupling limit. In the strong coupling limit, the large-$N$ results will have the correct qualitative trends for all quantities, barring the compressibility which will be shown to scale as the inverse of the coupling strength. A comparison with the simple Hartree-shifted BCS mean field theory, which is quite accurate in the strong coupling regime and captures the correct qualitative trend for the compressibility (can be obtained quite independently from considering the speed of sound), will indicate that the large-$N$ theory is actually quantitatively inferior in the strong coupling limit.
This limitation is explained by noting that the large-$N$ theory does not treat the pairing and density fluctuations at equal footing; the saddle point for the large-$N$ approach does not contain the Hartree shift, which (unlike the continuum) is a well defined quantity across the crossover and plays a significant role in the estimation of compressibility.

The current chapter is organized as follows: In section 2, we shall introduce the Hamiltonian and the large $N$ formalism used in this work. In section 3 we shall discuss the $T = 0$ results for chemical potential, pairing gap, ground state energy, compressibility, and speed of sound. In section 4 we calculate the zero temperature superfluid density. In section 5 we shall outline the calculation and results for the critical temperature. Having calculated various ground state physical quantities and the critical temperature using the large $N$ theory, we shall next compare the results with a Hartree-shifted mean field theory in section 6. In section 7 we shall summarize our conclusions.

### 2.2 Formalism

In this section we first introduce the Hamiltonian that describes fermions on a lattice and give an estimate of unitarity. We then generalize to the case of $N$ flavors with $\text{Sp}(2N)$ symmetry and describe the constraints imposed on the thermodynamics by a particle-hole transformation. In the following subsection we introduce the functional integral formalism for the large $N$ model used in the paper and obtain an effective action. We next develop the mean field theory as a saddle point of the effective action. In the last subsection we set up the theory of Gaussian fluctuations around the saddle point, discuss the spectrum of collective excitations at $O(1/N)$ and make the large $N$ expansions of the gap and number equations.
2.2.1 Hamiltonian

The study of the BCS-BEC crossover in the absence of an optical lattice uses the divergence of the scattering length near a Feshbach resonance to tune the strength of the interactions between the fermions. Although this same technique has been applied to fermions in optical lattices (Chin et al., 2006), the Hamiltonian that describes this system near resonance is poorly understood. This is due to the inherent multi-band nature of the system when the (continuum) scattering length between the atoms diverges (Diener and Ho, 2006). We do not, have a separation of energy scales that would allow us to study an effective Hamiltonian in a single band. As we will show below, however, the lattice strongly modifies the scattering properties of fermions restricted to the lowest band, to the point that it takes a finite amount of on-site interaction to form a (molecular) bound state. Thus, a Feshbach resonance is not needed to achieve a unitary gas in a lattice. The Hamiltonian we will study is the single-band attractive Hubbard Hamiltonian:

\[
H = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) - U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i, \sigma} n_{i\sigma}
\]  

(2.1)

Here \(c_{j\sigma}\) is the fermion annihilation operator at site \(j\), the pseudo-spin index \(\sigma = \uparrow, \downarrow\) represent the two-hyperfine states, \(t\) is the hopping matrix element between adjacent sites and the summation indices \(\langle i, j \rangle\) represent sum over nearest-neighbor sites. The on-site attractive coupling is given by \(-U\) with \(U > 0\), \(n_{i\sigma}\) is the number operator at site \(i\) and \(\mu\) is the chemical potential. For simplicity, we will study homogeneous systems; i.e. we neglect the effects of the (typically harmonic) external trapping potential, which can eventually be included using a local density approximation. Throughout the paper, we have set \(\hbar = k_B = 1\) and we shall use the convention that all 3-momenta sums are summed over the first Brillouin zone and then divided by the total number of lattice sites.
Unitarity is given by the condition for divergence of the two-particle scattering amplitude in vacuum. The quantity that contains the infinite sum over all scattering events between two (spin 1/2) fermions is the four-point vertex function \( \Gamma(q, \omega) = U/(1 + U\Pi(q, \omega)) \), where \( q \) is the total momentum of the pair, and \( \Pi(q, \omega) \) is the two-particle correlation function. Further, the vertex function is related to the scattering amplitude \( f \) by the simple relation \( \Gamma(0, 0) = 4\pi f/m \), \( m \) being the mass of the fermions. A divergence of scattering amplitude thus implies \( \Gamma(0, 0) \rightarrow \infty \) or \( 1 + U\Pi(0, 0) \rightarrow 0 \). Next, the two-particle correlation function is a product of two Green’s functions, and is given by,

\[
\Pi(q, \omega) = \int_{BZ} \frac{dk}{(2\pi)^3} \frac{1}{\omega + \epsilon_{q/2+k} + \epsilon_{q/2-k}},
\]

where the integration is over the Brillouin zone, the energy dispersion \( \epsilon_k = -2t[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)] \), and \( a \) being the lattice constant. The condition for unitarity is thus given by (Burovski et al., 2006):

\[
\frac{1}{U} = -\Pi(0, 0) = -\sum_k \frac{1}{2\epsilon_k} \approx \frac{1}{7.915t}
\]

For most experiments, the values of \( U \) and \( t \) can be more or less independently chosen. While \( U \) is primarily fixed by the magnetic field strength and this can be chosen such that one is always far from a Feshbach resonance, \( t \) can be adjusted by tuning the height of optical lattice. In reality, both \( U \) and \( t \) depend on the lattice depth \( (V_0) \). However, \( t \) has a much stronger exponential dependence on \( V_0 \) in comparison to a linear dependence of \( U \) on \( V_0 \). One can therefore fix \( U \) by fixing the B-field and tune \( t \) across the crossover such that \( U, t \ll \omega_0 \), where \( \omega_0 \) is the zero-point energy in the individual wells of the lattice. Therefore, the single Bloch band picture remains valid for the purpose of studying the BCS-BEC crossover as depicted by Hamiltonian (2.1). Finally, recall that in free space the 3-momenta sum in \( \sum_k 1/2\epsilon_k \) is unbounded at the...
top and hence suffers from ultra-violet divergence. This divergence is regulated by replacing the bare interaction parameter $g$ by the low energy limit of the two-body t-matrix: $m/4\pi a_s = -1/g + \sum_{|k|<\Lambda} 1/(2\epsilon_k)$, where $a_s$ is the s-wave scattering length. The condition for two-body bound state to appear in vacuum is therefore given by $a_s \to \infty$. In a lattice the presence of a Brillouin zone gives a natural cutoff for all momentum sums and hence modifies the condition for unitarity.

The starting point of our large $N$ formalism is a generalization of the Hamiltonian in equation (2.1) to include $N$ fermion flavors

$$H = -t \sum_{\langle ij \rangle, \alpha, \sigma} (c_{i\alpha,\sigma}^\dagger c_{j\alpha,\sigma} + \text{c.c.}) - \frac{U}{N} \sum_{i, \alpha, \alpha'} c_{i\alpha,\uparrow}^\dagger c_{i\alpha',\downarrow}^\dagger c_{i\alpha',\downarrow} c_{i\alpha,\uparrow} - \mu \sum_{i, \alpha, \sigma} n_{i\alpha,\sigma} \quad (2.4)$$

where $\alpha$ is the index for one of the $N$ flavors. This Hamiltonian is invariant under the Sp($2N$) symplectic group (see Appendix B for more details) and reduces to eq. (2.1) setting $N = 1$. As shown in section (2.1.3) the virtue of working with the above form of interaction is that it lends itself to a systematic expansion in the parameter $1/N$ around the mean field theory results, which are exact in the limit $N \to \infty$. Although such an expansion is strictly valid in the large $N$ limit, it is assumed that the general trends of the results found will be correct setting $N = 1$ at the end of the calculation. In addition to the Sp($2N$) symmetry, Hamiltonian (2.4) satisfies the particle-hole symmetry on a lattice, which puts some general constraints on thermodynamic quantities. This is discussed next.

### 2.2.2 Particle-Hole Constraints

Lattice systems have an additional symmetry stemming from the possibility of describing the physics in terms of either particles or holes; the choice of description is usually made in order to simplify the resulting Hamiltonian. In the lattice model the number of fermions per site in a single band model is restricted to $0 \leq n \leq 2$. On a
bipartite lattice (a lattice which can be broken up into two sublattices “A” and “B” such that one has hopping from one kind of site onto another but not on the same sublattice) this leads to a special symmetric point at \( n = 1 \), or half filling. In the case of the Hamiltonian (2.4) we can obtain an exact relationship between a system with \( n \) fermions (particles) per flavor and one with \( 2 - n \) fermions (holes) per flavor.

Let us for the moment work in the canonical ensemble and look for the ground state of the Hamiltonian (2.4) with the constraint that the number of particles per site is \( n = n_{\alpha,1} + n_{\alpha,\downarrow} \). If we now perform the particle-hole transformation \( c_{i,\alpha}\sigma\dagger = (-1)^i d_{i,\alpha}\sigma \) \(^1\) it can be easily verified that the kinetic energy term maintains its form with the replacement of the \( c \) operators with \( d \) operators. On the other hand, the on-site interaction term (with the site index omitted for clarity) transforms as

\[
\frac{U}{N} \sum_{\alpha,\alpha'} c_{i,\alpha}\dagger c_{i,\alpha'} c_{i,\alpha'}\dagger c_{i,\alpha}\dagger \to -\frac{U}{N} \sum_{\alpha,\alpha'} d_{i,\alpha}\dagger d_{i,\alpha'} d_{i,\alpha'}\dagger d_{i,\alpha}\dagger + \frac{U}{N} \left( -N + \sum_{\alpha,\sigma} d_{i,\alpha}\dagger d_{i,\alpha}\right)
\]

Given that \( d_{i,\alpha}\dagger d_{i,\alpha} + d_{i,\alpha}\dagger d_{i,\alpha} = 2 - n \) is fixed in the calculation the terms in the second line of (2.5) are constant within the Hilbert space of interest. Thus, the Hamiltonian maintains its operational form under the particle-hole transformation and the ground state wavefunction for a system of \( n \) particles per flavor is related to the ground state wavefunction for a system of \( 2 - n \) particles per flavor. Their corresponding energies related as

\[
\mathcal{E}(n) + \frac{Un^2}{4} = \mathcal{E}(2 - n) + \frac{U(2 - n)^2}{4}.
\]  
(2.5)

Differentiating with respect to \( n \) we see that the chemical potential, defined as \( \mu(n) = \partial \mathcal{E}(n)/\partial (Nn) \), satisfies

\[
\mu(2 - n) = -\mu(n) - \frac{U}{N}
\]  
(2.6)

\(^1\)In 3D, \( i \) at a given site can be thought of as a sum of the lattice indices in the 3 orthogonal directions. Note, the factor \((-1)^i\) then induces a relative (-) sign between adjacent pairs of sites on a bipartite lattice e.g. a cubic lattice.
Finally, the thermodynamic potential \( \Omega(\mu) = \mathcal{E}(n(\mu)) - \mu n N \) which is the quantity that we will calculate in the grandcanonical ensemble, satisfies

\[
\Omega(-\mu - \frac{U}{N}) = \mathcal{E}(2 - n) - (\mu - \frac{U}{N})(2 - n) N
\]

\[
= \Omega(\mu) + 2\mu N + U
\]

which can be written in the symmetric form

\[
\Omega(\mu) + \mu N = \Omega(-\mu - \frac{U}{N}) + (-\mu - \frac{U}{N})N
\]

We stress that any approximation method used to solve the problem would have to satisfy this symmetry in order to yield physically consistent results. In the case of the large-\(N\) theory that we will present in the rest of this article, we shall show that this symmetry is preserved up to linear order in \(1/N\).

In the passing, we note that it is possible to start with the attractive Hubbard model (2.1) and write down similar particle-hole constraints. These are given in Appendix A. We shall next develop a functional integral formalism for the large-\(N\) model.

### 2.2.3 Functional Integral Formalism for large-\(N\) model

In this section we give a brief account of the functional integral formalism used in this chapter. The thermodynamical properties of the system can be obtained from the partition function in the grand-canonical ensemble \( Z(\mu, \beta) \), where \( \beta^{-1} \) is the temperature \( T \) of the system. Indeed, \( Z \) is related to the thermodynamical potential as \( \Omega(\mu, \beta) = -\beta^{-1} \ln Z \). This partition function can be expressed as a Feynman path
integral over Grassmann fields \( \bar{\Psi}_{\alpha \sigma} \) and \( \Psi_{\alpha \sigma} \)

\[
Z = \int D\bar{\Psi}_{\alpha \sigma} D\Psi_{\alpha \sigma} \exp(-S_\Psi) 
\]  

(2.9)

with the action in imaginary time \( \tau \)

\[
S_\Psi = \int_0^\beta d\tau \sum_{i \alpha \sigma} (\bar{\Psi}_{i \alpha \sigma}(\tau) \partial_\tau \Psi_{i \alpha \sigma}(\tau) + H[\bar{\Psi}_{i \alpha \sigma}, \Psi_{i \alpha \sigma}]). 
\]

(2.10)

The quartic fermionic interaction term in the Hamiltonian can be decoupled by introducing a Hubbard-Stratonovich field \( \Delta(x) \) at each \( x = (x_i, \tau) \) which couples to \( \sum_\alpha \bar{\Psi}_{i \alpha \sigma}(\tau) \bar{\Psi}_{i \alpha \sigma}(\tau) \). The partition function can then be written as

\[
Z = \int D\Delta D\Delta^* D\bar{\Psi}_{i \alpha \sigma} D\Psi_{i \alpha \sigma} \exp(-S_{\Psi,\Delta}) 
\]  

with a full action

\[
S_{\Psi,\Delta} = \int d\tau \sum_i \left( \frac{N[\Delta(x)]^2}{U} - \int d\tau' \sum_{ij\alpha} \bar{\psi}_{i,\alpha}^\dagger(\tau) G_{ij}^{-1}(\tau, \tau') \psi_{j,\alpha}(\tau') \right), 
\]

(2.11)

where we have introduced the Nambu spinors \( \bar{\psi}_{i,\alpha}^\dagger(\tau) = (\bar{\Psi}_{i \alpha \sigma}(\tau), \bar{\Psi}_{i \alpha \sigma}(\tau)) \). The inverse Nambu-Gorkov Green's function \( G_{ij}^{-1}(\tau, \tau') \) is given by

\[
\begin{pmatrix}
(-\partial_\tau + \mu)\delta_{i,j} + t\delta_{<i,j>} & \Delta(x)\delta_{i,j} \\
\Delta^*(x)\delta_{i,j} & (-\partial_\tau - \mu)\delta_{i,j} - t\delta_{<i,j>} \end{pmatrix} \delta(\tau - \tau') 
\]

(2.12)

with the notation \( \delta_{<i,j>} = 1 \) only if the \( i \) and \( j \) sites are nearest neighbors and zero otherwise. The functional integral is now both Gaussian in the fermionic fields and diagonal in the flavor index \( \alpha \). After integrating over these Grassmann variables we get

\[
Z = \int D\Delta D\Delta^* \exp(-S_\Delta) 
\]

(2.13)
with an effective action $S_{\Delta}$ which only depends on the auxiliary fields $\Delta(x)$ in the form

$$S_{\Delta} = N \int dx \frac{|\Delta(x)|^2}{U} - N \int dx \text{Tr} \ln G^{-1}[\Delta(x)]$$  \hspace{1cm} (2.14)$$

where $\int dx = \sum_i \int d\tau$.

Looking at the effective action (2.14), we see that for infinitely large $N$ the value of the integral is completely dominated by the saddle point contribution. Assuming that the saddle-point auxiliary field is space and time independent (i.e. $\Delta(x) = \Delta_0$), the thermodynamical potential $\Omega$ is of the form $\Omega(\mu, \beta) \simeq N\Omega_0 = S_{\Delta}(\Delta(x) = \Delta_0)/\beta$. Fluctuations around the saddle point yield corrections that are smaller than this term by powers of $1/N$; thus the full thermodynamical potential will be expanded in the form

$$\frac{\Omega}{N} = \Omega_0 + \frac{1}{N}\Omega_g + \cdots$$  \hspace{1cm} (2.15)$$

The strategy for the above expansion is as follows: For the saddle point, note that $\Delta$ corresponds to two Grassmann fields of the same flavor, and hence summing up the contributions for each flavor, we find that the total saddle point contribution to the action is of the order $N$. In order to obtain the next leading order term in $1/N$, we expand $\Delta$ around $\Delta_0$ and write the action in terms of the fluctuations around $\Delta_0$. We observe that each diagram in the RPA loop expansion (fluctuations upto Gaussian order) is of the order 1. In order to see this we note that the $\text{Sp}(2N)$ interaction that we are considering is of the form shown in Figure (2.1), in which a pair of particles of opposite spin but the same flavor $a$ can scatter to another pair of particles with (possibly different) flavor $b$ with their spins unchanged. When we consider the first term (Hartree term) in $\Omega_g$ corresponding to this theory, we close the external lines which necessitates $a = b$. Each of the flavors $a$ and $b$ come with a summation over flavor indices, and the interaction between a pair of flavors is $(-U)/N$. Thus the Hartree term in $\Omega_g$ will be of overall order 1 or $O(1/N)$ relative to $\Omega_0$. Similarly, the
Figure 2.1: Feynman diagram depicting the interaction in the \( \frac{1}{N} \) theory at the Hartree level.

\[
\begin{align*}
\frac{U}{N} & \quad \frac{U}{N} \\
\downarrow & \quad \uparrow \\
\downarrow & \quad \uparrow \\
\end{align*}
\]

Figure 2.2: RPA loop expansion of the thermodynamic potential in the \( \frac{1}{N} \) order. The first diagram is the Hartree term.

\[
\Omega_g = \begin{array}{c}
\includegraphics[width=2cm]{diagram1} \\
\includegraphics[width=2cm]{diagram2} \\
\end{array} + \ldots
\]

\( m \)th diagram in the series (Figure 2.2) has \( m \) sums over \( N \) flavors and \( m \) interaction vertex, each contributing a factor \( \frac{1}{N} \) and therefore has an overall order 1.

In the following sections we shall derive expressions for \( \Omega_0 \) and \( \Omega_g \), as well as discuss how to obtain expansions of other thermodynamical variables in powers of \( \frac{1}{N} \). In the next section we give the form for \( S_0 \) and derive the mean field equations.
2.2.4 Saddle point approximation - Mean field theory at T=0

For the uniform static saddle point approximation, we replace $\Delta(x)$ by a space-time independent quantity $\Delta_0$. Fourier transforming all the fields to the reciprocal (momentum) lattice and Matsubara frequencies, the effective action is given by

$$S_\Delta[\Delta_0] = N{\beta \Delta_0^2 \over U} - N \sum_{k,i\k_n} \text{tr} \ln G_0^{-1}(k) \equiv NS_0$$  \hspace{1cm} (2.16)

with

$$G_0^{-1}(k) = \begin{pmatrix} ik_n - \xi_k & \Delta_0 \\ \Delta_0 & ik_n + \xi_k \end{pmatrix}$$  \hspace{1cm} (2.17)

Here $ik_n = (2n + 1)\pi/\beta$ are fermionic Matsubara frequencies, with $n \in \mathbb{Z}$, and $\beta$ being the inverse temperature. Using equation (2.16) we obtain for the mean-field thermodynamic potential (see Appendix C)

$$\Omega_0 = S_0/\beta = {\Delta_0^2 \over U} - \sum_k (E_k - \xi_k)$$  \hspace{1cm} (2.18)

where $E_k = (\xi_k^2 + \Delta_0^2)^{1/2}$. Then the spatially uniform, static saddle point at $T = 0$ is given by the following condition: $\delta S_0/\delta \Delta_0 = 0$, which written in terms of the thermodynamic potential is

$$\frac{\partial \Omega_0}{\partial \Delta_0} = 0 \quad \text{or} \quad \frac{1}{U} = \sum_k \frac{1}{2E_k}$$  \hspace{1cm} (2.19)

The mean field number equation can be obtained from the condition

$$\left( \frac{\partial \Omega_0}{\partial \mu} \right)_{T,V} = -n \quad \text{or} \quad n = \sum_k \left( 1 - \frac{\xi_k}{E_k} \right)$$  \hspace{1cm} (2.20)
Equations (2.19, 2.20) must be solved self-consistently to obtain the mean field gap parameter $\Delta_0$ corresponding to the mean field chemical potential $\overline{\mu}$, as well as finding the chemical potential which yields the desired density $n$. The results of this calculation are presented as dashed lines in Figure 2.4.

It is instructive to show that this mean field theory satisfies the particle-hole constraints in the lattice (see section 2.2.2) to the proper order, i.e. to zeroth order in $1/N$. From equation (2.6) we see that this corresponds to the chemical potentials on particle and hole sides being related by $\overline{\mu}(n) = -\overline{\mu}(2 - n)$. The validity of this equation can be seen by replacing $\mu \to -\mu$ without modifying $\Delta_0$; this leaves (2.19) unchanged while replacing $n \to 2 - n$ in (2.20).

The large $U/t$ limit of this theory can be easily obtained from the equations. To zero-th order in $t/U$, the chemical potential becomes $\overline{\mu} = (1 - n)U/2$ and the gap parameter is $\overline{\Delta}_0 = \sqrt{1 - (1 - n)^2} U/2$. We finally emphasize that our mean field theory results are quantitatively different from the ones discussed in references (Nozieres and Schmitt-Rink, 1985; Belkhir and Randeria, 1992), since the latter include a Hartree-shift in their chemical potentials at the mean field level. Such a term, which corresponds to terms in the particle-hole channel cannot be easily added into our formalism. We recover this important contribution in our theory as a $1/N$ order correction in what follows.

2.2.5 Leading order $1/N$ corrections - Gaussian fluctuations

at $T = 0$

In order to go beyond the mean field approximation we next consider fluctuations of the order parameter $\Delta$ around its static saddle point value $\Delta_0$

$$\Delta(x) = \Delta_0 + \eta(x) \quad (2.21)$$
where the complex bosonic field $\eta(x)$ describes space-time dependent fluctuations around the uniform static value $\Delta_0$. We next expand the action $S_\Delta$ to order $\eta^2$. The saddle point condition (2.19) ensures that there is no term linear in $\eta$ and we obtain $S_\Delta = NS_0 + S_g + \ldots$. The mean field piece $S_0$ has been defined above and Gaussian piece has the form

$$S_g = \frac{1}{2} \sum_{iq\iota} (\eta^*(q)\eta(-q)) M(q) \begin{pmatrix} \eta(q) \\ \eta^*(-q) \end{pmatrix}$$

where $iq\iota = i2\pi l/\beta$ are the Bose-Matsubara frequencies ($l \in \mathbb{Z}$) and the matrix elements of the inverse fluctuation propagator $M$ are given by (see Appendix D)

$$M_{11}(q) = M_{22}(-q) = \frac{1}{U} + \frac{1}{\beta} \sum_{ikl} G^0_{22}(k) G^0_{11}(k + q)$$

$$= \frac{1}{U} + \sum_k \left( \frac{v_k^2 v_k'^2}{iq\iota - E_k - E_k'} - \frac{v_k^2 v_k'^2}{iq\iota + E_k + E_k'} \right)$$

and

$$M_{12}(q) = M_{21}(q) = \frac{1}{\beta} \sum_{ikl} G^0_{12}(k) G^0_{12}(k + q)$$

$$= \sum_k u_k u_k' v_k v_k' \left( \frac{1}{iq\iota + E_k + E_k'} - \frac{1}{iq\iota + E_k + E_k'} \right)$$

Here $G^0$ is the Nambu propagator whose inverse is defined in equation (A.12) but now $\Delta_0$ has been replaced by $\Delta$, whose value after including $1/N$ corrections is yet to be determined, $u_k^2 = 1 - v_k^2 = (1/2)(1 + \xi_k/E_k)$ are the standard BCS coherence factors and $k' = k + q$. Writing the partition function upto Gaussian order

$$Z \simeq \exp(-NS_0) \int D\eta^\dagger \eta D \exp(-S_g)$$

29
and integrating out the Gaussian fluctuations we obtain

\[ Z = \exp(-NS_0) \int D\eta^\dagger \eta D\exp(-\eta^\dagger M\eta) = \exp(-NS_0) \frac{1}{\text{Det} M} \]  

(2.26)

The second equality holds even for non-Hermitian matrices \( M \), provided \( M \) is positive definite (for a proof see Appendix E). After putting in the right convergence factors, the Gaussian contribution to the thermodynamic potential is given by (see Appendix F)

\[ \Omega_g = \frac{1}{2\beta} \sum_{i\eta_n, q} \ln \left( \frac{M_{11}}{M_{22}} \text{Det} M(q) \right) e^{i\eta_n q^0+} \]

\[ = \frac{1}{2\beta} \sum_{i\eta_n, q} \ln (U^2 \text{Det} M(q)) + \frac{U}{2} \sum_k (u^2 - v^2) \]  

(2.27)

In the above equation and hereafter we use the following shorthand notation: \( u_k = u \), \( u_{k+q} = u' \) etc. The second term in equation (2.27) comes from taking into account the correct convergence factors.

The collective excitations are given by the poles of the fluctuation propagator i.e. roots of \( \text{Det} M(q, z) = 0 \). These excitations are the \( q \to 0 \) Goldstone modes of the order parameter in the broken symmetry superfluid state. In addition to simple poles, the fluctuation propagator has branch cuts on the real axis originating at \( E_c(q) = \pm \min(E_k + E_{k+q}) \). These branch cuts represent the two-particle continuum of states for scattering of gapped quasiparticles. To summarize the analytic properties of \( \Omega_g \), the Gaussian contribution (2.27) can be symbolically written as

\[ \Omega_g = \frac{1}{2} \sum_q \left[ \omega_0(q) - E_c(q) - \int_{-\infty}^{-E_c(q)} \frac{d\omega}{\pi} \delta(q, \omega) \right] + \mathcal{R} \]  

(2.28)

where \( \omega_0(q) \) is the frequency of collective excitations obtained from \( \text{Det} M = 0 \), and the last integral describes the contribution of the virtual scattering of quasiparticles.
with a phase shift $\delta(q, \omega)$ defined by $\delta(q, \omega) = \text{Im} \ln \det M(q, \omega + i0^+)$. The particle continuum for quasiparticle scattering begins at $E_c(q)$. The last term $\mathcal{R}$ comes from using the correct convergence factors in the calculation (see Appendix F for more details).

To illustrate these points, we plot (Figure 2.3) the two-particle continuum and the spectra of collective excitations along the main diagonal $q(1,1,1)$ of the Brillouin zone, at unitarity and for $n = 0.5$. For small $q$, the collective excitation spectrum is linear indicative of sound modes, eventually hitting the two-particle continuum. In the BEC limit, the two-particle continuum lies at a much higher energy scale and the low-energy excitations are entirely given by the gapless sound modes, a fact that will play a major role in deciding $T_c$ as illustrated in section (V). Further, at half-filling, due to the onset of CDW order one would expect the collective excitation spectrum to be gapless at $q = (\pi, \pi, \pi)$ indicating new Goldstone modes. However, this special feature of the attractive Hubbard model at half-filling is not captured in our theory since we only decouple the quartic interaction in the $p$-$p$ channel. We therefore do
not see the density (CDW) order and hence there is no softening of \((\pi, \pi, \pi)\) mode at half-filling within our theory. We shall present a discussion on CDW order in Appendix G.

2.2.6 Corrections of order \(1/N\)

Using the new approximation to the thermodynamical potential per flavor, \(\Omega_0(\mu) + (1/N)\Omega_q(\mu)\), we can obtain expressions for the properties of the system to linear order in \(1/N\). At this point, we want to emphasize the asymmetric way in which we treat the chemical potential \(\mu\) and the auxiliary field \(\Delta_0\). Indeed, in our approach the former is a thermodynamical variable while the latter is merely a calculational tool, obtained as the saddle point of a variable that is integrated over in the partition function. As such, it is not an independent variable but it is defined as a function of \(\mu\), i.e. \(\Delta_0(\mu)\) is the saddle point field used to calculate the partition function at such a chemical potential, obtained from the solution of the equation \(\partial S_0/\partial \Delta_0 = 0\). As we make expansions in powers of \(1/N\) this equation is left unchanged, as the saddle point condition is exact to all orders. Note that the saddle point condition for the integral (2.13) is the functional derivative \(\delta S_\Delta[\Delta(x)]/\delta \Delta(x) = 0\), or \(\delta S_\Delta[\Delta_q]/\delta \Delta_q = 0\) for all \(q\) in momentum space; this seems more general than the condition \(dS_0/d\Delta_0 = 0\) that we use and may suggest that we are using an approximate “mean-field” saddle-point condition. This, however, is not the case: if we make an expansion of \(S_\Delta\) around the static homogeneous saddle point \(\Delta_0\) we get

\[
S_\Delta(\Delta_0 + \eta_q) = S_0(\Delta_0) + (dS_0/d\Delta_0)\eta_0 + \sum_q \alpha_q\eta_q\eta_{-q},
\]

which shows that the only nontrivial saddle point equation for the full action is the one for \(q = 0\) which corresponds to \(dS_0/d\Delta_0 = 0\). For more on the question of
feedback we refer the reader to \(^2\) and the references therein.

For brevity, we shall change our notation from here onwards. The gap parameter \(\Delta_0\) will be represented as \(\Delta\) and the mean field value of \(\Delta_0\) namely, \(\Delta_0\) will be written as \(\Delta_0\). Similarly, the mean field value of \(\mu\), \(\bar{\mu}\) will be written as \(\mu_0\) (see Table 2.2.6).

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Old notation</th>
<th>New notation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gap parameter</td>
<td>(\Delta_0)</td>
<td>(\Delta)</td>
</tr>
<tr>
<td>MF Gap parameter</td>
<td>(\Delta_0)</td>
<td>(\Delta_0)</td>
</tr>
<tr>
<td>MF Chemical Potential</td>
<td>(\bar{\mu})</td>
<td>(\mu_0)</td>
</tr>
</tbody>
</table>

Table 2.1: Change of Notation for MF chemical potential and Gap parameter

In order to feedback the leading order corrections to the gap and number equations we expand the renormalized chemical potential and gap around their respective saddle point values to linear order in \(1/N\):

\[
\mu = \mu_0 + \frac{\delta \mu}{N} + ... \\
\Delta = \Delta_0 + \frac{\delta \Delta}{N} + ...
\]

Expanding equation (2.19) upto \(O(1/N)\) we obtain

\[
\frac{\partial \Omega_0}{\partial \Delta} + \frac{1}{N} \left( \frac{\partial^2 \Omega_0}{\partial \Delta^2} \delta \Delta + \frac{\partial^2 \Omega_0}{\partial \Delta \partial \mu} \delta \mu \right) = 0
\]

We do not have a \(\Omega_g\) term in equations (2.32) since the saddle point condition is not modified by Gaussian fluctuations (see the discussion in the previous paragraphs).

\(^2\)If one insists on treating \(\mu\) and \(\Delta\) on equal footing and wishes to feedback the fluctuations in the gap equation, the correct way to do so is to switch to an amplitude-phase representation for the fluctuations (Diener et al., 2008). One then gets a different form for the fluctuation propagator corresponding to the gapless phase fluctuations and the validity of Goldstone's Theorem is ensured. However, this approach leads to an unphysical negative compressibility in the BEC limit in the continuum (Diener et al., 2008).
Equating the coefficient of the $1/N$ term to zero we obtain a relation between $\delta \Delta$ and $\delta \mu$

$$\delta \Delta = -\frac{(\partial^2 \Omega_0/\partial \Delta \partial \mu)}{(\partial^2 \Omega_0/\partial \Delta^2)} \delta \mu$$  \hspace{1cm} (2.33)

Next, expanding the number equation to linear order in $1/N$ and writing $(d/d\mu)_{T,V} = (\partial/\partial \mu)_{T,V} + (d\Delta/d\mu)(\partial/\partial \Delta)_{T,V}$ we get

$$-n = \left( \frac{d \Omega}{d \mu} \right)_{T,V} = \left( \frac{d \Omega_0}{d \mu} \right)_{T,V} + \frac{1}{N} \left[ \left( \frac{d^2 \Omega_0}{d \mu^2} \right)_{T,V} \delta \mu + \left( \frac{d \Omega_0}{d \mu} \right)_{T,V} \right]_{\mu_0, \Delta_0} \hspace{1cm} (2.34)$$

which gives

$$\delta \mu = -\left( \frac{d \Omega_g}{d \mu} \right) / \left( \frac{d^2 \Omega_g}{d \mu^2} \right) \hspace{1cm} (2.35)$$

The derivative $d\Delta/d\mu = (\sum_k \xi/E^3)/(\sum_k \Delta/E^3)$ is obtained from equation (2.33). A summary of numerical methods used for the calculation of $\Omega_g$ is given in Appendix H. We note that the correction to the chemical potential to order $1/N$ obtained in equation (2.35) is the same as obtained in (Veillette et al., 2007). We refer the reader to Appendix I for details. The correction to the gap parameter $\delta \Delta$, corresponding to $\delta \mu$ and given by equation (2.33), is however different from (Veillette et al., 2007).

### 2.3 Zero-temperature Results to linear order in $1/N$

Using our formalism we can now calculate all thermodynamical quantities for the system. In this section we present our results, both for the mean field approximation and up to linear order in the $1/N$ expansion; in the figures we have set the number of flavors $N$ equal to 1 in the expansion.
2.3.1 Chemical potential, gap parameter and ground state energy

The chemical potential and the gap parameter across the entire crossover and for a typical density (quarter filling, \( n = 0.5 \)) are plotted in Figure 2.4; while the fluctuations are unimportant for small interactions \( U \), the correction becomes important at unitarity and in the BEC limit. The fluctuations decrease the value of the order parameter, as well as decrease the value of the chemical potential; as we shall see this is related to the Hartree shift in the energy of the system.

We can show that our theory satisfies particle-hole symmetry to first order in \( 1/N \). As we can see from (2.8) and the expansion (2.15), particle-hole symmetry at this order implies that

\[
\Omega_g(-\mu) = \Omega_g(\mu) - U(1-n)
\]  

(2.36)

where \( \mu = \bar{\mu}(n) \). This property of our \( \Omega_g(\mu) \) can be directly seen from the second line in (2.27); once again making the transformation \( \mu \rightarrow -\mu \) as well as switching variables to \( k \rightarrow -k \) and \( q \rightarrow -q \) we can see the first term is left unchanged while
in the second one $u \leftrightarrow v$. Thus, we recover (2.36).

Figure (2.5) shows our calculation of the ground state energy, which is obtained as $\mathcal{E} = \Omega(T = 0) + \mu n$ for a quarter-filled lattice across the entire crossover. Once again we see a large reduction in the value of the energy when compared with the mean-field prediction.

### 2.3.2 Compressibility

We next calculate the compressibility of the system defined as $\kappa = \frac{dn}{d\mu}$ to order $1/N$. Expanding the number equation to order $1/N$ we obtain the following expression for compressibility

$$
\frac{dn}{d\mu} = -\frac{d^2 \Omega_0}{d\mu^2} - \frac{1}{N} \left[ -\left(\frac{d^3 \Omega_0}{d\mu^3}\right) \frac{d\Omega_g/d\mu}{d^2\Omega_0/d\mu^2} + \frac{d^2 \Omega_g}{d\mu^2} \right]
$$

(2.37)

Figure (2.6) shows the compressibility as a function of filling in the strong coupling limit ($U/t = 30.0$) both at the mean field level and after including $1/N$ corrections. The positive compressibility in the BEC limit is a check that our theory gives phys-
Figure 2.6: The compressibility $dn/d\mu$ as a function of filling $n$ in the strong coupling limit ($U/t = 30.0$). The dashed line is the mean field compressibility. The solid line is the compressibility up to $O(1/N)$ and can be seen to be greater than zero and large (but finite) for smaller values of $n$. The inset shows how compressibility changes across the crossover for $n = 0.5$.

The inset in figure (2.6) shows the behavior of compressibility across the crossover. In the strong coupling limit $dn/d\mu \propto 1/U$ stemming from the fact that $\mu_0 = (1 - n)U/2$, a point we shall revisit when we compare the large-$N$ results with Hartree-shifted Mean Field Theory.

### 2.3.3 Speed of sound

The speed of sound is given by the roots of $\text{Det} \, M(q, \omega) = 0$ in the limit $q \to 0$, $\omega \to 0$. To this effect we expand $\text{Det} \, M(-\omega, q)$ up to quadratic order in small $\omega$ and $|q|$. For simplicity we choose $q$ to be pointing along the diagonal $q_x = q_y = q_z = q$. Then the single particle energy up to second order in $q$ is given by $\epsilon_{k+q} = \epsilon_k(1 - q^2/2) + \epsilon_k q$, where $\epsilon_k = 2t(\sin(k_xa) + \sin(k_ya) + \sin(k_za))$. Next expanding the energy up to second order gives

$$E_{k+q} = E_k[1 + \epsilon'_k \xi_k q/E^2_k + (\epsilon'_k \Delta)^2 - E^2_k \epsilon_k \xi_k]q^2/(2E^4_k)$$

(2.38)
The matrix elements of \( M(-\omega, q) \) are then given by

\[
\begin{align*}
M_{11}(-\omega, q) &= A + B\omega + (C - K)\omega^2 + D_{11}q^2, \\
M_{22}(-\omega, q) &= M_{11}(\omega, q), \\
M_{12}(-\omega, q) &= A + C\omega^2 + D_{12}q^2,
\end{align*}
\]

where 

\[
\begin{align*}
A &= (U/4) \sum_k X^2/E, \quad B = (U/4) \sum_k Y/E^2, \\
C &= (U/16) \sum_k X^2/E^3, \quad K = (U/8) \sum_k 1/E^3, \\
D_{11} &= (U/8) \sum_k (1/E)\{(3/2)X^2WY + (7/2)X^2Y^2Z^2 + X^2Z^2 - Y^2Z^2 - WY - X^4Z^2/2\}, \\
D_{12} &= (U/16) \sum_k (X/E)\{-2X^3Z^2 + 3XY^2Z^2 + XYZ + 4X\{YJ/(1 - Y^2) - Z^2X^4(1 + Y^2)/(1 - Y^2)^2\}\}, \text{ with } J = W/2 + Z^2Y + X^2YZ^2/2 - WY^2/2 - Z^2Y^3
\end{align*}
\]

and 

\[X = \Delta/E, \quad Y = \xi/E, \quad Z = \epsilon'/E, \quad W = \epsilon/E.\]

We therefore obtain for the speed of sound

\[
c_s = \sqrt{\frac{2A(D_{11} - D_{12})}{B^2 + 2AK}} \tag{2.40}
\]

The results for the speed of sound are shown as the black curves in Figure 2.7. The solid black line is the result obtained by using the mean field values for \( \Delta_0 \) and \( \mu \). The dashed black line is the result obtained after including the Gaussian fluctuations. As expected, Gaussian fluctuations tend to significantly reduce the speed of sound from its mean field value across the entire crossover.

### 2.4 Superfluid Density

The superfluid density is defined as a response of the system to a twist of the boundary conditions. In order to formulate this definition, let us consider an arbitrary many-
body system on a hypercubic lattice in \(d\) dimensions with a generic Hamiltonian

\[
\hat{H} = - \sum_{i,\alpha=1,...,d} t_{\alpha}(r_i) [\hat{c}^\dagger(r_i)\hat{c}(r_i + \hat{\alpha}) + h.c.] + \hat{V}
\]  

(2.41)

where \(t_{\alpha}(r)\) is the hopping amplitude between nearest neighbor, \(\hat{\alpha}\) denotes the unit vector in the \(\alpha\)th direction and \(\hat{V}\) denotes all possible interactions between particles as well as possible onsite random potentials. Note, at this stage we are making no assumption about the statistics obeyed by the particles. The ground state wavefunction \(\Psi_0\{r_i\}\) for boundary conditions at rest satisfies

\[
\hat{H}\Psi_0\{r_i\} = E(0)\Psi_0\{r_i\}
\]  

(2.42)

Now let us put the system on a ring in the \(\hat{1}\) direction and re-express the variable \(r_i\) in terms of an angular variable \(\theta_i\) and transverse co-ordinates \(\eta_i\). Then the single-valuedness boundary condition on the ground state wavefunction says that if one particle is taken around the ring, keeping the others fixed, we recover the original
wavefunction

\[ \Psi_0(\theta_1, \eta_1, ..., \theta_i, \eta_i, ..., \theta_N, \eta_N) = \Psi_0(\theta_1, \eta_1, ..., \theta_i + 2\pi, \eta_i, ..., \theta_N, \eta_N), \forall i \]  

(2.43)

In order to impose the twisted boundary conditions, we consider the wavefunction \( \Psi_{\phi}\{r_i\} \) that minimises the expectation value of \( H \) but now subject to the condition

\[ \Psi_{\phi}(\theta_1, \eta_1, ..., \theta_i, \eta_i, ..., \theta_N, \eta_N) = \exp(i\phi)\Psi_{\phi}(\theta_1, \eta_1, ..., \theta_i + 2\pi, \eta_i, ..., \theta_N, \eta_N), \forall i \]  

(2.44)

Let \( E(\Delta \phi) \) be the corresponding eigenvalue. Then the increase in energy due to the applied twist is given by

\[ E(\Delta \phi) - E(0) = t\rho_sL^d \left( \frac{\Delta \phi}{L} \right)^2 + ... \]  

(2.45)

where \( \rho_s \) is the superfluid density and \( L \) is the number of lattice sites in any direction. The superfluid density is thus defined as

\[ \rho_s = \frac{L^{2-d}}{2t} \lim_{\Delta \phi \to 0} \frac{\partial^2 E(\Delta \phi)}{\partial(\Delta \phi)^2} \]  

(2.46)

Next, it has been shown (Leggett, 1998a), on quite general grounds, that the superfluid density of a translationally invariant superfluid possessing time reversal invariance at \( T = 0 \), is equal to the total density

\[ \lim_{T \to 0} \frac{\rho_s(T)}{\rho} = 1 \]  

(2.47)

For a one component system barring pathologies, the statement can be proved using the Gibbs-Duhem relation. In order to do so, we invoke Landau's two-fluid hydrodynamics to write down the following relations between mass current density \( j(r, t) \),
pressure $P(r,t)$, superfluid velocity $\mathbf{v}_s(r,t)$ and chemical potential $\mu(r,t)$

\[
\begin{align*}
\frac{d\mathbf{j}}{dt} &= -\nabla P \\
\frac{d\mathbf{v}_s}{dt} &= -\nabla \mu
\end{align*}
\] (2.48)

In the limit $T \to 0$, the Gibbs-Duhem relation implies $\nabla P = \rho \nabla \mu$ which combined with the equations (2.48) give $\mathbf{j} = \rho \mathbf{v}_s + f(r)$, where $f(r)$ is an arbitrary function of position but not time. On the otherhand, Landau’s two-fluid description gives $\mathbf{j} = \rho_s \mathbf{v}_s + \rho_n \mathbf{v}_n$ and $\rho = \rho_s + \rho_n$. The only way these relations could still hold is when the function $f$ is identically zero. Thus at $T = 0$ equation (2.47) is satisfied.

In the case of a translationally invariant system, a phase twist in the boundary conditions for the order parameter, is uniformly distributed across the system. However, the situation is different on a lattice - because of the broken translation symmetry, the many-body wavefunction has very small amplitude between the lattice sites and now it is energetically advantageous to put the phase twists between the lattice sites. As a result, the superfluid density, which is the response of the system to this phase twist, turns out to be different on a lattice. In Kubo formalism, these considerations translate to a vanishing paramagnetic part of the current-current correlation function for a translationally invariant system. The superfluid density in such a system is therefore entirely given by the diamagnetic part of the response and turns out to be equal to the total density. However, on a lattice, the total momentum operator does not commute with the Hamiltonian and hence the paramagnetic part of the response is non-zero. Consequently, the superfluid density differs from the total density on a lattice even at $T = 0$. 

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2.4.1 Calculation of Superfluid density on a lattice

The superfluid density is computed by comparing the free energy \( F(n) = \Omega + \mu n \) of the gas at rest with the free energy of a gas moving with a superfluid velocity \( v_s = Q/(2m) \) in the limit \( Q \to 0 \); indeed, \( F(Q,n) - F(0,n) = \frac{1}{2} n_s m v_s^2 \) so that (Taylor et al., 2006)

\[
n_s = 4m \left( \frac{\partial^2 F}{\partial Q^2} (Q \to 0) \right) n.
\] (2.49)

where \( n_s = \rho_s/m \). ³ We can relate this derivative of \( F \) with derivatives of \( \Omega \) recognizing that \( \Omega \) and thus

\[
\left( \frac{\partial^2 F}{\partial Q^2} \right)_n = \left( \frac{\partial^2 \Omega}{\partial \mu^2} \right)_\mu + \left( \frac{\partial \Omega}{\partial \mu} \right)_Q + n \left( \frac{\partial^2 \mu}{\partial Q^2} \right)_n
\]

\[
= \left( \frac{\partial^2 \Omega}{\partial Q^2} \right)_\mu
\] (2.50)

where we have used the number equation at \( Q = 0 \) in the last line.

Here we extend our large \( N \) formalism to the calculation of the superfluid density (Taylor et al., 2006) in a lattice. We start by putting a (time-independent) phase twist \( \theta(x) = Q \cdot x_i = \theta_i \) on the order parameter

\[
\Delta(x) \to e^{i\theta_i} \Delta(x)
\] (2.51)

in the expression (2.12) for the Nambu-Gorkov propagator, which is used to calculate the full action \( S_{\psi,\Delta} \). We shall assume that the phase difference is a constant \( \theta \) for any two neighboring sites along the (arbitrarily chosen) \( x \)-direction; thus, we have

\[
Q = Q_x = \theta/a
\]

where \( a \) is the lattice spacing and the superfluid density is

\[
n_s = 4ma^2 \left( \frac{\partial^2 \Omega}{\partial \theta^2} \right)_\mu
\] (2.52)

³Unless, otherwise mentioned, we shall mean \( n_s \) for superfluid density
where the mass in the lattice is the combination \( m = 1/(2ta^2) \), i.e. the effective mass for fermions at the bottom of the band.

We can remove the phase twist from \( \Delta(x) \) by applying a unitary transformation to the Grassmann fields of the form

\[
\psi_i(\tau) = U_i \psi_{i\alpha}(\tau)
\]

with

\[
U_i = \begin{pmatrix}
e^{-i\theta_i/2} & 0 \\
0 & e^{i\theta_i/2}
\end{pmatrix}
\]

so that the inverse Green’s function in (2.12) now becomes \( \mathbf{G}_{ij}^{-1}(\tau, \tau') \rightarrow U_i \mathbf{G}_{ij}^{-1}(\tau, \tau') U^\dagger_j \). As can be easily verified, this leaves the form of \( \mathbf{G}_{ij}^{-1}(\tau, \tau') \) unchanged from (2.12) except for the hopping term, which now gains a phase difference. Under this transformation, the diagonal part of the action becomes

\[
\tilde{\Psi}_{i,1} e^{-i\theta_i/2} [ -t + (-\mu + \partial_x)^\delta_{i,j} > \Psi_j,1 e^{+i\theta_j/2} + \tilde{\Psi}_{i,1} e^{-i\theta_i/2} [ t - (\mu + \partial_x)^\delta_{i,j} > \Psi_j,1 e^{+i\theta_j/2}
\]

and therefore the hopping term gains a phase difference \( t \rightarrow t \exp(\pm i(\theta_j - \theta_i)/2) \) in the first (second) diagonal element. However, the relative phase \( \theta \) can be incorporated into the single particle dispersion

\[
\tilde{\epsilon}_k = -2t [\cos(k_x + \theta) + \cos(k_y) + \cos(k_z)]
\]

and hence the kinetic energy term, in the momentum space can be written as \( \tilde{\epsilon}_k \tilde{\Psi}_{k,\sigma} \Psi_{k,\sigma} \).

Transforming to the reciprocal lattice, we obtain an inverse Green’s function of the
form
\[
\tilde{G}_0^{-1} = \begin{pmatrix}
(i_k - \tilde{\xi}_k)e^{-ik_0^+} & \Delta_0 \\
\Delta_0 & (i_k + \tilde{\xi}_k)e^{+ik_0^+}
\end{pmatrix}
\] (2.57)

where \(\tilde{\xi}_k = \tilde{\xi}_k - \mu\). Taking the limit of small \(\theta\), we see that this corresponds to shifting the Matsubara frequencies and the energy dispersion as

\[
i\tilde{k}_n = ik_n - \frac{\theta}{2a}(\partial \epsilon_k / \partial k_x)
\] (2.58)

\[
\tilde{\xi}_k = \xi_k + \frac{\theta^2}{8a^2} \frac{\partial^2 \epsilon_k}{\partial k_x^2}
\]

The effective action at a fixed \(\theta\), from which the saddle point condition is derived, satisfies

\[
\frac{S_0(\Delta_0; \mu, \theta)}{N\beta} = \frac{\Delta_0^2}{U} - \frac{1}{\beta} \sum_{i\tilde{k}, \kappa} \text{Tr} \ln \tilde{G}_0^{-1}(\kappa)
\] (2.59)

\[
= \frac{S_0(\Delta_0; \mu, \theta = 0)}{N\beta} + \frac{\theta^2}{8a^2} \sum_k \left(1 - \frac{\xi_k}{E_k}\right) \frac{\partial^2 \epsilon}{\partial k_x^2}
\]

where we have used the fact that the shift in the Matsubara frequencies is not important once they are summed over as long as \(\theta\) is small, as well as the shift in the energy dispersions to quadratic order in \(\theta\) (see Appendix K for more details).

The saddle point condition \(\delta S_0 / \delta \Delta_0 = 0\) yields the small \(\theta\) expansion \(\Delta_0(\mu, \theta) = \Delta_0(\mu, 0) + \alpha(\mu)\theta^2\), where

\[
\alpha(\mu) = -\frac{3}{8\Delta_0 a^2} \frac{\sum_k (\partial^2 \epsilon_k / \partial k_x^2) \xi_k / E_k^3}{\sum_k (1 / E_k^3)}
\] (2.60)

and all quantities are evaluated at \(\theta = 0\).
2.4.2 Mean Field Superfluid Density

The mean field thermodynamic potential per flavor at $T = 0$ for a system with a phase twist is given by

$$\tilde{\mathcal{O}}_0(\mu, \theta) = \frac{1}{N\beta} \tilde{\mathcal{O}}_0(\Delta_0(\mu, \theta); \mu, \theta)$$

(2.61)

Using that the $\Delta_0$ dependence on $\theta$ is obtained from the saddle point condition $\delta S_0/\delta \Delta_0 = 0$ we can obtain the superfluid density as

$$n_s^0 = \frac{1}{N\beta} \left( \frac{\partial^2 \tilde{\mathcal{O}}_0}{\partial \theta^2} \right)_{\mu, \Delta}$$

(2.62)

$$= \left( \frac{d^2 \tilde{\Omega}_0}{d\theta^2} \right)_{\theta=0}$$

(2.63)

As before, the terms containing first order derivatives with respect to $\theta$, are zero from parity and the term $(\partial^2 \Delta/\partial \theta^2)(\partial \mathcal{O}_0/\partial \Delta) = 0$ from the saddle point condition. The mean field thermodynamic potential in presence of the phase twist at $T = 0$ is given by (see equation 2.16)

$$\tilde{\tilde{\mathcal{O}}}_0 = \frac{\Delta_0^2}{U} - \frac{1}{\beta} \sum_{ikn} \text{Tr ln} \tilde{G}_0^{-1}(k)$$

(2.64)

Using the following expansions for $\tilde{E}_k$ and $\tilde{\xi}_k$ up to $O(\theta^2)$:

$$\tilde{\xi}_k \approx \xi_k + \frac{\theta^2}{2} \partial^2 \xi_k$$

(2.65)

$$\tilde{E}_k \approx E_k + \frac{\theta^2}{2} \frac{\xi_k}{E_k} \partial^2 \xi_k$$

$$\partial k^2$$

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in equation (2.64) we find that the mean field thermodynamic potential for an arbitrary dispersion \( \epsilon_k \) is given by (see Appendix K)

\[
\tilde{\Omega}_0 = \frac{\Delta_0^2}{U} - \sum_{k} (E_k - \xi_k) + \frac{\theta^2}{2} \sum_{k} \left( 1 - \frac{\xi_k}{E_k} \right) \frac{\partial^2 \epsilon_k}{\partial k^2}
\]

Using equation (2.49) and again assuming that the phase twist is in the \( x \) direction, we obtain the mean superfluid density on the lattice as

\[
n_s^0 = \sum_k \left( 1 - \frac{\xi_k}{E_k} \right) \cos(k_x a)
\]  

From this formula we can see that for a lattice with a dispersion \( \epsilon_k \) defined above we have \( n_s^0 < n \). The Galilean invariant result in the dilute, continuum limit is recovered as the limit of small density \( n \) and interaction \( U/t \), in which the chemical potential \( \mu \) is near the bottom of the band. Thus, expanding \( \cos(ka) \) to \( O(k^2) \) we obtain \( n_s^0 = n \).

2.4.3 Calculation of \( n_s \) including Gaussian fluctuations

In order to include Gaussian fluctuations, we need to calculate the Gaussian part of the action \( S_g(\Delta; \theta, \mu) \) in the presence of the phase twist \( \theta \). This corresponds to replacing the elements of \( G^0 \) The inclusion of the effects of Gaussian fluctuations in the calculation of the superfluid density follows the same methodology used in section 2.3. The thermodynamic potential per flavor to first order in \( 1/N \) is of the form

\[
\frac{\Omega(\mu, \theta)}{N} = \frac{\Omega_0(\mu, \theta)}{N} + \frac{1}{N} \Omega_g(\mu, \theta).
\]
where again \( \Omega_g(\mu, \theta) = S_g(\Delta(\mu, \theta); \mu, \theta)/\beta \). The Gaussian correction to the thermodynamic potential has the same form as the one without the phase twist

\[
\tilde{\Omega}_g = \frac{1}{2\beta} \sum_{i\mathbf{q}, \mathbf{q}} \ln(\det \tilde{\mathbf{M}}(\mathbf{q})) + \frac{U}{2} \sum_{\mathbf{k}} (\tilde{\mathbf{u}}^2 - \tilde{\mathbf{v}}^2)
\]  \hspace{1cm} (2.69)

**Continuum**

Before we calculate the superfluid density including Gaussian fluctuations on a lattice, let us go back to the continuum limit and outline the calculation of the \(1/N\) corrections to \(n_s\) in the continuum. This would help in elucidating some of the technical points that makes a lattice calculation different from the continuum. To this effect we first prove that for a translationally invariant system, the relation \(n_s = n\), is respected even at the \(1/N\) level. For an energy dispersion \(\epsilon_k = k^2/2m\), the shift in single particle energies due to the introduced twist (see second equation in 2.59) is only a constant and can be incorporated into the chemical potential. Since, the phase twist is uniformly distributed across the system the order parameter transforms as:

\(\Delta(x) \rightarrow \Delta(x)e^{i\mathbf{Q}\cdot\mathbf{r}}\) and the Green’s function transforms as

\[
G_{ij}(i\tilde{k}_n, \mathbf{k}, \mu) \rightarrow G_{ij}(i\tilde{k}_n, \mathbf{k}, \mu - \mathbf{Q}^2/8m)
\]  \hspace{1cm} (2.70)

where the \(i\tilde{k}_n = i\mathbf{k}_n - \mathbf{k}.\mathbf{Q}/2m\) are the Doppler shifted Matsubara frequencies. Then,

\[
\tilde{\mathbf{M}}_{11}(i\mathbf{q}, \mathbf{q}) = \frac{1}{U} + \sum_{i\mathbf{k}_n, \mathbf{k}} G_{22}(i\tilde{k}_n - \frac{\mathbf{k}.\mathbf{Q}}{2m}, \mathbf{k}; \mu - \frac{\mathbf{Q}^2}{8m})G_{11}(i\tilde{k}_n - \frac{(\mathbf{k} + \mathbf{q}).\mathbf{Q}}{2m} + i\mathbf{q}, \mathbf{k} + \mathbf{q}; \mu - \frac{\mathbf{Q}^2}{8m})
\]

\[
\quad = M_{11}(i\mathbf{q} - \frac{\mathbf{q}.\mathbf{Q}}{2m}, \mathbf{q}; \mu - \frac{\mathbf{Q}^2}{8m})
\]  \hspace{1cm} (2.71)

The effects of the phase twist at \(T = 0\) is therefore to shift the contour of integration for the Matsubara sum by an amount proportional to \(Q\) along the real axis and to
shift the chemical potential $\mu$ by a constant amount $Q^2/8m$. In the limit $Q \to 0$, the shift of the contour of integration to the right keeps the Matsubara sum invariant and hence the phase twist enters the thermodynamic potential only through a shift of the chemical potential. This means that the saddle point condition in presence of the phase twist remains unchanged from the one in absence of the same. Further, $\tilde{\Omega}$ only contains terms in powers of $Q^2$ and therefore we obtain,

$$4m \left( \frac{\partial^2 \tilde{\Omega}_g}{\partial Q^2} \right)_{\mu_0, Q \to 0} = - \left( \frac{\partial \Omega_g}{\partial \mu} \right)_{\mu_0}$$  \hspace{1cm} (2.72)

By the same logic, $4m(\partial \tilde{\Omega}_0/\partial Q^2)_{\mu_0, Q \to 0} = -(\partial \Omega_0/\partial \mu)_{\mu_0}$. Since, the number equation is given by $\partial (\Omega_0 + \Omega_g/N)/\partial \mu = -n$ we obtain

$$n_s = 4m \left( \frac{d^2 \tilde{\Omega}}{dQ^2} \right)_{Q \to 0} = - \left( \frac{\partial \Omega_0}{\partial \mu} \right)_{\mu_0} - \frac{1}{N} \left( \frac{\partial \Omega_g}{\partial \mu} \right)_{\mu_0} = n$$ \hspace{1cm} (2.73)

We have thus proved that the superfluid density at $T = 0$ in the continuum remains pinned to the total density even after including the effects of Gaussian fluctuations. At finite temperatures we can use Landau's two fluid model to write down

$$\rho_s = \rho - \rho_n$$ \hspace{1cm} (2.74)

where, $\rho$, $\rho_s$, and $\rho_n$ are the total, superfluid, and normal densities respectively (for notational convenience here, we shall use $\rho = mn$ for density). Next, the normal fluid density can be written as a sum of Fermi quasiparticles and Bose collective modes contribution

$$\rho_n \equiv \rho_n^F + \rho_n^B$$ \hspace{1cm} (2.75)
where

$$\rho_n^F = -\frac{m}{\beta} \sum_k \left( \frac{k \hat{Q}}{m} \right)^2 \text{Tr}[G_0(k)G_0(k)]$$  \hspace{1cm} (2.76)$$

and

$$\rho_n^B = -\frac{2m}{\beta} \sum_q \frac{1}{(\text{Det} \tilde{M})^2} \left[ \text{Det} \tilde{M} \left( \frac{\partial^2 \text{Det} \tilde{M}}{\partial Q^2} \right) \hat{\mu} - \left( \frac{\partial \text{Det} \tilde{M}}{\partial Q} \right)^2 \right]_{Q \rightarrow 0}$$  \hspace{1cm} (2.77)$$

where $\hat{Q} = Q/|Q|$. The fermionic contribution to the normal fluid density $\rho_n^F$ can be identified as the long-wavelength static limit of the current-current correlation function up to a factor of $-m$. After doing the Matsubara sum in equation (2.76), we obtain

$$\rho_n^F = -\frac{2}{m} \int d^3k \frac{2}{(2\pi)^3} \hat{k} \hat{\mu} \frac{\partial f(E_k)}{\partial E_k}$$

$$= \frac{2}{3m} \int d^3k \frac{2}{(2\pi)^3} \hat{k} \hat{\mu} \left( -\frac{\partial f(E_k)}{\partial E_k} \right)$$  \hspace{1cm} (2.78)$$

where $f(E_k)$ is the Fermi distribution function. Equation (2.78) is the well-known Landau formula for the normal fluid density of a uniform weak-coupling BCS superfluid. This formula only takes into account the thermally excited Fermi BCS quasiparticles. The effect of the bosonic collective modes can be incorporated in (2.78) by renormalizing, from their BCS mean field values, the quantities $\mu$ and $\Delta$ involved in $f(E_k)$ in presence of Bose fluctuations (Taylor et al., 2006).

**Lattice**

We next consider the lattice. Now the shift to the single-particle dispersion due to the phase twist is no longer a constant (since it is proportional to $\partial^2 \epsilon_k / \partial k^2$) and hence cannot be absorbed into the chemical potential. Consequently, the above argument that applies to the continuum does not hold on the lattice and we expect the superfluid density at $T = 0$ to deviate from the total density. In order to calculate the superfluid
density on the lattice, we start by writing the 1/N corrections to the thermodynamic potential as follows

\[ \Omega(\mu, \Delta(\mu, \theta), \theta) = \Omega_0(\mu, \Delta(\mu, \theta), \theta) + \frac{1}{N} \Omega_\delta(\mu, \Delta(\mu, \theta), \theta) \] (2.79)

Further, \( \mu = \mu_0 + \delta \mu/N \), which then combined with equation (2.52) gives

\[ n_s = \left( \frac{d^2 \tilde{\Omega}}{d \theta^2} \right)_\mu = \left( \frac{d^2 \tilde{\Omega}_0}{d \theta^2} \right)_{\mu_0} + \frac{1}{N} \left( \frac{d^2 \tilde{\Omega}_0}{d \mu d \theta^2} \right)_{\mu_0} \delta \mu + \frac{1}{N} \left( \frac{d^2 \tilde{\Omega}_\delta}{d \theta^2} \right)_{\mu_0} \] (2.80)

In the first line \( d/d\mu = \partial/\partial \mu + (\partial \mu/\partial \Delta) \partial/\partial \Delta \). Note the presence of an explicit \( \partial/\partial \Delta \) derivative which was absent in the expression for \( n^0_s \) because of the saddle point condition \( \partial \Omega_0/\partial \Delta = 0 \). All the terms involving \( \tilde{\Omega}_0 \) in equation (2.8) are calculated analytically. The third term \( \left( \frac{d^2 \tilde{\Omega}_\delta}{d \theta^2} \right) \) is evaluated numerically by writing it as a first derivative with respect to \( \theta^2 \) since \( \theta \) does not appear in linear order due to symmetry and we truncate all expansions in \( \theta \) upto quadratic order. Finally, the
derivative \(\frac{\partial^2 \tilde{\Omega}}{\partial \theta^2}\) in the fourth term in equation (2.8) is evaluated numerically and the term \(\frac{\partial^2 \Delta}{\partial \theta^2}\) is evaluated analytically as follows: We start by writing out the expansions of the gap \(\Delta\) and the energy dispersion \(\tilde{\xi}\) in presence of a small phase twist \(\theta\):

\[
\Delta = \Delta + \frac{\theta^2}{2} \Delta + ... \tag{2.81}
\]

\[
\tilde{\xi} = \xi + \frac{\theta^2}{2} \epsilon'' + ...
\]

where \(\Delta = \frac{\partial^2 \Delta}{\partial \theta^2}\) and \(\epsilon'' = \frac{\partial^2 \epsilon_k}{\partial k^2}\). Keeping terms only upto \(O(\theta^2)\), the above expansions give \(\tilde{E} \approx E[1 + \theta^2(\xi'' + \Delta \tilde{\Delta})/E^2]^{1/2}\). Substituting in the gap equation \(1/U = \sum_k 1/(2\tilde{E})\) we find

\[
\Delta \tilde{\Delta} \sum_k \frac{1}{E^3} = - \sum_k \frac{\xi \epsilon''}{E^3} \quad \text{or} \quad \Delta = -\frac{B}{A \Delta} \tag{2.82}
\]

where \(A = \sum_k 1/E^3\), and \(B = \sum_k \xi \epsilon''/E^3\).

After obtaining the \(1/N\) correction to \(n_s\), we finally set \(N = 1\). In figure (2.8) we plot the mean field superfluid density and the one including \(1/N\) corrections as a function of coupling strength. As it can be seen, Gaussian fluctuations reduce the superfluid number density from its mean field value across the entire crossover with an increased suppression in the strong coupling regime. This is expected because the BCS mean field theory reduces the problem to one of non-interacting Bogoliubov quasiparticles with a gapped excitation spectrum. However, the low lying excitations in the strong coupling regime, are the gapless collective modes of the composite bosons, which are not captured by the BCS mean field theory. Since our theory of Gaussian fluctuations gives a correct account of these collective modes in the strong coupling regime, we get a reduction of the superfluid density from its mean field value. Further, \(n_s\) falls off like \(t^2/U\) in the strong coupling limit which can be explained by
noting that the system in this regime comprises of hard-core bosons on a lattice with an effective hopping parameter $\sim t^2/U$.

2.5 Critical temperature

The question of critical temperature across the BCS-BEC crossover was first addressed by Noziéres and Schmitt-Rink (NSR) (Noziéres and Schmitt-Rink, 1985). They extended Leggett's analysis of the crossover phenomenon in the continuum to lattice models and also to finite temperatures. Using a diagrammatic theory NSR calculated the scattering t-matrix and obtained the critical temperature from the condition of divergence of the t-matrix. Within their set of approximations, NSR were able to show that in the continuum, the critical temperature smoothly interpolates between the two physically distinct regimes and, more importantly, has a sensible strong coupling limit. A few years later, Sá de Melo, Randeria, and Engelbrecht addressed (Sa de Melo et al., 1993) the same problem in the continuum using a functional integral formalism and underlined the importance of quantum fluctuations in the intermediate and strong coupling normal states in order to recover the NSR results. There are two temperature scales in the problem: $T^*$, or “pair formation temperature” and $T_c$, or “critical temperature”. $T^*$ in the BCS limit is the same as $T_c$ but in the BEC regime it is the Saha dissociation temperature for the molecule to dissociate into two atoms, whose scale is set by the pair binding energy (Randeria et al., 1992). $T_c$ on the other hand, is the temperature below which there is a condensate. The phase diagram reveals, in the strong coupling regime, a region in which pre-formed fermion pairs exist but there is no condensate (Randeria et al., 1992; Trivedi and Randeria, 1995). After the discovery of the copper-oxide based high temperature superconductors, this region of pre-formed pairs was identified with the proposed pseudogap phase of the cuprates and there was a resurgence of interest in the crossover phenomenon.
Since the cuprates have a highly anisotropic lattice structure where the copper and oxygen atoms are arranged in a 2D plane, there have been several papers addressing the crossover phenomenon on a 2D lattice (Randeria et al., 1989, 1990; Scalettar et al., 1989; Moreo and Scalapino, 1991; Randeria et al., 1992; Trivedi and Randeria, 1995). We shall quickly review the physics in two dimensions in the next section before moving on to the three dimensional case.

In two dimensions, there is a jump discontinuity in the density of states at the bottom of the band and this leads to a logarithmic singularity of the 2D propagator and t-matrix. This leads to the corollary that for s-wave pairing in 2D, a necessary and sufficient condition for Cooper instability is the existence of a two-body bound state in vacuum (Randeria et al., 1989). In the continuum, a constant density of states in 2D allows an exact solution of the $T = 0$ gap and number equations for a dilute system at all couplings. However, the situation is much more complicated on a lattice, particularly at finite temperatures and hence, numerical approaches like QMC have been employed (Scalettar et al., 1989; Moreo and Scalapino, 1991; Randeria et al., 1992; Trivedi and Randeria, 1995). Away from half-filling there is a Kosterliz-Thouless type phase transition with off-diagonal algebraic order (Moreo and Scalapino, 1991) and at half-filling ($n = 1$) there is a coexistence of superconductivity and charge density wave (CDW) ordering, along with a vanishing $T_c$ at $n = 1$. The last result can be obtained by mapping the system near $n = 1$ to a two-dimensional Heisenberg antiferromagnet in a magnetic field. One then obtains for the critical temperature

$$T_c \simeq -\frac{2\pi J}{\ln |1 - n|}$$

(2.83)

where $J = t^2/U$ is the effective hopping parameter of the composite bosons. From equation (2.83) one can clearly see that $T_c \to 0$ when $n \to 1$.

In this section we calculate on a three dimensional lattice the pairing temperature $T^*$ (below which pairs form) and the critical temperature $T_c$. We shall show that
in the BCS regime $T_c$ approaches $T^*$ with decreasing coupling strength. The two temperatures differ, however, in the equation of state that is used to calculate the density. The pairing temperature is obtained using the mean field approximation to the thermodynamical potential, in which only fermionic excitations are included (i.e. the breaking up of pairs at that temperature). The calculation of the critical temperature corresponds to the addition of the effects of Gaussian fluctuations in which bosonic excitations (Goldstone modes) are included, leading to a large renormalization of the equation of state. Therefore, in the BEC regime we expect a large deviation of $T_c$ from $T^*$ since in this regime the former is governed by a mechanism different from pair breaking, namely phase fluctuations. In other words, in the large $U/t$ limit, $T_c$ is governed by the center-of-mass motion of the pairs. If we further consider the dilute limit, and ignore the interactions between the (hardcore) bosons, then the energy spectrum for the free bosons can be written as $\omega_q = -\epsilon_0 + \epsilon_q$. The occupancy of the $q^{th}$ state is given by the usual Bose distribution: $g(\omega_q - 2\mu) = [\exp(\beta(\omega_q - 2\mu) - 1)]^{-1}$. The condition for BEC is met when $2\mu$ reaches the bottom of the bound state band, $-\epsilon_0$. This happens at a critical temperature $T_c = (2\pi/m_{eff})(N_0/2.612)^{2/3}$, where $m_{eff}$ is the effective mass of the bosons. However, note that a boson on the lattice can only move by virtual ionization and a simple perturbation theory in $t/U$ suggests that $m_{eff} \sim U/t^2$. Hence, we find $T_c \sim (t^2/U)n^{2/3}$ in the BEC limit. The $t^2/U$ scaling of $T_c$ can also be motivated in the following way. Since phase fluctuations control $T_c$ in this regime, $T_c$ should scale like the zero temperature superfluid stiffness $D_s$. It has been shown in the previous section that $D_s \sim t^2/U$ and therefore $T_c \sim t^2/U$ in the strong coupling regime. To contrast this with the continuum, the superfluid density at $T = 0$ in the continuum is fixed to the total density and hence $T_c$ goes to a constant in the strong coupling limit (Sa de Melo et al., 1993).

One of the limitations of the large $N$ formalism developed here is that it fails to capture the onset of charge density wave order at half-filling. Due to the absence of the
CDW order at \( n = 1 \), the large \( N \) formalism overestimates \( T_c \) near half-filling. It has been shown by Tamaki et al., (Tamaki et al., 2008) that due to a competition between superfluid order and CDW order at \( n = 1 \), the maximum \( T_c \) occurs away from \( n = 1 \). In this section we therefore focus our attention to fillings away from \( n = 1 \) where the large \( N \) theory gives better quantitative results for the critical temperature. The procedure we follow here for calculating the transition temperature \( T_c \) is essentially a large \( N \) analog of the diagrammatic approach of Noziéres and Schmitt-Rink (Nozieres and Schmitt-Rink, 1985).

2.5.1 Calculation of \( T^* \)

We approach the transition from above \( T_c \) and look for the condition when the t-matrix diverges. In terms of the fluctuation matrix \( \mathbf{M} \) this translates to \( M_{11}(q) = 0 \) (one can easily verify that above \( T_c \) the matrix element \( M_{12} = 0 \) by setting \( \Delta = 0 \)). We thus obtain a t-matrix condition for \( T_c \)

\[
\frac{1}{U} = \sum_k \frac{1}{2\xi_k} \tanh\left(\frac{\beta \xi_k}{2}\right)
\] (2.84)

where \( \beta = 1/T \). Since, we anticipate that in the strong coupling regime, the critical temperature would be much smaller than the pairing energy scale which is given by \( T^* \) (i.e. \( 1/N \) corrections to \( T^* \) are large), we note that it is important to choose the right quantity between \( T_c \) and \( \beta_c = 1/T_c \) for the large \( N \) expansion. A failure to make the right choice here has led to incorrect results for \( T_c \) in the literature (Veillette et al., 2007). These authors incorrectly report \( T_c < 0 \) for the strong coupling limit using a large-\( N \) theory in the continuum. In the current work \( \beta = 1/T \) is used in all calculations in order to get positive results for \( T_c \). We note that the above condition (2.84) is also derived by setting \( \Delta = 0 \) in the finite temperature gap equation \( 1/U = \sum_k 1/(2E_k) \tanh(\beta E_k/2) \). This later derivation of equation (2.84)
is not entirely consistent, since the derivation of the finite temperature gap equation itself assumes $\Delta(T) \neq 0$. We shall therefore consider the divergence of the t-matrix to be the correct condition. Next, in order to set up the number equation we use the same functional integral formalism developed so far to first calculate (see Appendix L for more details) the mean field thermodynamic potential at temperatures $T \geq T_c$

$$\Omega_0 = -\frac{2}{\beta} \sum_{\mathbf{k}} \ln(1 + e^{-\beta \xi_k}), \quad (2.85)$$

The mean field number equation at $T = T_c$ is then given by $\partial \Omega_0 / \partial \mu = -n$, or

$$n = \sum_{\mathbf{k}} \frac{2}{\exp(\beta \xi_k) + 1} \quad (2.86)$$

where $\xi_k = \epsilon_k - \mu$ as usual. We next solve equations (2.84, 2.86) self-consistently to obtain the mean field $\beta_c$ and denote it by $\beta_c^0$. In figure (2.9) we plot the mean field transition temperature $T^* = (\beta_c^0)^{-1}$ as a function of the gap parameter $\Delta$. One can see that the for small $\Delta$ (BCS regime) $T^*$ scales linearly with $\Delta$.

In the continuum, the binding energy of the pairs when $1/k_F a_s \to +\infty$, is given by $E_b = 1/ma_s^2$. In this limit, it is the gap equation that determines the chemical potential and one finds that the chemical potential for the fermions is one-half of the binding energy: $\mu = -E_b/2$. Thus in the strong coupling regime, the temperature $T^*$ is given by: $T^* \simeq E_b/2 \ln(E_b/\epsilon_F)^{3/2}$, where $\epsilon_F$ is the Fermi energy. On the other hand, the dissociation temperature $T_{\text{dissoc}}$ can be obtained by noting that for $T \sim T_{\text{dissoc}}$ both the fermions and the bosons are non-degenerate and hence the chemical potential for the bosons is simply twice the same for the fermions: $\mu_b = 2\mu_f$. This gives $T_{\text{dissoc}} \simeq E_b/\ln(E_b/\epsilon_F)^{3/2}$, where the logarithmic factor comes from entropic considerations. We thus conclude, that the temperature scale $T^*$ is the pair dissociation energy scale upto factors of order unity.
2.5.2 Calculation of $T_c$

To obtain the thermodynamic potential upto Gaussian order for $T \geq T_c$, we note that $u_k = 1$ and $v_k = 0$ and hence $M_{12} = M_{21} = 0$. Therefore

$$\Omega_q = \frac{1}{2\beta} \sum_{q,iq} \ln |M_{11}(q)|^2$$  \hspace{1cm} (2.87)

For $T \geq T_c$, $M_{11}(q) = 1 + U \sum_k (1 - f - f')/(iql - \xi - \xi')$, where $iql = i2\pi l/\beta$ are the Bose Matsubara frequencies and $f(\xi) = 1/[\exp(\beta \xi) + 1]$ is the Fermi distribution function.

Following NSR, we maintain the same form of the $t$-matrix equation (2.84). Nevertheless, just like at $T = 0$ the $1/N$ corrections to the thermodynamic potential will renormalize the chemical potential and hence change $\beta_c$. The inverse temperature $\beta$ and the chemical potential $\mu$ are in general independent thermodynamic variables but are related to each other at $T = T_c$ through the $t$-matrix equation. Expanding equation (2.84) upto $O(1/N)$ we obtain

$$\frac{\partial \Omega_0}{\partial \Delta} + \frac{1}{N} \left( \frac{\partial^2 \Omega_0}{\partial \Delta \partial \mu} \delta \mu + \frac{\partial^2 \Omega_0}{\partial \Delta \partial \beta} \delta \beta \right) = 0$$  \hspace{1cm} (2.88)
In the above equation all the derivatives are evaluated at $\Delta = 0$, $\mu = \mu_0$ and $\beta = \beta_0^0$. Setting the coefficient of the $1/N$ term to zero we obtain

$$\delta \beta = -\frac{(\partial^2 \Omega_0/\partial \Delta \partial \mu)}{(\partial^2 \Omega_0/\partial \Delta \partial \beta)} \delta \mu$$

(2.89)

We remind the reader that terms containing $\Omega_g$ are absent in equation (2.89) since we have insisted, following NSR, to keep the form of the t-matrix equation unchanged after $1/N$ corrections are included. Similarly we expand the number equation and obtain

$$-n = \frac{\partial \Omega_0}{\partial \mu} + \frac{1}{N} \left( \frac{\partial^2 \Omega_0}{\partial \mu^2} \delta \mu + \frac{\partial^2 \Omega_0}{\partial \mu \partial \beta} \delta \beta + \frac{\partial \Omega_g}{\partial \mu} \right)$$

(2.90)

and setting the coefficient of the $1/N$ term to zero we get

$$\delta \mu = -\frac{(\partial \Omega_g/\partial \mu) + (\partial^2 \Omega_0/\partial \mu \partial \beta) \delta \beta}{(\partial^2 \Omega_0/\partial \mu^2)}$$

(2.91)

Equations (2.89, 2.91) are then simultaneously solved to obtain the $1/N$ corrections to $\beta_0^0$ and $\mu_0$. We obtain the critical temperature $T_c$ from $T_c = (\beta_0^0 + \delta \beta)^{-1}$ (after setting $N = 1$). Note, we work with inverse temperature $\beta$ and expand in orders of $1/N$. Since we expect a large deviation for $T_c$ from its mean field value, it is important to work with $1/T_c$, expand in orders of $1/N$ and then set $N = 1$ at the end. This way we always obtain $T_c \geq 0$, unlike some of the unphysical results in the literature (Veillette et al., 2007).

The results are shown in Figures (2.10, 2.11). As expected, there is a large deviation of $T_c$ from its mean field value $T^*$ in the strong coupling regime. The phase diagram is as follows: above $T^*$ the system is described by fermionic degrees of freedom, for temperatures below $T^*$ and above $T_c$ there are preformed uncondensed pairs and below $T_c$ we have a condensate of pairs. In the weak coupling limit $T_c$ approaches
Figure 2.10: The chemical potential $\mu/t$ as a function of $U/t$ for $n = 0.5$. The chemical potential is suppressed from its mean field value when $1/N$ fluctuations are included.

Figure 2.11: The transition temperature $T_c/t$ as a function of $U/t$ for $n = 0.5$. The dashed line is the mean field transition temperature denoted by $T^*/t$. The solid line includes fluctuations upto $O(1/N)$.
Figure 2.12: The ratio of gap $\Delta$ and the transition temperature $T_c$ as a function of $U/t$ for $n = 0.5$. For small $U/t$ the $\Delta/T_c$ approaches the known BCS value of 1.75.

Figure 2.13: Plot shows $n_sT_c$ as a function of $U/t$ for $n = 0.5$. In the BEC regime $T_c$ is seen to scale like $n_s$ times a constant ($\approx 6.67$).

the BCS value $\Delta/1.75$ (see Figure 2.12). Beyond the BCS regime, the pairing temperature grows linearly with $U/t$ while $T_c$ goes through a maximum near unitarity and then falls off as $t^2/U$. The precise value of $U/t$ for which $T_c$ goes to a maximum depends on filling (see Figure 2.14). In the BEC limit, the critical temperature scales like the superfluid density and hence like $t^2/U$. This can seen in Figure (2.13). As explained earlier, the reason why $T_c$ scales like $t^2/U$ in the BEC limit can be explained by considering hardcore bosons on a lattice. A simple second order perturbation the-
Figure 2.14: (color online) Plot shows $T_c/t$ as a function of $U/t$ for various fillings: $n = 0.4$ (black), $n = 0.5$ (red), $n = 0.6$ (green), $n = 0.7$ (blue)

ory in $t/U$ then gives an effective hopping parameter proportional to $t^2/U$ for the composite bosons. Since the superfluid density is proportional to the effective hopping parameter and $T_c$ in this regime is governed by phase fluctuations of the lattice Bose gas, hence $T_c \sim t^2/U$ in this limit (Emery and Kivelson, 1995; Toschi et al., 2005).

### 2.5.3 Scaling of $T_c$ in the two regimes

Here we discuss the scaling of the critical temperature in the two regimes. First of all, there is only one finite temperature phase transition at $T = T_c$ in this problem, which is from a normal state to a superconducting state in 3D. However, the nature of the transitions are quite different in the two regimes. In the BCS regime, the normal state is an ordinary Fermi liquid which undergoes Cooper pairing and condensation at the same temperature $T_c$. Hence, in this regime the critical temperature is expected to scale with $U/t$ like the $T = 0$ gap ($\sim \Delta$). In the BEC regime, however, the energy scales for pair formation and for condensation of the pairs become widely separated. At any given temperature, the Cooper pairs become more tightly bound with increasing coupling strength, and the kinetic energy cost is overcompensated by
the gain in potential energy. In other words, the energy scale to dissociate a pair is a large one. While approaching the transition from above, by the time one has reached $T_c$ would have already formed. The nature of phase transition in the Bose limit is therefore between a normal Bose gas and a condensed one. One can then ask, what is the mechanism that governs $T_c$ in this regime? In order to answer that we note that the relevant low energy excitations in the strong coupling limit are the phase fluctuations of the lattice Bose gas. We therefore expect $T_c$ to scale like the $T = 0$ superfluid stiffness ($\sim n_s t$). In order to test these claims we plot $T_c/t$, $\Delta/t$, and $n_s$ as a function of $U/t$ in Figure (2.15) The most non-trivial aspect of Figure (2.15) is that $T_c$ scales like two zero temperature quantities in the two limits. This indicates that the mechanism for the destruction of condensation at a higher temperature is intricately related to the physics in the ground state of the system.

A more detailed calculation of $T_c$ that takes into account the CDW order at $n = 1$ has been done by Tamaki et al. (Tamaki et al., 2008). These authors use a self-consistent t-matrix approximation for pairing fluctuations and a fluctuation exchange approximation to take into account the CDW and Spin Density Wave (SDW)
fluctuations.

2.6 Hartree + BCS Theory, Hartree + NSR

Theory, and Comparison with large $N$ results

We begin this section with a brief account of the Hartree + BCS (HBCS) Theory (Belkhir and Randeria, 1992, 1994; Randeria et al., 1992; Trivedi and Randeria, 1995). We shall first discuss the results from HBCS theory for chemical potential, and superfluid density and compare them with the large-$N$ results. Next, we shall discuss a Hartree-shifted Noziéres and Schmitt-Rink theory for $T_c$ and compare the results with those from large-$N$. We shall then explain the differences between HBCS and large-$N$ results in detail in sections (2.6.3) and (2.6.4).

2.6.1 Hartree + BCS Theory at $T = 0$

The starting point of the Hartree + BCS theory is the attractive Hubbard model (2.1). In mean field theory the contribution of the interaction term $V^i = -Uc^{\dagger}_{k,1}c^{\dagger}_{-k,1}c_{-k,1}c_{k,1}$ to the ground state energy can be written as

$$
\langle \hat{V} \rangle = -U \sum_k \langle c^{\dagger}_{k,1}c_{k,1} \rangle \langle c^{\dagger}_{-k,1}c_{-k,1} \rangle - U \sum_k \langle c^{\dagger}_{k,1}c^{\dagger}_{-k,1} \rangle \langle c_{-k,1}c_{k,1} \rangle
$$

$$
= -\frac{Un^2}{4} - U \sum_k F_k F^*_k \tag{2.92}
$$

The first term is a constant and is the Hartree correction to the ground state energy. Note that since the chemical potential is a derivative of the ground state energy w.r.t. $n$, we can absorb the overall shift of the ground state energy due to the Hartree term in the chemical potential by adding $nU/2$ to it. The quantity $F_k$ in the second term is self-consistently obtained by minimizing the ground state energy w.r.t. $F_k$ and this
Figure 2.16: Figure shows a comparison of the chemical potentials obtained within Hartree shifted BCS theory and large-$N$ respectively. The filling fraction $n = 0.5$.

The gap and number equations in HBCS respectively read,

\[
\frac{1}{U} = \sum_k \frac{1}{2E_k} \tag{2.93}
\]

\[
n = \sum_k \left( 1 - \frac{\xi_k}{E_k} \right) \tag{2.94}
\]

where $E_k = \sqrt{\xi_k^2 + \Delta^2}$. We note that the gap and number equations in HBCS have the same form as obtained at the zeroth order in the large $N$ theory, except the single particle energies $\xi_k$ in HBCS include a Hartree shift: $\xi_k = \epsilon_k - \mu - nU/2$, where the last term is the Hartree term. It can be easily verified that the HBCS theory satisfies the particle-hole constraints on thermodynamics derived from the attractive Hubbard model (see Appendix A). Equations (2.93, 2.94) are then solved for a given value of $n$ and the results are compared in Figure (2.16) with results upto $O(1/N)$ in the large $N$ theory. When $U/t \gg 1$,

\[
\mu_{\text{HBCS}} \approx -(U/2) + 12(t^2/U)(n - 1) \tag{2.95}
\]
Figure 2.17: Figure shows a comparison of the superfluid densities obtained within Hartree shifted BCS theory and large $N$ respectively. The filling fraction $n = 0.5$. Both the superfluid densities have the same $t/U$ scaling in the large $U/t$ limit. However, prefactors being different, $n_s^{HBCS} > n_s^{MF+1/N}$ across the crossover.

On the other hand, the strong coupling limit of the chemical potential within the large-$N$ theory scales like

$$
\mu \simeq -(U/2)(2 - n) + O(t^2/U),
$$

which has a different leading order term compared to the HBCS $\mu$. We already see that there are quantitative differences between the HBCS and the large-$N$ results. We shall discuss these differences later in section (2.6.3) and section (2.6.4). For the moment we shall continue with the HBCS theory and calculate the superfluid density.

The superfluid density within HBCS is defined as (see equation 2.67)

$$
n_s^{HBCS} = \frac{1}{\beta} \left( \frac{\partial^2 \hat{S}_0}{\partial \theta^2} \right)_{\mu, \Delta} = \sum_k \left( 1 - \frac{\xi_k}{E_k} \right) \cos(k_x a)
$$

where $\xi_k = \epsilon_k - \mu - nU/2$ has the Hartree shift. As shown in Figure (2.17) the superfluid densities for both the approaches scale like $t/U$ in the strong coupling...
regime. However, the two have quantitative differences between them.

Having discussed some of the results from introducing a Hartree shift to the BCS theory at \( T = 0 \), we next move on to a calculation of \( T_c \) where now the Nozieres and Schmitt-Rink approach (Nozieres and Schmitt-Rink, 1985) is adapted to include Hartree shifts in the single-particle propagators.

### 2.6.2 Critical temperature using Hartree shifted NSR

For calculating the critical temperature we shall use the Nozieres and Schmitt-Rink approach (Nozieres and Schmitt-Rink, 1985) with the modification that the single particle Green's function \( G_0 \) now includes a Hartree shift which we call \( \Sigma \). We shall work in the grand canonical ensemble at a fixed \( \mu \) and hence \( \Sigma \) is a function of \( \mu \) and \( T \). We approach the transition from above \( T_c \) and look for the divergence of the \( t \)-matrix. This gives us a relation between \( T_c \) and \( \mu \)

\[
\frac{1}{U} = \sum_k \frac{1}{2\xi_k} \tanh\left(\frac{\beta \xi_k}{2}\right)
\]

Here the Hartree shift is contained in \( \xi_k = \epsilon_k - \mu + \Sigma \). Since we are working in the grand canonical ensemble the filling fraction would depend on the value of \( \mu \) we choose. At a fixed temperature this dependence is given through the number equation

\[
n = -\left. \frac{\partial \Omega(T, \mu)}{\partial \mu} \right|_T
\]

The Hartree shift, which depends on the filling fraction, is then given by

\[
\Sigma(\mu, T) = -n(\mu, T)U/2
\]

In order to implement the number equation (2.100) we proceed as follows: For a given \( U \) and \( \mu \), we calculate \( T_c \) and \( \Sigma(\mu, T_c) \) by simultaneously solving equations (2.99) and
With these values of $T_c$ and $\Sigma$, we evaluate $\Omega(\mu, T = T_c)$. Next, keeping the temperature fixed we change $\mu$ to $\mu + \delta \mu$ and evaluate $\Sigma(\mu + \delta \mu, T = T_c)$ from equation (2.101). This lets us evaluate $\Omega(\mu + \delta \mu, T = T_c)$. The number equation can then be written in the form

$$n = -\frac{\Omega(\mu + \delta \mu, T = T_c) - \Omega(\mu, T = T_c)}{\delta \mu} \quad (2.102)$$

We next give an explicit formula for the thermodynamic potential $\Omega = \Omega_0 + \Omega_g$. In presence of the Hartree shift, the mean field thermodynamic potential $\Omega_0$ is given by

$$\Omega_0 = -\frac{2}{\beta} \sum_k \ln(1 + e^{-\beta \xi_k}) + \frac{\Sigma^2}{U} \quad (2.103)$$

As a check, note that setting $\Omega = \Omega_0$ in equation (2.100) the above form for $\Omega_0$ gives us the familiar mean field number equation

$$n = \sum_k \frac{2}{\exp(\beta \xi_k) + 1} \quad (2.104)$$

To obtain the thermodynamic potential upto Gaussian order for $T > T_c$, we note that $u_k = 1$ and $v_k = 0$ and hence $M_{12} = M_{21} = 0$. Therefore

$$\Omega_g = \frac{1}{\beta} \sum_{q, i q_i} \left[ \ln(M_{11}(q)) - (M_{11}(q) - 1) \right] \quad (2.105)$$

where, we are justified to drop the convergence factor in the last line of equation (2.105) since $(M_{11} - 1)$ takes out the leading $1/iq_i$ piece from $\ln(M_{11})$ (see Appendix A for more details). For $T > T_c$, $M_{11}(q) = 1 + U \sum_k (1 - f - f')/(iq_i - \xi - \xi')$, where $iq_i = i2\pi l/\beta$ are the Bose Matsubara frequencies and $f(\xi) = 1/[\exp(\beta \xi) + 1]$ is the Fermi distribution function. We numerically calculate $\Omega_g$ using equation (2.105) and set up the number equation using the procedure outlined above. In order to obtain the $n$ dependence of $T_c$, the procedure is repeated for various values of $\mu$. The results
Figure 2.18: Figure shows a comparison of the critical temperatures obtained within Hartree shifted NSR and large $N$ respectively. The filling fraction $n = 0.5$. The maximum $T_c$ for the Hartree shifted NSR and the large $N$ theory can be compared to the results of Tamaki et al. ($T_c^{\text{max}} \approx 0.66t$ for $n = 0.5$) Tamaki et al. (2008) are plotted in Figure (2.18). We notice that there are quantitative differences between the HNSR and large-$N$ results. At this stage, we do not understand why the $T_c$ from HNSR is lower than the $T_c$ from large-$N$ theory.

2.6.3 Comparison in the BEC limit

In order to understand the results (2.95) and (2.96), we next solve the problem exactly in the atomic limit: $t/U = 0$ and show that the Hartree Mean Field theory gives exact answers in this limit. For $t/U = 0$ the Hamiltonian is a single site one

$$H = -Un_{\uparrow}n_{\downarrow} - \mu(n_{\uparrow} + n_{\downarrow})$$  \hspace{1cm} (2.106)$$

and has four eigenstates: $|0\rangle, |\uparrow\rangle, |\downarrow\rangle$ and $|\uparrow \downarrow\rangle$ with respective energies $0, -\mu, -\mu$ and $-2\mu - U$. To study the broken symmetry state we now introduce a fictitious pairing field $h$ to obtain a Hamiltonian

$$H = -Un_{\uparrow}n_{\downarrow} - \mu(n_{\uparrow} + n_{\downarrow}) - h(c_{\uparrow}^\dagger c_{\downarrow}^\dagger + c.c.)$$  \hspace{1cm} (2.107)$$
After setting up the gap and number, we shall finally take $h = 0$. The eigenvalues of (2.107) are: $-\mu$, $-\mu$, $(-U - 2\mu + \sqrt{4h^2 + (U + 2\mu)^2})/2$ and $(-U - 2\mu - \sqrt{4h^2 + (U + 2\mu)^2})/2$. The ground state eigenvalue $\lambda = (-U - 2\mu - \sqrt{4h^2 + (U + 2\mu)^2})/2$ corresponds to the eigenvector

$$|\Psi_G\rangle = [-\left(U + 2\mu + \sqrt{4h^2 + (U + 2\mu)^2}/2\right)|0\rangle + |\uparrow\downarrow\rangle] (2.108)$$

upto an overall normalization factor $(1 + h^2/\lambda^2)^{-1}$. The gap and number equations at $T = 0$ then read

$$\Delta = U \langle c^\dagger_1 c_1 \rangle = \frac{-U h/\lambda}{1 + (h/\lambda)^2} (2.109)$$

$$n = \langle c^\dagger_1 c_1 + c^\dagger_1 c_1 \rangle = \frac{2}{1 + (h/\lambda)^2} (2.110)$$

In the limit $h = 0$, when the above equations are solved for $\mu$ and $\Delta$, we find $\mu = -U/2$ and $\Delta = U \sqrt{n(2 - n)}/2$. These are exactly the values obtained from solving the HBCS number and gap equations (Garg et al., 2005). Physically, the result $\mu = -U/2$ in the atomic limit makes sense. In this limit we have a single site problem with bosons. The chemical potential of the bosons is just the binding energy $\sim U$ and the chemical potential of the fermions is just one-half of that value. From these considerations, we conclude that the large-$N$ theory gives quantitatively incorrect results for the density ($n$) dependence of the chemical potential in the atomic limit. This also leads to problems with the compressibility since the compressibility is the derivative of $\mu$ with respect to $n$. We turn to this next.

In order to calculate the compressibility $dn/d\mu$ within HBCS we note that the Hartree shift to the single particle energies can be incorporated into the chemical potential. Following Trivedi and Randeria (1995) we write the renormalized chemical
potential as $\tilde{\mu} = \mu + nU/2$, and evaluate $dn/d\mu$ as

$$\frac{dn}{d\mu} = \frac{\partial n/\partial \tilde{\mu}}{1 - (U/2)\partial n/\partial \tilde{\mu}} \quad (2.111)$$

The quantity $\partial n/\partial \tilde{\mu}$ can be calculated from equations (2.93 and 2.94)

$$\frac{\partial n}{\partial \tilde{\mu}} = \Delta^2 \sum_k \frac{1}{E_k^3} + \frac{(\sum_k \frac{\xi_k}{E_k^3})^2}{\sum_k \frac{1}{E_k^3}} \quad (2.112)$$

Figures (2.19 and 2.20) show a comparison of $dn/d\mu$ as obtained from HBCS using equations (2.111, 2.112) and large-$N$ respectively. In the strong coupling limit the HBCS compressibility scales as

$$\frac{dn}{d\mu} \approx \frac{U}{12t^2} \left(1 - \frac{24t^2}{U^2}\right) \quad (2.113)$$

This is again expected on general grounds, when one notes that the chemical potential $\mu$, written in powers of $t/U$, has a zeroth term equal to $-U/2$ (atomic limit). Any $n$ dependence of $\mu$ is hence at least $O(t^2/U)$, which implies that the compressibility must increase with $U$. From these considerations we come to the conclusion that the

Figure 2.19: Compressibility $dn/d\mu$ obtained within Hartree shifted BCS theory for filling fraction $n = 0.5$. 

Figure 2.20: Compressibility $dn/d\mu$ obtained within Hartree shifted BCS theory for filling fraction $n = 0.5$. 


compressibility should be a monotonically increasing function of $U/t$. In contrast, the compressibility for large-$N$ seems to scale like $dn/d\mu \sim 2/U$.

### 2.6.4 HBCS vs. large-$N$ - final remarks

To summarize we find that the much simpler BCS plus Hartree theory works better in the BEC limit compared with the more sophisticated large-$N$ approach where we included the $1/N$ Gaussian fluctuation corrections to the saddle point result, where both approximations satisfy the particle-hole constraints on the thermodynamics. By better we mean that BCS + Hartree reproduces the atomic limit behavior of the chemical potential and the strong coupling behavior of the compressibility expected for a BEC of hard-core lattice bosons, while the large-$N$ approach (with $N$ set equal to 1 at the end) does not. We can also compare our results with the available Quantum Monte Carlo data, which however is only for the two-dimensional attractive Hubbard model. We find that the results for the chemical potential (Randeria et al., 1992) and for the compressibility (Trivedi and Randeria, 1995) at moderately large $|U|/t$ are both in good (semi-quantitative) agreement with the Hartree + BCS theory. Although there exists no QMC data on the 3D attractive Hubbard model at $T = 0$,
we note that fluctuations should be less important in 3D than in 2D. It is therefore reasonable to expect, that the agreement between Hartree + BCS theory and QMC should only improve in 3D.

The comparison between the two approaches (large-\(N\) and HBCS) is quite surprising and unexpected. We should emphasize that the two theories start with quite different mean field solutions (or saddle points). The BCS + Hartree solution incorporates both the particle-particle (p-p), or pairing, and the particle-hole (p-h) Hartree physics on an equal footing at the mean field level. The large-\(N\) solution, on the other hand, is designed to focus only on the p-p channel at the saddle point level, and include all other effects as fluctuations about the saddle point. One might have thought that since the Hartree correction to the thermodynamics is included at the \(1/N\) level (along with higher order terms), the large-\(N\) approach would "go beyond" the simpler BCS + Hartree approach. But we find that "more" (diagrams, for instance) is not necessarily "better" for quantum many-body systems!

It might also be worth contrasting the optical lattice calculations presented here from BCS-BEC crossover in the continuum. In the continuum, one does not in general have a Hartree term in thermodynamics, which is proportional to both the interaction and the density (except in the BCS limit). The reason is as follows: the bare interaction \(g(\Lambda)\) actually goes to zero as the ultraviolet cutoff (inverse range of potential) goes to infinity. Thus a "bare Hartree term" proportional to \(g(\Lambda)n\) vanishes throughout the crossover. Also there can be no term proportional to the renormalized interaction \(a_s\) in the ground state energy in general, since that would diverge at unitarity! As shown by Diener et al. (2008), the Hartree diagram in the Gaussian fluctuation correction to the BCS theory does indeed lead to the expected Hartree correction of relative order \(k_f a_s\) in the BCS limit. But it is not possible to isolate "the Hartree correction" to the ground state energy or chemical potential at arbitrary values of \(1/k_f a_s\) in the continuum problem.
In conclusion we have learned a valuable lesson for optical lattice calculations in the future. A simple mean field calculation that takes into account both pairing and Hartree shifts, and thus satisfies the p-h constraints on thermodynamics, is expected to be more reliable than a large-\(N\) theory which includes \(1/N\) corrections, but does not treat pairing and Hartree shifts on an equal footing.

2.7 Conclusions

In this Chapter we have developed a large \(N\) approach for the attractive Hubbard model in 3D. We have calculated the ground state chemical potential, gap, ground state energy etc. away from half-filling. The superfluid density at \(T = 0\) on the lattice is found to deviate from the total density and in the BEC limit is determined by the single-boson hopping matrix element which scales as \(t/U\). We also calculate the transition temperature by approaching the superfluid state from above \(T_c\). The transition temperature is shown to scale like two different ground state quantities in the two regimes: in the BCS regime \(T_c\) scales like the gap, while in the BEC regime \(T_c\) scales like the zero temperature superfluid density. These two different scalings show that in the weak coupling regime coherence is lost due to pair breaking and in the strong coupling the superfluid order is destroyed by phase fluctuations of the lattice Bose gas.

We also find, quite contrary to our expectations, that in the strong coupling limit, the large-\(N\) theory gives inaccurate results for quantities like chemical potential and qualitatively wrong trends for compressibility. A comparison with a simple Hartree shifted BCS theory, which correctly recovers the atomic limit and predicts the right qualitative trends for compressibility, reveals that the large-\(N\) theory on the lattice, although considers a larger number of diagrams, is in fact inferior to the simpler Hartree shifted BCS theory. The limitation of the large-\(N\) approach is explained by
noting (i) the importance of Hartree shift in lattice problems, and (ii) inability of the large-$N$ approach to treat particle-particle and particle-hole channels at equal footing at the saddle point level.
Chapter 3

Dynamics of Bose Josephson junctions

In the past few years, experiments on Josephson tunnel junctions in superconductors (Carmi et al., 2000; Monaco et al., 2002, 2009) and Bose-Einstein condensates (Scherer et al., 2007; Schweikhard et al., 2007) have addressed the role of non-adiabaticity in the spontaneous production of topological defects, a question that has bearing on early-universe cosmology (Kibble, 1976; Zurek, 1985; Freire et al., 2005; Donaire, 2006). While a first type of experiments (Monaco et al., 2002, 2009) have used a temperature quench through a second-order phase transition from a normal to a superconducting phase, a second type (Scherer et al., 2007; Schweikhard et al., 2007) uses interference between initially independent condensates as a mechanism to trap vortices. In the case of superconductors the Kibble-Zurek scaling law (Zurek, 1985) relating the probability to trap vortices to the quench rate has been tested. Experiments connecting the independent BECs have similarly tried to test the role of the merging rate in determining the probability for observing vortices in the final BEC. Motivated by these experiments we have studied numerically the related problem of a ring-shaped Bose-Josephson junction array. We would like to stress that, while there are similarities between our initial conditions and those of the aforementioned experiments, there are also qualitative differences that will be discussed later. Nevertheless, it is quite conceivable that our findings here can be tested in future experiments with ultra-cold atomic gases (Amico et al., 2005).
3.1 Kibble-Zurek scenario

In 1976, Kibble proposed a scenario for the formation of cosmological strings in the early universe (Kibble, 1976). Under this scenario, symmetry-breaking phase transitions in causally disconnected regions during the early expansion of the universe gave rise to independent order parameters. A concrete example would be causally disconnected Higgs fields coming out of electroweak symmetry breaking during the cosmological expansion. When these regions with independent order parameters became causally connected, they incorporated long lived topological structures like cosmic strings. Even though the existence of cosmic strings is yet to be confirmed from cosmological data, the Kibble scenario remains a general mechanism for the formation of topological defects under quench situations. Kibble’s idea was adapted to superfluid He$^4$ by Zurek in 1985 when he estimated the velocities of superflows after realistic quenches in cryogenic experiments and concluded that such topological defects could be detected (Zurek, 1985). The starting point of Zurek’s analysis is the Landau energy functional

\[ V = \alpha |\psi(r)|^2 + \frac{1}{2} \beta |\psi(r)|^4 \]  

(3.1)

that describes the potential energy contribution to the free energy near a second order phase transition. In the broken symmetry state $\alpha < 0$ and $V$ has the shape of a “Mexican hat” with a central hump $\Delta V = \alpha^2/\beta$. $\Delta V$ can be interpreted as the difference in free energies of the normal and the broken symmetry states. A length scale that characterizes a second order phase transition is the correlation length $\xi(T) = \hbar/\sqrt{2m\alpha}$. Further, in the broken symmetry phase the order parameter can be described by a magnitude and an arbitrary overall phase: $\psi = |\psi|e^{i\theta}$. The superfluid velocity is then proportional to the gradient of the $\psi$: $v_s = (\hbar/m)\nabla \theta$. The order parameter $\psi$, in superfluid He$^4$, satisfies the Gross-Pitaevskii equation with the Landau energy
The geometry that Zurek considers is an annulus with circumference \( C = 2\pi R \) and cross-sectional radius \( r \), such that \( r \ll R \). The further assumption is that the system arrives with a pre transition correlation length \( \xi_i \) at the phase transition point after which the system evolves under a sudden approximation. The length scale \( \xi_i \) is therefore a frozen length scale over which the order parameter is well defined and unique. This defines a domain. For a circumference \( C \), the number of such domains is \( N = C/\xi_i \). Two points separated by a distance greater than \( \xi_i \) are causally disconnected and have different order parameters with an arbitrary relative phase to begin with. When the two domains start to overlap, an arbitrary relative phase is chosen between \(-\pi\) and \(\pi\). Since the relative phases are randomly chosen, the total phase winding around the circumference follows a normal distribution with a width

\[
\delta \theta = \int_C \nabla \theta \cdot d\vec{s} \sim \sqrt{N} \tag{3.3}
\]

The third assumption that Zurek makes is that equation (3.3) determines the final circulation of stable vortices thus created during the quench, an assumption that we shall question in the following section. Assuming equation (3.3) as the final phase winding around the loop, Zurek estimates the superfluid velocity as

\[
v_s = \frac{\hbar/m}{(C\xi_i)^{1/2}} \tag{3.4}
\]

Equation (3.4) suggests that a rapid quench would leave the superfluid circulating around the annulus. In order to give an estimate of \( v_s \), one needs to calculate the frozen out correlation length \( \xi_i \). This is done by multiplying the correlation time with a characteristic velocity, which in this case would be the second sound velocity. The dynamics of the system is divided into three time stages: An adiabatic stage...
during which the system evolves close to equilibrium arriving at the transition with a frozen correlation length $\xi_0$, followed by a non-adiabatic stage (treated under sudden approximation) during which the system goes out of equilibrium since the correlation time $\tau = \hbar/\alpha$ at the transition diverges. After going through $T_c$, if we wait long enough, the system will eventually come back to equilibrium. Further changes in temperature or pressure would be adiabatic. We shall exclude this last stage and only focus on the first two stages. Proximity to the transition can be characterized by a parameter $\epsilon$ such that

$$\epsilon = (T_\lambda - T)/T_\lambda = t/\tau_Q$$  

(3.5)

where $T_\lambda$ is the temperature for the $\lambda$-transition and $\tau_Q$ is the time over which the quench is accomplished. Since, we want to quench the system at a rate such that it goes out of equilibrium at an early time (this will ensure more number of domains and hence larger $v_s$), we do this using a pressure quench. Close to the transition, the first sound velocity $c_1$, associated with a pressure wave, would be much larger than the second sound velocity $c_2$ which is inversely proportional to the response time of the system, and hence becomes zero at $T = T_\lambda$. The way $\xi$ and $c_2$ scale with the parameter $\epsilon$ is as follows:

$$\begin{align*}
\xi &= \xi_0 |\epsilon|^\nu \\
c_2 &= c_2^0 \epsilon^{1-\nu}
\end{align*}$$

(3.6)

where, $\xi_0$ and $c_2^0$ are the $T = 0$ correlation length and second sound velocity respectively, and the critical exponent $\nu = 1/2$ for Landau-Ginzburg theory and equal to $2/3$ for RG. The correlation time $\tau$ is given by

$$\tau = \frac{\xi}{c_2} = \frac{\tau_0}{\epsilon}$$

(3.7)
where \( \tau_0 = \xi_0/c_0^2 \). If \( t > \tau \), then the system evolves close to the equilibrium and if \( t < \tau \), then the system is out of equilibrium. The two regimes meet at \( t = \hat{\tau} \) when

\[
\hat{\tau} = \tau(\hat{\tau}) = \tau_0/\varepsilon(\hat{\tau})
\]

\[ \hat{\tau} = \sqrt{\tau_0 \tau_Q} \] (3.8)

We can now estimate the size of the frozen out configurations

\[
\xi_t(\hat{\tau}) = \xi_0 \left( \frac{\tau_Q}{\tau_0} \right)^{\nu/2}
\] (3.9)

Using, \( C = 1 \text{ cm} \) for the circumference, \( \tau_Q = 10^{-2} \text{s} \), and \( \xi_0 = 5.6 \text{ Å} \) and \( \tau_0 = 8.5 \times 10^{-12} \text{s} \) from Ginzburg-Landau theory, we obtain \( v_s = 1 \text{mm/s} \), a detectable velocity in experiments.

The final point in Zurek’s scenario is the conservation of angular momentum. Zurek proposes that the angular momentum can be conserved for reasonable geometries if the superfluid current is equated to thermal current due to Brownian motion. Even though the average current due to Brownian motion is zero, the instantaneous current is non-zero. Further, the supercurrent is proportional to the superfluid density which itself scales with temperature. Hence, close to \( T_c \) one can have a sizeable superfluid velocity but a small supercurrent that can be balanced by the instantaneous thermal current. A superflow can thus be set up while conserving the total angular momentum. The thermal angular momentum can obviously be transferred to the walls of the container while the superfluid keeps circulating around the annulus.

One of the criticisms of the Kibble-Zurek scenario is (a) the use of local hydrodynamics for estimating the size of the uncorrelated domains (Leggett, 2002). Let us consider the kinetics of Cooper pair formation starting with a normal state that is supercooled below \( T_c \). We remind ourselves that the Cooper instability arises due to scattering of pairs of electrons with opposite spins and momenta. As a superconducting gap opens up, Leggett (2002) argues that in order for the gap to reach its
equilibrium value, the reservoir of normal quasiparticles must be in thermal equilib­rium. In other words, the thermal distribution should have enough time to adjust itself, and this time scale is governed by the quasiparticle scattering time scale and not the gap frequency ($\Delta/\hbar$). However, we have stated earlier that $k_B T_c \tau(T_c)/\hbar \gg 1$ and hence the requirement of thermal equilibrium will impose severe restrictions on the applicability of local hydrodynamics close to $T_c$. In other words, Zurek's estimate of $v_s$ outlined above involves $\epsilon \sim 10^{-4}$, which puts one extremely close to $T_c$, where the applicability of the hydrodynamic formulation is doubtful. A second point (b) that has been addressed by Zurek (Zurek, 1996) is by invoking the Ginzburg crite­rion. He concludes that very close to critical point, the Ginzburg-Landau theory can only be used as a "qualitative guide" for He$^4$. Whether it is point (a), or point (b), or both that would eventually restrict the applicability of KZ scenario in a certain experiment, will depend on the details of quenching rate etc.

3.2 Statistics of Vortex trapping in circular Josephson junction arrays

In this section, we revisit Zurek's assumption that the final circulation around the loop is proportional to the dispersion of sum total of initial relative phases between adjacent condensates. As it will be shown in the next section, the initial configuration right after the relative phases are established between adjacent pairs of condensates, is a highly unstable one. The question we ask is: if we allow the system to reach a stable circulation where the currents in all the links are same, do we still have the same scaling for final winding numbers? In order to address this, we shall define a similar problem and make a few comments at the end on the relevance of our results to the Kibble-Zurek scenario.

The problem we study is that of $N$ independent Bose-Einstein condensates which
upon sudden connection become arranged on a ring of weakly coupled condensates. We assume that the phase inside each condensate is uniform, the condition for which is outlined in Ref. (Zapata et al., 1998). This condition further ensures that no vortices form within the individual condensates, leaving us only with vortices caused by the phase variation along the ring. At \( t = 0 \), simultaneous Josephson contacts are made between each adjacent pair of condensates. As shown in Ref. (Zapata et al., 2003) for the case of two initially independent condensates, a relative phase is quickly established once a few condensate atoms have hopped from one side to another. Each pair of neighboring condensates behaves as if a random relative phase \( \phi \in (-\pi, \pi] \) is chosen locally. However, due to the single-valuedness of the macroscopic wave function, there are only \( N-1 \) independent variables. Therefore, in our simulations we choose \( N-1 \) relative phases independently, each following a flat distribution within the interval \( (-\pi, \pi] \). The \( N^{th} \) relative phase lies in the same interval and is determined by the constraint that the total phase variation around the ring should be \( 2\pi n \) (\( n \in \mathbb{Z} \)). From the central limit theorem, we know that for \( N \rightarrow \infty \) the distribution of \( n \) approaches a normal distribution with FWHM = 2.354 \( \sigma N^{1/2} \), where \( \sigma = 1/\sqrt{12} \) is the standard deviation for a flat distribution in the interval \( (-\frac{1}{2}, \frac{1}{2}] \).

A key point is to realise that the classically stable fixed points correspond to all the relative phases being equal (modulo \( 2\pi \)) to a value \( 2\pi m/N \), where \( m \in \mathbb{Z} \) is the winding number or charge of the final vortex configuration. To allow our system to converge to one of these fixed points we let each link follow a semiclassical Josephson equation which includes a phenomenological dissipation term characterized by a single parameter \( \gamma \). Such dynamics allows the system to go through phase slips at individual junctions. Thus, generally \( m \neq n \).
3.3 Hamiltonian and equations of motion

We shall begin by deriving, under conditions to be stated below, a Hamiltonian that describes the case of two BECs connected to each other through a weak Josephson link. After presenting the Hamiltonian for the case of two BECs, we shall generalize to the case of \( N \) BECs arranged in a ring. We start our analysis for the system of two BECs with the canonical Josephson Hamiltonian:

\[
H = -\frac{E_J}{2} (a_1^\dagger a_2 + a_2^\dagger a_1) + \frac{E_C}{8} (a_1^\dagger a_1 - a_2^\dagger a_2)^2 - \frac{\Delta \mu}{2} (a_1^\dagger a_1 - a_2^\dagger a_2)
\]  

(3.10)

where, \( a_1 \) and \( a_2 \) are the annihilation operators for condensate 1 and 2 respectively, \( E_J \) is the Josephson coupling energy proportional to the tunneling through the barrier that separates the two BECs, \( E_C \) is the charging energy or bulk modulus, and \( \Delta \mu \) is the difference in chemical potentials between the two BECs. The conditions under which the canonical Hamiltonian (3.10) is valid are explicitly given in (Leggett, 2001). If we now define an operator \( \hat{n} = (a_1^\dagger a_1 - a_2^\dagger a_2)/2 \), we note that one of the conditions mentioned in (Leggett, 2001) is the condition that the eigenvalue \( n \ll N \), where \( N \) is the total number of particles. The second condition for the validity of (3.10) is that the trap asymmetry \( \Delta \mu \ll V_0 \), where \( V_0 \) is the barrier height. Failure to meet these requirements might result in inter alia, \( \mu \) in each well becoming a non-linear function of \( N \), and \( E_J \) being significantly modified from its \( n = 0 \) value. In the current problem we shall set the bias \( \Delta \mu = 0 \) for simplicity and always assume \( n \ll N \). We next define a relative phase operator \( \hat{\phi} \) such that it satisfies the commutation relation

\[
[\hat{n}, \hat{\phi}] = -i
\]  

(3.11)
and a coherent Gross-Pitaevskii state of the form

$$\Psi_N = \frac{1}{\sqrt{N!}}(\cos \chi e^{i\phi/2}a_1^\dagger + \sin \chi e^{-i\phi/2}a_2^\dagger)N|\text{vac}\rangle$$  \hspace{1cm} (3.12)

is an eigenstate of $\hat{\phi}$. One can define such a relative phase operator provided that the amplitude of the states with $N/2 - |n| \leq N^{1/2}$ is small and we neglect effects of relative order $N^{-1/2}$. The Hamiltonian (3.10) can then be written in the familiar form

$$H = -E_J\sqrt{1 - \frac{4\hat{n}^2}{N^2}} \cos \hat{\phi} + \frac{E_C\hat{n}^2}{2}$$  \hspace{1cm} (3.13)

It is important to note that we have set $E_J \equiv NE_J$ in the above equation. The ratio $E_C/E_J$ by its order of magnitude characterizes three distinct regimes. These are summarized in Table (3.1). For real systems with dilute alkali gases, the Rabi regime can never be attained under the conditions stated above.

<table>
<thead>
<tr>
<th>Regime</th>
<th>Condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rabi</td>
<td>$E_C/E_J \ll N^{-2}$</td>
</tr>
<tr>
<td>Josephson</td>
<td>$N^{-2} \ll E_C/E_J \ll 1$</td>
</tr>
<tr>
<td>Fock</td>
<td>$1 \ll E_C/E_J$</td>
</tr>
</tbody>
</table>

Table 3.1: Different regimes described by the ratio $E_C/E_J$

We next generalize to the case of $N$ BECs arranged on a ring and with nearest neighbors connected through weak Josephson links (the system we study is always in the Josephson regime defined in the above table). The Hamiltonian for such a system, ignoring terms of $O(n^2/N^2)$, is given by

$$H = -E_J \sum_i \cos \phi_{i,i+1} + (E_C/2) \sum_i n_i^2$$  \hspace{1cm} (3.14)
where $\phi_{i,i+1}$ is the relative phase between $i$ and $i+1$ (with $i = N + 1$ identified to $i = 1$) and $n_i = N_i - N_i^{(0)}$ is the deviation of the number of particles $N_i$ from the equilibrium value $N_i^{(0)}$ at condensate $i$. We assume all $N_i^{(0)}$s to be the same and initially $n_i = 0$, so that $\sum_i n_i = 0$ throughout the entire evolution. In the classical limit this Hamiltonian can be mapped into that of coupled rigid pendula, with the first term denoting the “potential energy” and the second term the “kinetic energy” of the pendula system.

We start our analysis of the Josephson dynamics by stating a theorem: If $N$ BECs with random relative phases are coupled by a nearest-neighbor Josephson coupling on a one-dimensional lattice with periodic boundary conditions, a necessary condition to obtain a metastable non-zero circulation of winding number $2\pi m$ is $N > 4m$, the case of $4m$ links being marginal. The proof is as follows:

Let us consider a system with $N$ links and a total phase difference of $2\pi m$ around the loop. As stated earlier, the fixed point corresponding to a circulation of charge $m$ is given by the configuration where all the phases are $\Phi_m = 2\pi m/N$ (modulo $2\pi$). Hereafter, we simplify the notation $\phi_i \equiv \phi_{i,i+1}$. To determine whether this fixed point is stable we consider a configuration where $\phi_i = \phi_m + \epsilon_i$ with $\sum_i \epsilon_i = 0$ and $\epsilon_i \to 0$.

The potential energy of this new configuration with respect to the fixed point is, up to second order in $\epsilon_i$, given by $\Delta E(\epsilon_i) = (\cos \phi_m) \sum_i \epsilon_i^2$. For the fixed point to be stable we should have $\Delta E(\epsilon_i) > 0$, which requires $N > 4m$. This theorem can equally be applied to a system of $XY$ spins coupled by Heisenberg interaction. A corollary is that final configurations satisfying $N/4 \leq m \leq N/2$ are unstable (Paraoanu, 2003).

For a more generic analysis of the fixed points and their basins of attraction we derive from Hamiltonian (3.14) a set of semiclassical equations of motion for the relative phases and currents at each junction. It is important to note that for cyclically coupled Josephson junctions the variable canonically conjugate to, say, $\phi_i$ is not $(n_i - n_{i+1})$ but rather the quantity $\int_0^t j_i(t) dt$. To see this we remind ourselves that...
\(
\phi_i \) is the relative phase between the \(i^{th}\) and \((i+1)^{th}\) condensates. However, if we write 
\(n_i = n_{i,i+1} + n_{i,i-1}\), where \(n_{i,i+1}\) is the number of atoms transferred from condensate \(i\) to \(i + 1\), then \(n_{i,i+1}\) and \(\phi_i\) (\(\phi_i\) is the shorthand notation for \(\phi_{i,i+1}\)) are conjugate to each other. We can then write the charging term as \((E_c/2)(n_{i,i+1} + n_{i,i-1})^2\). The equations of motion for \(\phi_i\) and \(n_{i,i+1}\) are given by

\[
\frac{\partial \phi_i}{\partial t} = \frac{\partial H}{\partial n_{i,i+1}} \quad \text{and} \quad \frac{\partial n_{i,i+1}}{\partial t} = -\frac{\partial H}{\partial \phi_i} \quad (3.15)
\]

The first equation gives

\[
\frac{\partial \phi_i}{\partial t} = \frac{\partial H_i}{\partial n_{i,i+1}} + \frac{\partial H_{i,i+1}}{\partial n_{i,i+1}}
\]

\[
= E_c(n_{i,i+1} + n_{i,i-1}) + E_c(n_{i+1,i} + n_{i+1,i+2})(\frac{\partial n_{i+1,i}}{\partial n_{i,i+1}}) \quad (3.16)
\]

However, \(n_{i+1,i} = -n_{i,i+1}\) and hence \(\dot{\phi}_i = E_c(n_{i,i-1} + 2n_{i,i+1} - n_{i+1,i+2})\). Written in terms of currents

\[
\ddot{\phi}_i(t) = E_C [2j_i(t) - j_{i+1}(t) - j_{i-1}(t)] \quad (3.17)
\]

The equation of motion for \(n_{i,i+1}\) reads \(\dot{n}_{i,i+1} = -E_J \sin \phi_i\). Here time and energies are expressed in units of \(E_J^{-1}\) and \(E_J (\hbar = 1)\), respectively. The detailed dynamics of the few site case without dissipation has been studied by Dziarmaga et al. (Dziarmaga et al., 2002). Here we shall add a phenomenological dissipative term of the form \(-\gamma \dot{\phi}_i\) in the equation of motion for \(j_i\) while neglecting finite-temperature noise (Dziarmaga et al., 2002).

\[
j_i(t) = -\sin \phi_i(t) - \gamma \dot{\phi}_i(t) \quad (3.18)
\]

It is important to add the damping term for the system to converge to one of the fixed points. From our knowledge of three or more coupled pendula we know that the system of equations (3.17)-(3.18) is chaotic (Nerenberg et al., 1987) and without any damping would typically explore the whole phase space without converging to
a fixed point. To verify this point, we have investigated the dynamics of Lyapunov exponents for the case of $N = 3$. To ensure that the system is in the Josephson regime we take $E_C/E_J = 0.01$ in all our simulations. We find that three out of six Lyapunov exponents are positive, indicating chaotic behavior. We note that the Ohmic nature of the dissipative term is justified at temperatures higher than the chemical potential between sites (Zapata et al., 1998) or at low temperatures if each condensate lives in a large box (Meier and Zwerger, 2001).

An interesting property of equation (3.17) is that $\sum_i \phi_i$ is a mathematical constant of motion. This can be checked by summing $\dot{\phi}_i$, $\forall i = 1, ..., N$ and noting that the total number of atoms for our closed system is a constant. The outcome that $\sum_i \phi_i$ is a constant of motion is important in maintaining the single-valuedness of the total wavefunction of the system at all times during the process of evolution once it is ensured in the initial conditions. However, physically the system can still change its winding number by going through phase slips at any junction. It will be useful to incorporate the above constant of motion by imposing the restriction $\phi_i \in (-\pi, \pi]$ only at $t = 0$ and removing it for later times. Of course the physical quantity which is observed at the end of the evolution is the Josephson current at each junction, which depends on the relative phase modulo $2\pi$. Thus, for accounting purposes we count states as different if they have had different histories, even if at the time in question they are physically indistinguishable.

Let us next look at the continuum limit of equations (3.17 and 3.18): $\ddot{\phi}_{i,i+1} = E_c (2j_{i,i+1} - j_{i-1,i} - j_{i+1,i+2})$ and $j_{i,i+1} = -E_J \sin \phi_{i,i+1} - \gamma \dot{\phi}_{i,i+1}$ Inserting equation for $j_i$ into the equation for $\phi_i$ we obtain

$$\ddot{\phi}_{i,i+1} = E_c \left[ E_J (\sin \phi_{i-1,i} + \sin \phi_{i+1,i+2} - 2 \sin \phi_{i,i+1}) - \gamma (\dot{\phi}_{i-1,i} + \dot{\phi}_{i+1,i+2} - 2\dot{\phi}_{i,i+1}) \right]$$

(3.19)

Now lets us denote $\phi_{i,i+1} = \phi_i - \phi_{i+1}$ as $\tilde{\phi}(x)$. Note $\tilde{\phi}(x)$ is not the absolute phase.
at position $x$ but is proportional to the gradient of the phase at position $x$ in the
continuum limit. Then $\phi_{i-1,i} = \tilde{\phi}(x-a)$ and $\phi_{i,i+1} = \tilde{\phi}(x+a)$, where $a$ is the lattice
constant. We now have to make some approximations. Suppose we assume that the
relative phase has only slow spatial variations (this would rule out phase slips). Then

$$\tilde{\phi}(x+a) \approx \tilde{\phi}(x) + a\tilde{\phi}'(x) + \frac{a^2}{2}\tilde{\phi}''(x) + ...$$

(3.20)

Then our discrete equation (3.19) has the following continuum form

$$\frac{\partial^2 \tilde{\phi}(x,t)}{\partial t^2} = (E_cE_J)a^2 \left[ \cos \tilde{\phi}(x,t) \left( \frac{\partial^2 \tilde{\phi}(x,t)}{\partial x^2} \right) \right] + \sin \tilde{\phi}(x,t) \left( \frac{\partial \tilde{\phi}(x,t)}{\partial x} \right)^2$$

+ $E_c\gamma a^2 \frac{\partial}{\partial t} \left( \frac{\partial^2 \tilde{\phi}(x,t)}{\partial x^2} \right)$

(3.21)

The constraint of motion for equation (3.21) is

$$\frac{\partial}{\partial t} \int \tilde{\phi}(x,t)dx = 0$$

Note that in the limit of no damping and small $\tilde{\phi}(x,t)$ equation (3.21) reduces to the
familiar wave equation. If we now set the wavelength equal to the cutoff value $a$, then the frequency $\omega$, upto factors of order unity, is equal to the Josephson plasma
frequency $\omega_{JP} = \sqrt{E_cE_J}$.

### 3.4 Numerical procedure

In order to generate statistics, we consider a large number of different initial con­
figurations, with the relative phases and numbers chosen as explained earlier. A
histogram is plotted for the sum total of initial relative phases for every initial con­
figuration. Since the initial phases are chosen randomly, their sum total follows a
normal distribution as discussed earlier. Equations (3.17)-(3.18) are then numerically integrated for each set of initial conditions. After the average current has reached its final equilibrium value, its magnitude equals \( \sin(2\pi m/N) \) and the value of the final winding number \( m < N/4 \) is uniquely extracted. Another histogram is then plotted for all values of \( m \) and its width is recorded. To obtain the scaling law we have calculated the width as a function of \( N \) and fitted it to a function of the form \( \lambda N^\alpha \). The process is repeated for different values of \( \gamma \). The numerical routine to solve large sets of differential equations was implemented in parallel for a large number of initial conditions using MPI. All the computation was done on the UIUC Digital Computer Laboratory's Turing Cluster consisting of Apple Xserves, each with two 2 GHz G5 processors and 4 GB of RAM.

### 3.5 Summary of results

Here time and energies are expressed in units of \( E_j^{-1} \) and \( E_J (\hbar = 1) \), respectively. We obtain a number of interesting results:

(i) The distribution of the final winding number deviates from the initial distribution for all values of \( N \) and \( \gamma \). That final distribution for \( m \) is narrower than the initial distribution for \( n \), indicating an increased probability for low-charge vortex configurations (see Figure 3.1).

(ii) The width of the final distribution scales with the size of the system as \( \lambda N^\alpha \), where \( \alpha = 0.47 \pm 0.01 \), independent of \( \gamma \) and \( \lambda < 0.67 \) (normal distribution value), indicating a shrinking of the basins of attraction for higher winding numbers (see Figures 3.2, 3.3). For \( \gamma \leq 3 \) the width of the final distribution shrinks upon decreasing \( \gamma \) (see inset of Figure 3.3).

(iii) If one focuses on initial configurations with \( n = 0 \), the final distribution of
Figure 3.1: Initial distribution of total phases and final distribution of stable winding numbers for $N = 10^3$ and $\gamma = 5$ for $10^5$ runs.

Figure 3.2: (Color online) Red plot shows how the FWHM of the final distribution of winding numbers scales with $N$ for $\gamma = 6$. The scaling exponent is $\alpha = 0.47 \pm 0.01$ and the prefactor $\lambda = 0.55 \pm 0.05$. Blue plot shows the scaling of FWHM of the initial distribution of total relative phases: $\alpha = 0.50 \pm 0.01$, $\lambda = 0.67 \pm 0.05$. 
winding numbers in the limit of large $N$ is still a Gaussian centered around $m = 0$ with a nonzero spread (see Figure 3.4). This reflects the fact that a finite fraction of the initial configurations with zero total phase have Josephson coupling energies higher than those which correspond to nonzero final winding numbers. The width of the final distribution generated from this initially restricted configuration is clearly smaller than the width of the final distribution for unrestricted initial conditions (see Figures 3.1, 3.4). This suggests that while the reconnection process can result in the generation of a finite winding number with a sum total of zero for the initial phases, there is also significant evidence of memory of the initial conditions.

### 3.6 Stability analysis of superflows

We begin with a summary of notations (Table 3.2) we shall use in this section.

To get a qualitative idea of the dynamics and the role of dissipation, we consider a certain class of initial configurations where $\phi_1 = \Phi_m + \epsilon$ while $\phi_i = \Phi_m - \epsilon/(N - 1)$
Figure 3.4: Restricted to configurations $\sum_i \phi_{i,i+1} = 0$, this histogram for final winding numbers shows that even in the high friction limit one can obtain a non-zero circulation. The above simulation uses $N = 10^3$ and $\gamma = 50$.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Notation for</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi_i$</td>
<td>Relative phase between $i^{th}$ and $(i + 1)^{th}$ sites: $\phi_i - \phi_{i+1}$</td>
</tr>
<tr>
<td>$\Phi_m$</td>
<td>$\Phi_m = 2\pi m/N$</td>
</tr>
</tbody>
</table>

Table 3.2: Summary of notations used in the stability analysis

for $2 \leq i \leq N$. Given $\phi_1$, this configuration has the lowest potential energy. Figure (3.5) shows the potential energy for such a configuration as a function of $\epsilon$ for $N = 10$ and $m = 2$. The first minimum corresponds to the fixed point $K_2$ ($\phi_i = \Phi_2$ for all $i$) followed by the fixed point $K_1$ ($\phi_1 = \Phi_1 + 2\pi; \phi_i = \Phi_1$ for all $i > 1$) and so on so forth. The global minimum of the energy landscape is the configuration $K_0$ with zero winding number. Starting with the initial configuration mentioned above, Figure (3.5) shows the path of steepest descent from $K_2$ to $K_0$. Starting from a local minimum one can characterize the size of the basins of attraction by the value $\epsilon_c$ which $\epsilon$ takes at the next nearest local maximum. However, one should be warned that such an estimate applies only to the specific class of initial configurations described above.
Figure 3.5: Potential Energy landscape for $N = 10$ and a certain class of configurations: $m = 2; \phi_i = 4\pi/10 + \epsilon, \phi_j = 4\pi/10 - \epsilon/9; j \neq i$. Winding number zero is the global minimum of energy landscape and here occurs at $\epsilon = 3.6\pi$.

The role played by dissipation can also be elucidated by studying that class of configurations. Suppose $\epsilon > \epsilon_{c1}$, where $\epsilon_{c1}$ is the first critical value of $\epsilon$. The system starts at an unstable point and as it rolls down to the fixed point with one less winding number, loses kinetic energy due to friction. If it arrives at the next stable point with kinetic energy less than what is needed to overcome the next barrier, then it settles down at the fixed point $K_{m-1}$. However, if it has enough kinetic energy to roll over the next barrier then the final winding number would be less than $(m - 1)$. This is elucidated in Figure (3.6). Starting with 10 condensates and with same set of initial conditions, it is shown that the final circulation can depend on the strength of dissipation. Inspection of Figure (3.5) also suggests a qualitative understanding of the effect of dissipation in the general case: The particle always starts with zero kinetic energy. In the limit of large friction, it lands in a typically close lake (fixed point) to which it is connected through the steepest descent path. For weak friction, and depending on the initial direction of motion, the particle may alternatively escape the initial basin and glide over the multidimensional landscape gradually lowering its
Figure 3.6: The above two plot shows how the average current $\frac{\sum J_i(t)}{10}$ varies with time for $N = 10$ and the same set of initial conditions with $\sum_i \phi_i = 4\pi$ for two different values of $\gamma$. Note that when $\gamma = 5.0$ the final current saturates to a value corresponding to winding number $2\pi$ and for $\gamma = 0.5$ the same set of initial conditions yields no circulation.
energy to eventually land in a lower lake, i.e. in a lower-charge vortex configuration. Thus low friction enhances, by a moderate factor, the probability of ending in a low-charge configuration, as revealed by Figure (3.3). Hence on a multidimensional landscape: For large $\gamma$, the system settles down in the nearest valley; for small $\gamma$, the particle may escape the initial basin and lower its winding number. Thus low friction enhances, by a moderate factor, the probability of ending in a low-charge configuration as suggested by Figure (3.5) and confirmed by Figure (3.3).

### 3.7 Estimation of areas for basins of attraction

For a semi-analytical discussion of the basins of attraction we focus on the case of $N = 5$ (stable $m = 0, \pm 1$) and high friction. Let $P(m)$ be the probability of landing in a final vortex configuration of charge $m$, $Q(n)$ the initial probability for $\sum_i \phi_i = 2\pi n$, and $P(m|n)$ the probability to obtain a final charge $m$ conditioned to $\sum_i \phi_i = 2\pi n$. Below we estimate $P(1)$ and show that $P(1) < Q(1)$. From the theorem of conditional probabilities we note:

$$P(1) = P(1|1)Q(1) + P(1|0)Q(0) + P(1|-1)Q(-1) \quad (3.22)$$

We therefore begin by estimating $P(1|1)$. The limit of high friction ensures that the system follows the path of steepest descent towards the nearest stable fixed point. The system always resides on the hypersurface $S_n$ defined by the constant of motion $\sum_i \phi_i = 2\pi n$. Note that, on the surface $S_1$, most of the $m = 1$ configurations correspond to the fixed point $\phi_i(t) = 2\pi/5 \ (i = 1, \ldots, 5)$, whereas $m = 0$ can emerge from five different fixed points on $S_1$, namely, those of the type $\phi_i(t) = 2\pi$ with $\phi_j(t) = 0$ for all $j \neq i \ (i = 1, \ldots, 5)$. Likewise, $m = -1$ is dominated by two sets of fixed points on $S_1$: five corresponding to one link having undergone a $4\pi$ total slip, and ten corresponding to two different links each having undergone a $2\pi$ slip.
Note that, even for \( m = 1 \) on \( S_1 \), there are many other configurations different from the dominant ones mentioned above e.g. \( \phi_i = 2\pi/5 + 2\pi, \phi_j = 2\pi/5 - 2\pi, \) and \( \phi_k = 2\pi/5 \) for \( k \neq i, j \ (i, j = 1, \ldots, 5) \). However, in the limit of large \( \gamma \), those configurations involving many different, mutually cancelling phase slips should have negligible probability.

To calculate the area of the basin of attraction for \( m = 1 \), we define a set of five orthonormal vectors \( \hat{x}_i \) such that four of them lie on \( S_1 \) and the fifth vector is perpendicular to \( S_1 \). We define our origin on \( S_1 \) by shifting that of \( S_0 \) along \( x_5 \) by an amount \( \Phi_1 = 2\pi/5 \). The five vectors are then given by:

\[
\begin{align*}
\hat{x}_1 &= (1/\sqrt{2})(1, -1, 0, 0, 0), \\
\hat{x}_2 &= (1/\sqrt{2})(0, 0, 1, -1, 0), \\
\hat{x}_3 &= (1/\sqrt{20})(1, 1, 1, 1, -4), \\
\hat{x}_4 &= (1/2)(1, 1, -1, -1, 0), \\
\hat{x}_5 &= (1/\sqrt{5})(1, 1, 1, 1, 1) \end{align*}
\]

To obtain the basin boundaries on the four-dimensional hypersurface we next write the four independent \( \phi_i \)'s in terms of the in-plane basis vectors \( \hat{x}_i \)’s \((i = 1, \ldots, 4)\)

\[
\begin{align*}
\phi_1 &= \frac{1}{\sqrt{2}} x_1 - \frac{\sqrt{5}}{6} x_3 + \frac{1}{2} x_4 \\
\phi_2 &= -\frac{1}{\sqrt{2}} x_1 - \frac{\sqrt{5}}{6} x_3 + \frac{1}{2} x_4 \\
\phi_3 &= \frac{1}{\sqrt{2}} x_2 - \frac{\sqrt{5}}{6} x_3 - \frac{1}{2} x_4 \\
\phi_4 &= -\frac{1}{\sqrt{2}} x_2 - \frac{\sqrt{5}}{6} x_3 - \frac{1}{2} x_4 \end{align*}
\]

and then transform to spherical co-ordinates \((r, \theta_1, \theta_2, \theta_3)\). We then obtain:
\[ \phi_1 = rf_1(\theta_1, \theta_2, \theta_3), \phi_2 = rf_2(\theta_1, \theta_2, \theta_3), \phi_3 = rf_3(\theta_1, \theta_2, \theta_3), \phi_4 = rf_4(\theta_1, \theta_2, \theta_3), \]

where

\[
\begin{align*}
 f_1(\theta_1, \theta_2, \theta_3) &= \frac{\cos \theta_1 \sin \theta_2 \sin \theta_3}{\sqrt{2}} - \frac{\sqrt{5}}{6} \cos \theta_2 \sin \theta_3 + \frac{\cos \theta_3}{2} \\
 f_2(\theta_1, \theta_2, \theta_3) &= -\frac{\cos \theta_1 \sin \theta_2 \sin \theta_3}{\sqrt{2}} - \frac{\sqrt{5}}{6} \cos \theta_2 \sin \theta_3 + \frac{\cos \theta_3}{2} \\
 f_3(\theta_1, \theta_2, \theta_3) &= \frac{\sin \theta_1 \sin \theta_2 \sin \theta_3}{\sqrt{2}} - \frac{\sqrt{5}}{6} \cos \theta_2 \sin \theta_3 - \frac{\cos \theta_3}{2} \\
 f_4(\theta_1, \theta_2, \theta_3) &= -\frac{\sin \theta_1 \sin \theta_2 \sin \theta_3}{\sqrt{2}} - \frac{\sqrt{5}}{6} \cos \theta_2 \sin \theta_3 - \frac{\cos \theta_3}{2}
\end{align*}
\]

Now, the potential energy is given by \( \mathcal{E} = -E_J \sum_i \cos \phi_i \) and the condition \( \partial \mathcal{E}/\partial r = 0 \) defines the boundary of the basin of attraction. Shifting the origin back to \( S_0 \), the basin boundary for \( m = 1 \) on \( S_1 \) is then given by:

\[
f_1 \sin (rf_1 + \Phi_1) + f_2 \sin (rf_2 + \Phi_1) + f_3 \sin (rf_3 + \Phi_1) + f_4 \sin (rf_4 + \Phi_1) = 0, \quad (3.25)
\]

where the various \( f_k = f_k(\theta_1, \theta_2, \theta_3) \) are obtained from a coordinate transformation.

The probability \( P(1|1) \) to end up with \( m = 1 \) having started from any point on \( S_1 \) is given by the ratio \( A_1/B_1 \), where \( A_1 \) is the area enclosed by the curve (3.25) on \( S_1 \) and \( B_1 \) is the total area on \( S_1 \) subject to the initial constraints \( \phi_i(0) \in (-\pi, \pi) \). Using Monte Carlo, we obtain \( P(1|1) = 0.03 \). Similarly we also calculate \( P(0|1) \) and \( P(0|0) \) by Monte Carlo, both yielding 0.94. Using this second result, the symmetry between \( m = 1 \) and \( m = -1 \), and the fact that \( P(1|0) + P(0|0) + P(-1|0) = 1 \), we can also obtain \( P(1|0) = P(-1|0) = 0.03 \). By contrast, the initial distributions are \( Q(0) = 0.6 \) and \( Q(1) = Q(-1) = 0.2 \). Hence in the limit of large \( \gamma \), \( P(1)/Q(1) = 0.15 \), which indicates a shrinking of the initial distribution in favor of final zero winding number. Full scale simulations based on Eqs. (3.17)-(3.18) yields for the same ratio 0.14. An exact agreement would require consideration of infinitely many phase-slip histories.
3.8 A few final comments

Inspired by the Kibble-Zurek scenario and the Scherer et al. (2007) experiments, we have studied the dynamics of independent quasi-condensates. While this situation definitely arises in the Zurek scenario, the ensuing dynamics have qualitative differences with our situation. Our analysis of the dynamics holds true strictly in the Josephson regime; throughout the evolution the BECs are connected through weak Josephson links. Analogously, experiments with fully merging independent BECs (Scherer et al., 2007) or the scenario of quasi-condensates in BEC formation as envisaged by Zurek (1985), always go through an intermediate Josephson regime when adjacent condensates start to overlap. However, a complete study of the dynamics there would require going beyond the two-mode Josephson Hamiltonian (3.14) for each junction, since some of the assumptions (e.g. \( n \ll \mathcal{N} \)) that went in deriving (3.14) would no longer be valid. This could be reflected in the outcome of experiments by Scherer et al. (2007) where three independent BECs have been merged to form stable vortices in the final BEC. A further complication that arises in the (Scherer et al., 2007) experiments is the fact that the Josephson contacts between the BECs are not really point contacts. If one considers the possibility of a non-uniform phase along the wavefront of the merging BECs, then one can not \textit{apriori} rule out the possibility of trapping vortex-anti-vortex pairs at the boundaries between the two BECs. In such a situation one can generate in the bulk BEC vorticities that are not accounted for by counting relative phases around the loop. The phase-counting arguments presented in (Scherer et al., 2007) are therefore somewhat misleading.

To conclude, we have investigated the possibility of vortex trapping in a circular array of Josephson junctions when adjacent BECs, that are initially pair-wise independent, are suddenly connected. We find that the system, right after the sudden connection, finds itself in a highly unstable state with unequal currents in each junction. In presence of Ohmic damping, the system relaxes to a (meta)stable con-
figuration with a stable winding number. The final distribution of stable winding numbers is shown to be significantly narrower than the initial distribution of phase windings. It is even possible to generate a non-zero circulation starting with zero sum total of relative phases. Future work in this direction could study the microscopic mechanism of and the role played by dissipation during the kinematics of overlapping condensates in Zurek's geometry.
Chapter 4

Conclusions

In this dissertation we have addressed two problems in the general field of ultracold atomic gases. In the first problem, we have studied the BCS-BEC crossover in a system of two-component fermions with attractive interactions on a 3-dimensional optical lattice. We first derive a set of particle-hole constraints on the thermodynamics for a bipartite lattice. We then develop a large-$N$ approach to include Gaussian fluctuations around the saddle point. We show that the large-$N$ theory satisfies the particle-hole constraints for the Sp(2N) Hamiltonian, both at the saddle point and $O(1/N)$ level. Using this approach we next calculate various physical quantities e.g. chemical potential, gap parameter, ground state energy, compressibility etc. at $T = 0$. The superfluid density at $T = 0$, is shown to have a non-trivial dependence on $U/t$, due to broken translational invariance. We next calculate the critical temperature and show that while the pair breaking energy scale $T^*$ grows linearly with $U/t$, the critical temperature is actually non-monotonic across the crossover. In the weak coupling regime, $T_c$ scales with the zero temperature gap $\Delta$, and in the strong coupling regime it scales like the zero temperature superfluid density. This is explained by noting that in the BCS regime, coherence is lost due to pair breaking. However, in the BEC regime, the energy scale to break a pair is very high and phase fluctuations destroy superfluidity. Since, the superfluid stiffness becomes increasingly small with coupling in this regime, large phase fluctuations eventually destroy the superfluid order. We next compare our large-$N$ results with a simple Hartree shifted BCS theory that also satisfies the p-h constraints imposed by the attractive Hubbard model, and find that
the large-$N$ theory incorrectly predicts a decreasing compressibility with increasing coupling strength. On the other hand, the simple Hartree shifted BCS theory is shown to correctly recover the atomic limit ($t/U = 0$) and predict the correct trend for compressibility. We ascribe this limitation of the large-$N$ theory to its inability, at the saddle-point level, to treat the particle-hole channel in interactions at the same footing as the particle-particle channel. As a result of that, the large-$N$ theory is unable to recover the Hartree shift, which plays a significant role in lattice problems. This is one of the rare occurrences in quantum many-body problems, where a simple mean field theory gives better results compared to a more sophisticated theory that takes more diagrams into account.

The second problem we address in this dissertation is a study of kinematics of vortex trapping in a circular array of suddenly connected Bose-Josephson junctions. Starting with $N$ independent BECs we couple the condensates through Josephson links and allow the system to reach a stable circulation by adding a dissipative term in our semiclassical equations of motion. The central question we address is what is the probability to trap a vortex with winding number $m$. Our numerical simulations reveal that the final distribution of winding numbers is narrower than the initial distribution of total phases, indicating an increased probability for no-vortex configurations. Specifically, the final width of the distribution of winding numbers for $N$ sites scales as $\lambda N^\alpha$, where $\alpha = 0.47 \pm 0.01$ and $\lambda < 0.67$ (value predicted for the initial distribution). The actual value of $\lambda$ is found to depend on the strength of dissipation. The nonlinearity of the problem also manifests itself in the result that it is possible to obtain a non-zero circulation starting with zero total phase around the loop.
Appendix A

Diagrammatic Approach for the attractive Hubbard model

In this chapter we develop a diagrammatic formulation of the crossover problem in the lattice and discuss the connections of the same with the large $N$ approach and their differences. The starting point of this discussion is the attractive Hubbard Hamiltonian

$$H = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) - U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i, \sigma} n_{i\sigma} \quad (A.1)$$

Under a particle-hole transformation: $d_{i\sigma}^\dagger = (-1)^i c_{i\sigma}$, this Hamiltonian obeys the following particle-hole constraints for the ground state energy ($\mathcal{E}$), the chemical potential ($\mu$) and the thermodynamic potential ($\Omega$) respectively:

$$\mathcal{E}(n) + \frac{Un^2}{4} = \mathcal{E}(2-n) + \frac{U(2-n)^2}{4}$$
$$\mu(n) + \frac{Un}{2} = -\mu(2-n) - \frac{U(2-n)}{2}$$
$$\Omega(\mu) + \mu = \Omega(-\mu - U) - \mu - U \quad (A.2)$$

A.1 Need for a Diagrammatic Approach

It is easy to see that starting with Hamiltonian (A.1) if we use a functional integral formalism as before we would find that the consequent mean field theory where the Hubbard-Stratonovich field $\Delta(x, \tau)$ couples to $\bar{\Psi}_1 \tilde{\Psi}_1$ violates the constraints imposed by particle-hole transformation (A.2). In order to see this, let us write the mean field
theory as a saddle point of the effective action: \( \tilde{S}_0 = \beta \tilde{\Omega}_0 \), where

\[
\tilde{\Omega}_0 = \frac{\Delta_0^2}{U} - \sum_k (\tilde{E}_k - \xi_k)
\]  

(A.3)

with \( \tilde{E}_k = (\tilde{\xi}_k^2 + \Delta^2)^{1/2} \) and \( \xi_k = \epsilon_k - \mu \). However, \( \tilde{\Omega}_0 \) in equation (A.3) and its counterpart, after the particle-hole transformation satisfy

\[
\tilde{\Omega}_0(\mu) + \mu = \tilde{\Omega}_0(-\mu) - \mu
\]  

(A.4)

which is not the same as the constraint in equation (A.2). The reason why a functional integral method fails to satisfy the particle-hole constraints, can be traced back to the type of Hubbard-Stratonovich transformation used to decouple the quartic interaction term in equation (A.1). In our case, the Hubbard-Stratonovich field \( \Delta \) couples only to the particle-particle (p-p) channel and hence the theory fails to satisfy the constraints (A.2). In order to find a fix to this problem let us express how the chemical potential in the above theory on the particle side relates to the one on the hole side

\[
\mu(n) = -\mu(2 - n)
\]  

(A.5)

Comparing with the correct particle-hole constraint in equation (A.2), we see what is missing in the current theory is a Hartree shift \( -nU/2 \) to the mean field chemical potential. At this stage let us anticipate that a Hartree shift to the mean field chemical potential would correct this problem. In the diagrammatic procedure that follows, we use a Luttinger-Ward formalism to write down a Hartree shifted mean field theory and then develop an RPA on top of the mean field analysis.
A.2 Luttinger-Ward formalism

In this section we shall use the Luttinger-Ward formalism (Luttinger and Ward, 1960) to systematically introduce a Hartree shift at the saddle point level to take care of the particle-hole constraints on the thermodynamics. We shall then develop an RPA around the saddle point to account for Gaussian fluctuations. We introduce the Luttinger-Ward functional $\Phi[G]$ and write the thermodynamic potential $\Omega$ as

$$\Omega = \Phi + \text{Tr} \ln G - \text{Tr} \Sigma G$$  \hspace{1cm} (A.6)

where $\text{Tr} \equiv (1/\beta) \sum_{k,i,n} \text{tr}$ and the self-energy $\Sigma$ is obtained by evaluating the functional derivative of $\Phi[G]$ at the exact Green’s function

$$\beta \frac{\delta \Phi[G]}{\delta G} = \Sigma[G] = \Sigma$$  \hspace{1cm} (A.7)

Note that the relation $\Sigma[G] = \Sigma$ is independent from the Dyson equation $G^{-1} = G_0^{-1} - \Sigma$, where $G_0$ is the non-interacting Green’s function. In the Luttinger-Ward formalism $\Phi$ is obtained by summing up an infinite series of closed diagrams without any self-energy insertion (generally called skeleton diagrams) and replacing all free propagators by fully interacting ones. At the mean field level we need to retain only the first diagram in the series and thus

$$\Phi[G] = -U(\text{Tr} G_{12})(\text{Tr} G_{21}) + U(\text{Tr} G_{11})(\text{Tr} G_{22})$$  \hspace{1cm} (A.8)

We define $\frac{\delta \Phi[G]}{\delta G_{11}} = U \text{Tr} G_{22} = \Sigma$ which implies $\frac{\delta \Phi[G]}{\delta G_{22}} = U \text{Tr} G_{11} = -\Sigma$. We can further associate $\text{Tr} G_{21} = \text{Tr} G_{12}$ with the Hubbard-Stratanovich field $\Delta$ and therefore $\frac{\delta \Phi[G]}{\delta G_{12}} = -U \text{Tr} G_{21} = -\Delta$. The Luttinger-Ward functional at the
mean field level is therefore given by

$$\Phi[G] = -\frac{\Delta^2}{U} - \frac{\Sigma^2}{U}$$  \hspace{1cm} (A.9)

and the self-energy matrix is given by

$$\Sigma = \begin{pmatrix} \Sigma & -\Delta \\ -\Delta & -\Sigma \end{pmatrix}$$  \hspace{1cm} (A.10)

We next use the form of the free Green's function given by

$$G_0^{-1} = \begin{pmatrix} ik_n - \epsilon_k + \mu & 0 \\ 0 & ik_n + \epsilon_k - \mu \end{pmatrix}$$  \hspace{1cm} (A.11)

and the Dyson equation to calculate the inverse of the full Green's function

$$G^{-1} = \begin{pmatrix} ik_n - \epsilon_k + \mu - \Sigma & \Delta \\ \Delta & ik_n + \epsilon_k - \mu + \Sigma \end{pmatrix}$$  \hspace{1cm} (A.12)
Note, the Green's function in equation (A.12) has its single particle propagators Hartree shifted.

**A.2.1 Mean field theory at \( T = 0 \)**

Using equation (A.6) and the fact that \( \text{Tr} \, \Sigma = 0 \) we can obtain an expression for the mean field thermodynamic potential

\[
\Omega_0 = \frac{\Delta_0^2}{U} - \sum_k (E_k - \xi_k) + \frac{\Sigma^2}{U} \tag{A.13}
\]

where \( E_k = \sqrt{\xi_k^2 + \Delta_0^2} \) and \( \xi_k = \epsilon_k - \mu + \Sigma \). This form of thermodynamic potential, as anticipated earlier, obeys the correct particle-hole constraints. Then the spatially uniform, static saddle point at \( T = 0 \) is given by the following condition

\[
\frac{\partial \Omega_0}{\partial \Delta_0} = 0 \quad \text{or} \quad \frac{1}{U} = \sum_k \frac{1}{2E_k} \tag{A.14}
\]

The mean field number equation can be obtained from the condition

\[
\frac{\partial \Omega_0}{\partial \mu} = -n \quad \text{or} \quad n = \sum_k \left( 1 - \frac{\xi_k}{E_k} \right) \tag{A.15}
\]

and the Hartree shift \( \Sigma \) is given by

\[
\frac{\partial \Omega_0}{\partial \Sigma} = 0 \quad \text{or} \quad \Sigma = -\frac{U}{2} \sum_k \left( 1 - \frac{\xi_k}{E_k} \right) \tag{A.16}
\]

Equations (A.14, A.16, A.15) are then solved self-consistently and we obtain the mean field values for \( \Delta_0, \mu \) and \( \Sigma \).
A.2.2 Gaussian fluctuations at $T = 0$

In order to go beyond the mean field approximation we next consider fluctuations of the order parameter $\Delta$ around its static saddle point value $\Delta_0$ and expand the action $S_\Delta$ to Gaussian order. The first order term vanishes due to the saddle point condition (A.14) and we obtain

$$ S_\Delta = S_0 + S_g + ... $$

(A.17)

The mean field piece $S_0$ has been defined above and Gaussian piece has the form

$$ S_g = \frac{1}{2} \sum_{i\eta, \eta'} (\eta^*(q)\eta(-q))M(q) \begin{pmatrix} \eta(q) \\ \eta^*(-q) \end{pmatrix} $$

(A.18)

where $i\eta = i2\pi l/\beta$ are the Bose-Matsubara frequencies and the matrix elements of the inverse fluctuation propagator $M$ are given by

$$ M_{11}(q) = M_{22}(-q) = 1 + \sum_{ik, k'} G^0_{22}(k)G^0_{11}(k + q) $$

$$ = \frac{1}{U} + \sum_{k} \left( \frac{u_k^2}{i\eta_l - E_k - E_{k'}} - \frac{v_k^2}{i\eta_l + E_k + E_{k'}} \right) $$

(A.19)

and

$$ M_{12}(q) = M_{21}(q) = \sum_{ik, k'} G^0_{12}(k)G^0_{12}(k + q) $$

$$ = \sum_{k} u_k u_{k'} v_k v_{k'} \left( \frac{1}{i\eta_l + E_k + E_{k'}} - \frac{1}{i\eta_l - E_k - E_{k'}} \right) $$

(A.20)

Here $G^0$ is the same Nambu propagator defined in equation (A.12) with $\Delta = \Delta_0$, $u_k^2 = 1 - v_k^2 = (1/2)(1+\xi_k/E_k)$ are the standard BCS coherence factors and $k' = k + q$.

While calculating the thermodynamic potential including Gaussian fluctuations we need to remember that the first term in the Gaussian part ($\Omega_g$) is indeed the Hartree
Since the Hartree contribution has already been included at the mean field level to preserve particle-hole symmetry, we need to take it out from $\Omega_g$ to avoid double counting. Writing the partition function upto Gaussian order and integrating out the Gaussian fluctuations we obtain the Gaussian contribution to the thermodynamic potential

$$\Omega_g = \frac{1}{2\beta} \sum_{i\mathbf{q},\mathbf{k}} \ln \left( \frac{\mathbf{M}_{11}}{\mathbf{M}_{22}} \text{Det} \mathbf{M}(q) \right) e^{i\mathbf{q}_0 \mathbf{0} +} + \frac{\Sigma^2}{U} \tag{A.21}$$

where the matrix elements $\mathbf{M}_{11}$ etc. have been rescaled as $\mathbf{M}_{11} \to U\mathbf{M}_{11}$. It is easy to see that in the limit of large $i\mathbf{q}$

$$\text{Det} \mathbf{M}(q) \sim 1 - \frac{U^2}{(i\mathbf{q})^2} \left[ \sum_{\mathbf{k}} (u_{\mathbf{k}u_{\mathbf{k}'}}^2 - v_{\mathbf{k}v_{\mathbf{k}'}}^2) \right] \tag{A.22}$$

However

$$\ln \frac{\mathbf{M}_{11}}{\mathbf{M}_{22}} \sim \ln \left[ 1 + \frac{2U}{i\mathbf{q}} \sum_{\mathbf{k}} (u_{\mathbf{k}u_{\mathbf{k}'}}^2 - v_{\mathbf{k}v_{\mathbf{k}'}}^2) \right] \tag{A.23}$$

and hence the Matsubara sum $\sum_{i\mathbf{q}} \ln \mathbf{M}_{11} \text{Det} \mathbf{M}/\mathbf{M}_{22}$ without the convergence factor diverges for large $i\mathbf{q}$. However, the correct $\Omega_g$ also has a correction term given by

$$\frac{\Sigma^2}{U} = -\frac{U}{2} \sum_{i\mathbf{q},\mathbf{k}} \sum_{i\mathbf{q},\mathbf{k}} [G_{11}(\mathbf{k})G_{22}(\mathbf{k}') + G_{11}(\mathbf{k}')G_{22}(\mathbf{k})]
= -\frac{1}{2\beta} \sum_{i\mathbf{q},\mathbf{k}} \left[ (\mathbf{M}_{22} - 1)e^{-i\mathbf{q}_0} + (\mathbf{M}_{11} - 1)e^{+i\mathbf{q}_0} \right] \tag{A.24}$$

Upon changing the sign of $\mathbf{q}$ in the second term of the second line and noting that the sum over $\mathbf{q}$ is over both positive and negative values we have for large $i\mathbf{q}$

$$\frac{\Sigma^2}{U} = -\frac{1}{2\beta} \sum_{i\mathbf{q},\mathbf{k}} \frac{2U}{i\mathbf{q}} \sum_{\mathbf{k}} (u_{\mathbf{k}u_{\mathbf{k}'}}^2 - v_{\mathbf{k}v_{\mathbf{k}'}}^2)e^{+i\mathbf{q}_0} \tag{A.25}$$

which exactly cancels the linear term in the large $(i\mathbf{q})$ expansion in equation (A.23).
Summing up the above results we obtain the Gaussian correction to the thermodynamic potential

\[
\Omega_g = \frac{1}{2\beta} \sum_{i\mathbf{q}, \mathbf{q}} \ln \left[ \frac{\left( \frac{\mathcal{M}_{11}(q)}{\mathcal{M}_{22}(q)} \right) \text{Det} \mathcal{M}(q)}{\exp \left( U \sum_k \left( \frac{\mathcal{M}_{11}(q) \mathcal{M}_{22}(q)}{i\mathbf{q}_k - E_k - \mathcal{E}_k'} - \frac{\mathcal{M}_{11}(q) \mathcal{M}_{22}(q)}{i\mathbf{q}_k + E_k + \mathcal{E}_k'} \right) \right)} \right] \tag{A.26}
\]

where we are justified to drop the convergence factor \( e^{+i\eta^0} \) from the right hand side of equation (A.26) since in the large \((i\eta)\) limit, the leading order term in the sum is now of the order \(1/(i\eta)^2\) and thus the Matsubara sum is convergent. Thus the same scheme that restores the correct particle-hole symmetry in our theory, also makes the Matsubara sum convergent at the Gaussian level. To evaluate the Matsubara sum in equation (A.26) we analytically continue in the complex plane and convert the sum over the bosonic Matsubara frequencies to an integral over a closed contour enclosing the imaginary axis counter clockwise \((1/\beta) \sum_{i\mathbf{q}} \rightarrow \oint \frac{dz}{2\pi i} n_B(z)\) where \(n_B(z)\) is the Bose distribution function. We evaluate the integral over \(z\) along a contour parallel to the Matsubara axis: \(z \rightarrow 0^- + iy\) keeping in mind that the phase of \(\ln \mathcal{M}_{11}(\mathbf{q}, y)/\mathcal{M}_{22}(\mathbf{q}, y)\) and the imaginary part of \((\mathcal{M}_{11}(\mathbf{q}, y) - 1)\) are both odd functions of \(y\) and hence do not contribute when integrated over positive and negative values of \(y\). Therefore, we obtain at \(T = 0\)

\[
\Omega_g = \frac{1}{2\beta} \sum_{i\mathbf{q}, \mathbf{q}} \ln \left( \frac{\mathcal{M}_{11} \text{Det} \mathcal{M}}{\mathcal{M}_{22} \exp(-\Sigma^2/U)} \right) \\
= \int_0^\infty dy/(2\pi) \sum_{\mathbf{q}} \left[ \ln (\text{Det} \mathcal{M}(y)) - 2 \text{Re}(\mathcal{M}_{11} - 1) \right] \tag{A.27}
\]

To obtain \(\Delta_0, \mu\) and \(\Sigma\) including gaussian corrections we start with a grand canonical ensemble and treat both \(\mu\) and \(\Sigma\) as thermodynamic variables. For convinience we switch to \(\bar{\mu} = \mu - \Sigma\) and \(\Sigma\) as our independent variables. Then, the thermodynamic
potential can be written as

\[ \Omega(\tilde{\mu}, \Delta(\tilde{\mu}); \Sigma) = A(\tilde{\mu}, \Delta(\tilde{\mu})) + \Sigma^2 / U, \tag{A.28} \]

where the function \( A(\tilde{\mu}, \Delta(\tilde{\mu})) \) has no explicit dependence on \( \Sigma \). The gap \( \Delta(\tilde{\mu}) \) is obtained from the saddle point equation (A.14). To obtain the number equation and the equation for \( \Sigma \) we construct a function \( F(\tilde{\mu}, \Sigma) = \Omega(\tilde{\mu}, \Sigma) + (\tilde{\mu} + \Sigma) n \). The condition for \( \Sigma \) is then given by

\[ \left( \frac{\partial F}{\partial \Sigma} \right)_{\tilde{\mu}} = 0 \quad \text{or} \quad \Sigma = -\frac{nU}{2} \tag{A.29} \]

The number equation reads

\[ \left( \frac{\partial F}{\partial \tilde{\mu}} \right)_{\Sigma} = 0 \quad \text{or} \quad \left( \frac{\partial A}{\partial \tilde{\mu}} \right)_{\Sigma} + \left( \frac{\partial A}{\partial \Delta} \right)_{\Sigma} \left( \frac{\partial \Delta}{\partial \tilde{\mu}} \right)_{\Sigma} + n = 0 \tag{A.30} \]

We next switch to a canonical ensemble and for a fixed \( n \) numerically calculate \( A[\tilde{\mu}, \Delta(\tilde{\mu})] = A_0[\mu, \Delta(\mu)] + A_g[\mu, \Delta(\mu)] \). Equation (A.30) then gives the value of the renormalized Hartree shifted chemical potential \( \tilde{\mu} \) for the corresponding value of \( n \) which when combined with equation (A.29) gives the renormalized chemical potential \( \mu \) without the Hartree shift.

### A.2.3 Results from Diagrammatic Approach

The problem with this diagrammatic approach is that it predicts an unphysical negative compressibility in the BEC limit. In Figure (A.2) we have plotted \( \mu \) as a function of \( n \) for \( U/t = 20.0 \). Clearly, the slope of \( \mu \) versus \( n \) is negative for a large range of \( n \) indicating negative compressibility. However, we know that in this limit the system is a lattice Bose-gas with a hard-core repulsion coming from Pauli exclusion.
Figure A.2: The chemical potential $\mu$ plotted as a function of the filling $n$ for $U/t = 20.0$. Note that the slope is negative upto $n \approx 0.7$ indicating a negative compressibility. The range of fillings for which $dn/d\mu < 0$ increases with $U/t$, so that eventually for very large couplings the system is unstable for all fillings.

and a nearest neighbor repulsion proportional to $t^2/U$. Hence the system is stable in the BEC limit and the negative compressibility within the diagrammatic approach is therefore an unphysical result.
Appendix B

Sp(2N) symmetry of the large-N model

The 2N-dimensional Hilbert space on each site for the large N Hamiltonian (2.4) can be arranged as a direct product between an N-dimensional and a two-dimensional space. In the 2N-dimensional space the large N Hamiltonian can be rewritten as

\[ H = -t \sum_{\langle i,j \rangle} (c_i^\dagger c_j^\alpha + \text{c.c.}) - \frac{U}{2N} \sum_i (\mathcal{J}^{\alpha\beta} c_i^\dagger c_{i\beta}^\dagger)(\mathcal{J}_{\gamma\delta} c_i^\gamma c_i^\delta) - \mu \sum_i c_i^\dagger c_i^\alpha \]  

(B.1)

where \( \mathcal{J}^{\alpha\beta} \) is the Sp(2N) invariant tensor given by the \( 2N \times 2N \) matrix

\[
\mathcal{J}_{\alpha\beta} = \mathcal{J}^{\alpha\beta} = \begin{pmatrix}
1 & \cdots & -1 \\
-1 & \ddots & \ddots \\
\vdots & \ddots & \ddots
\end{pmatrix}
\]

and repeated spin indices are summed over. The interaction term in (B.1) favors on-site pairing of electrons into Sp(2N) singlets. Since the interaction in the singlet channel is non-zero while all pairings in higher spin channels are forbidden, the Sp(2N) group of Hamiltonian (B.1) is only a sub-group of the more general SU(2N) group. A full SU(2N) symmetry would require that the interaction parameters in all the spin channels be equal. For \( N = 1 \), the Sp(2) group is isomorphic to SU(2) which is the correct symmetry group of the Hubbard model. For more details please refer to Wu.
and Zhang (2005) and the references therein.
Appendix C

Calculation of the Mean Field thermodynamic potential using functional integrals

The mean field thermodynamic potential at $T = 0$ is given by

$$\Omega_0 = \frac{\Delta_0^2}{\beta} - \frac{1}{\beta} \sum_{i k l k} \text{Tr} \ln G_0^{-1}(k)$$  \hspace{1cm} (C.1)

where

$$G_0^{-1} = \begin{pmatrix}
(i k_l - \xi_k) e^{-i q 0^+} & \Delta_0 \\
\Delta_0 & (i k_l + \xi_k) e^{+i q 0^+}
\end{pmatrix}$$  \hspace{1cm} (C.2)

We would like to show how to evaluate the Matsubara sum in $-1/\beta \sum_{k, i k} \text{Tr} \ln G_0^{-1}$.

To proceed, we shall use the identity $\text{Tr} \ln G_0^{-1} = \ln \det G_0^{-1}$. Then,

$$-1/\beta \sum_{k, i k} \text{Tr} \ln G_0^{-1} = -\frac{1}{\beta} \sum_{k, i k} \ln \left[ (i k_l - \xi_k) e^{-i q 0^+} (i k_l + \xi_k) e^{+i q 0^+} - \Delta_0^2 \right]$$ \hspace{1cm} (C.3)

$$= -\frac{1}{2 \pi i} \sum_{k} \int_{c} dz f(z) \left[ \ln (z - \xi) e^{-z 0^+} + \ln (z + \xi) e^{+z 0^+} + \ln (1 - \frac{\Delta_0^2}{(z + \xi)(z - \xi)}) \right]$$

$$= -\frac{1}{2 \pi i} \sum_{k} \int_{c} dz f(z) \left[ \ln (z - \xi) e^{-z 0^+} + \ln (z + \xi) e^{+z 0^+} + \ln \left( \frac{x^2 - \Delta_0^2}{z^2 - \xi^2} \right) \right]$$

$$= I_1 + I_2 + I_3$$

Now at $T = 0$, the Fermi distribution $f(z) = \frac{1}{e^{x^2 + 1}} = 0$ for $z > 0$ and $f(z) = 1$ for $z < 0$. Then,

$$I_3 = -\frac{1}{2 \pi i} \sum_{k} \int_{c} dz \frac{(z + E)(z - E)}{(z + \xi)(z - \xi)}$$  \hspace{1cm} (C.4)
where, the factors $\ln(z-E)$ and $\ln(z-\xi)$ have branch cuts along the positive frequency line and gives zero contribution at $T = 0$. We next evaluate the following integral along the real axis by choosing the branch cut to run from $-E$ to $+\infty$

$$-\frac{1}{2\pi i} \int_c dz \ln(z + E) = -\int_{-E}^0 \frac{d\omega}{2\pi i} \ln(\omega + i\eta + E) - \ln(\omega - i\eta + E)$$ (C.5)

$$= -\int_{-E}^0 \frac{d\omega}{2\pi i} \ln(|\omega + E|e^{i\theta}) - \ln(|\omega + E|e^{i2\pi})$$

$$= -\frac{1}{2\pi i}(-2\pi i)|\omega + E|_{-E}^0$$

$$= -|E| = -E \quad (\because E > 0)$$

Similarly,

$$\frac{1}{2\pi i} \int_c dz \ln(z + \xi)(z - \xi) = |\xi|$$ (C.6)

and hence

$$I_3 = -(E - |\xi|)$$ (C.7)

We next note that since the integrals in $I_1$ and $I_2$ are over both $z > 0$ and $z < 0$ and at $T = 0$ only the left half plane contributes. Following a similar algebra as above, we obtain

$$I_1 + I_2 = \xi - |\xi|$$ (C.8)

Combining equations (L.5 and C.8) we obtain

$$-1/\beta \sum_{k,i\xi} \text{Tr} \ln G_0^{-1} = -\sum_k (E_k - \xi_k)$$ (C.9)

and hence the mean field thermodynamic potential is given by

$$\Omega_0 = \frac{\Delta^2}{U} - \sum_k (E_k - \xi_k)$$ (C.10)
Appendix D

Derivation for $M_{11}$ and $M_{12}$

In this appendix we shall derive the explicit forms of the matrix elements $M_{11}$ and $M_{12}$.

$M_{11}$ calculation: We begin with

$$M_{11}(q) = M_{22}(-q) = \frac{1}{U} + \frac{1}{\beta} \sum_{i k_n, k} G_{22}^0(k) G_{11}^0(k + q)$$

The denominator in the last line can be written as

$$\frac{1}{4 EE'} \left[ \frac{1}{(i k_l - E)(i k_l + i q_l - E')} + \frac{1}{(i k_l + E)(i k_l + i q_l + E')} \right] - \frac{1}{(i k_l + E)(i k_l + i q_l - E')} - \frac{1}{(i k_l - E)(i k_l + i q_l + E')}$$

Each term in (D.1) in general contributes two poles to the Matsubara sum over $i k_l$. However, at $T = 0$ all contributions from the right hand side of the complex lane is zero due to the fermi factors. Hence, at $T = 0$ the first term contributes nothing, second term gives two poles, and third and fourth term contribute a pole each. After doing the Matsubara sum and summing up the contributions from each term, we obtain

$$M_{11}(q) = M_{22}(-q) = \frac{1}{U} \sum_k \left( \frac{u_k^2 u_{k'}^2}{i q_l - E_k - E_{k'}} - \frac{v_k^2 v_{k'}^2}{i q_l + E_k + E_{k'}} \right)$$
\textbf{M}_{12} \text{ calculation:} \quad \text{For } M_{12} \text{ we have}

\begin{align*}
M_{12}(q) &= M_{21}(q) = \frac{1}{\beta} \sum_{ikn,k} G_{22}^0(k) G_{11}^0(k + q) \\
&= \frac{1}{\beta} \sum_{ikn,k} \frac{\Delta_0^2}{\{(ik_l)^2 - E^2\}\{(ik_l + iq_l)^2 - E'^2\}}
\end{align*}

We again split the denominator and perform the Matsubara sums over \(ik_l\). We then obtain

\begin{align*}
M_{12}(q) &= \sum_k \frac{uv\Delta_0}{(iq_l - E - E')(iq_l - E + E')} + \frac{u'v'\Delta_0}{(iq_l + E + E')(iq_l - E + E')}
\end{align*}

After cancellation of terms we obtain

\begin{align*}
M_{12}(q) &= M_{21}(q) = \sum_k u_k u_{k'} u_{k'}' \left( \frac{1}{iq_l + E_k + E_{k'}} - \frac{1}{iq_l - E_k - E_{k'}} \right)
\end{align*}
Appendix E

Proof of equation (2.25) for a non-Hermitian matrix M

Theorem 1 For any non-Hermitian positive definite matrix M, the partition function Z written as a path integral over bosonic fields \( \eta \)

\[
Z = \int D\eta^\dagger D\eta \exp(-\eta^\dagger M\eta) = \frac{1}{\det M}
\]

Proof To begin with, let us write M as a sum of Hermitian and anti-Hermitian matrices: \( M = A + B \), where Hermitian \( A = (M + M^\dagger)/2 \) and anti-Hermitian \( B = (M - M^\dagger)/2 \). Then \( \det M = \det A + \det(1 + A^{-1}B) \). Let us define \( D = A^{-1}B \). Then,

\[
\frac{1}{\det(1 + D)} = \exp[-\text{Tr} \ln(1 + D)] = \exp[-\text{Tr} (D - D^2/2 + D^3/3 + \ldots)] \quad (E.1)
\]

In order to prove the theorem we shall use the expansion (E.1) and show that \( \ln Z = -\ln \det M \). We next note that \( Z \) can be written as

\[
Z = \frac{1}{\det A} \langle \exp[-\eta^\dagger B\eta] \rangle, \quad \text{where } \langle X \rangle = \frac{\int D\eta^\dagger D\eta \exp(-\eta^\dagger A\eta)X}{\int D\eta^\dagger D\eta \exp(-\eta^\dagger A\eta)} \quad (E.2)
\]

We next use the expansion

\[
\ln(e^X) = \langle X \rangle + \frac{1}{2!} \langle X^2 \rangle - \langle X \rangle^2 + \frac{1}{3!} \langle X^3 \rangle - 3\langle X \rangle \langle X^2 \rangle + 2\langle X \rangle^3 \quad (E.3)
\]
For $X = -\eta^\dagger B\eta$, the first term on the R.H.S. of expansion E.3 is given by

$$\langle X \rangle = -\text{Tr} (\langle \eta^\dagger \eta \rangle B) = -\text{Tr} (A^{-1}B) = -\text{Tr} D \quad (E.4)$$

where we have used $\langle \eta^\dagger \eta A \rangle = 1$, which can be shown to be true by expanding $A$ in its eigen basis. We note that the R.H.S. of equation (E.4) is the first term in the exponent of equation (E.1). Next,

$$\frac{1}{2}[(X^2) - \langle X \rangle^2] = \frac{1}{2}[\langle \eta^\dagger \eta \eta^\dagger \eta \rangle BB - (\langle \eta^\dagger \eta \rangle B^2)] \quad (E.5)$$

$$= \frac{1}{2}[(\langle \eta^\dagger \eta \rangle B)^2 - (\langle \eta^\dagger \eta \rangle B)^2 - (\langle \eta^\dagger \eta \rangle B^2)] = \frac{1}{2} \text{Tr} D^2$$

which we recognize as the second term in the exponent of equation (E.1). Similarly, one can show that at the third order $(X^3)/3! = -(1/3) \text{Tr} D^3$. Thus order by order, we obtain

$$\ln Z = - \ln \text{Det} A + \ln(\exp[-\eta^\dagger B\eta]) = - \ln \text{Det} A - \text{Tr} D + \frac{1}{2} \text{Tr} D^2 - \frac{1}{3} \text{Tr} D^3 + ... \quad (E.6)$$

Now using $\text{Tr} \ln A = \ln \text{Det} A$ we obtain

$$\ln Z = - \ln \text{Det} A - \ln(1 + \text{Det} D) = - \ln(\text{Det} A \text{Det}[1 + A^{-1}B]) \quad (E.7)$$

and hence

$$Z = \frac{1}{\text{Det} M}$$
Appendix F

Convergence scheme in the $1/N$ expansion

The Gaussian part of the thermodynamic potential is given by

$$\Omega_g = \frac{1}{2\beta} \sum_{iq} \ln(M_{11}(q)M_{22}(q) - M_{12}^2(q)) \quad (F.1)$$

where

$$M_{11}(q) = \frac{1}{U} + \sum_k \left( \frac{u^2v'^2}{iq_l - E - E'} - \frac{v^2u'^2}{iq_l + E + E'} \right) \quad (F.2)$$

$$M_{12}(q) = \sum_k uuv'u' \left( \frac{1}{iq_l + E + E'} - \frac{1}{iq_l - E - E'} \right)$$

The expression for $\Omega_g$ in equation (F.1) is formally divergent in the limit $U \to \infty$. In order to remove this divergence we first remind ourselves that $M_{11}$ and $M_{22}$ have different convergence factors. We next split $\ln[M_{11}M_{22} - M_{12}^2]$ as

$$\ln(M_{11})e^{+iq0^+} + \ln(M_{22})e^{-iq0^+} + \ln \left( 1 - \frac{M_{12}^2}{M_{11}M_{22}} \right) \quad (F.3)$$

Note, the last term does not need a convergence factor. We next note that $M_{22}(-q) = M_{11}(q)$ and so upon summation over positive and negative values of $q$, $M_{22}$ can be combined with $M_{11}$ to give

$$\Omega_g = \frac{1}{2\beta} \sum_{iq} \ln \left( \frac{M_{11}}{M_{22}} \det M(q) \right) e^{+iq0^+} \quad (F.4)$$

We have now endowed $\Omega_g$ with a single convergence factor and in order to remove the log divergence at large $U$ we now simply add to $\Omega_g$ a term $\sum_{iq} \ln(U^2)e^{+iq0^+},$ which
has no poles or singularities in the left-half plane and therefore contributes nothing to the Matsubara sum except rendering $\Omega_g$ finite in the limit $U \to \infty$.

We redefine $M \to UM$ and split the sum in equation (F.4) into two parts:

$$\Omega_g = \frac{1}{2\beta} \sum_{i\eta_i, q} \left[ \ln \left( \frac{M_{11}}{M_{22}} \right) e^{i\eta q_0^+} + \ln \text{Det} M \right]$$

(F.5)

Again, the last term in equation (F.5) is manifestly convergent and hence does not require a convergence factor. However, the first term is ultra-violet divergent since in the large $iq_1$ limit it goes like

$$\frac{M_{11}}{M_{22}} \sim 1 + \frac{2\alpha(q)}{iq_1},$$

(F.6)

where $\alpha(q) = U \sum_k (u^2 w^2 - v^2 v^2)$. To regulate the offending term, we subtract and add a term $\sum_{i\eta_i, q} \alpha(q)[1/(iq_1 + a) + 1/(iq_1 - a)]e^{i\eta q_0^+}$, where $a$ is any real number to obtain

$$\frac{1}{2\beta} \sum_{i\eta_i, q} \left[ \ln \left( \frac{M_{11}}{M_{22}} \right) - \alpha(q) \left( \frac{1}{i\eta_1 + a} + \frac{1}{i\eta_1 - a} \right) \right] e^{i\eta q_0^+}$$

(F.7)

Now the first term is explicitly convergent and hence the convergence factor can be dropped. However, without the convergence factor, the first term is an odd function of $q_1$ and hence the Matsubara sum gives zero. So, we are left with only the second term, where the Matsubara sum can again be converted into an integral along the imaginary axis. We can further analytically continue on the left half of the complex plane (contribution from right half is zero at $T = 0$ due the Bose distribution function) and close the contour counter-clockwise to enclose the only singularity at $z = -a$. The contour integration gives $(U/2) \sum_k (u^2 - v^2)$ for the second term and thus $\Omega_g$ is
given by

$$\Omega_g = \frac{1}{2\beta} \sum_{i_0,q} \ln \text{Det} \ M(q) + \frac{U}{2} \sum_{k} (u^2 - v^2)$$

(F.8)
Appendix G

Charge Density Wave order at half-filling

In this section we show that at half-filling a short range CDW order appears in addition to the long range superfluid order. The emergence of the CDW order can be shown, within the RPA, as the condition for divergence of the static charge susceptibility

\[ \chi_{CDW}^{RPA} = \chi_{CDW}^0 \frac{1}{1 - U\chi_{CDW}^0}, \]  

where

\[ \chi_{CDW}^0(k, t - t') = i\Theta(t - t')\langle [\hat{\rho}(k, t), \hat{\rho}^\dagger(k, t')] \rangle_0 \]  

and the density operator

\[ \hat{\rho}_i = \sum_\sigma c_{i,\sigma} c_{i,\sigma}^\dagger \]  

The computation of \( \chi_{CDW}^0 \) is analogous to the RPA in section (2.2.3), except now the Hubbard-Stratanovich field couples to the particle-hole channel. After some algebra, one obtains

\[ \chi_{CDW}^0(q) = \sum_k \left[ \frac{(u_{k-q}v_k + v_{k-q}u_k)^2}{iq_n + E_{k-q} + E_{-k+q}} - \frac{(u_kv_k + v_ku_{k+q})^2}{iq_n - E_{k+q} - E_{-k+q}} \right] \]  

where the wavevector \( Q = (\pi, \pi, \pi) \) points to the Brillouin zone corner, where the CDW instability would be shown to occur. The condition for half-filling is given by \( \bar{\mu} = 0 \). In that case, one can easily verify that \( \xi_{k+Q} = -\xi_k \) and \( E_{k+Q} = E_k \). This leads to

\[ u_{k+Q}^2 = \frac{1}{2} \left( 1 + \frac{\xi_{k+Q}}{E_{k+Q}} \right) = \frac{1}{2} \left( 1 - \frac{\xi_k}{E_k} \right) = v_k^2 \]
Similarly, $v_{k+Q}^2 = v_k^2$. Hence, the charge susceptibility evaluated at $q = Q$ is given by

$$
\chi_{CDW}^0(iq_n, q = Q) = \sum_k \left[ \frac{(u_k^2 + v_k^2)}{iq_n + E_k + E_{-k}} - \frac{(u_k^2 + v_k^2)}{iq_n - E_k - E_{-k}} \right]
$$

where the last equality comes from the gap equation (2.19). One can immediately see that the denominator in the R.H.S. of equation (G.1) becomes zero and hence the RPA charge susceptibility at $(q = Q)$ diverges leading to a density order.

Further, when $\mu = 0$, $E_{-k} = E_k$ and after doing the Matsubara sum one obtains

$$
\chi_{CDW}^0(q = Q) = \sum_k \frac{1}{2E_k} = \frac{1}{U}
$$

where the last equality comes from the gap equation (2.19). One can immediately see that the denominator in the R.H.S. of equation (G.1) becomes zero and hence the RPA charge susceptibility at $(q = Q)$ diverges leading to a density order.

A few comments are in order here. First, the CDW order is a staggered order since the instability occurs at $Q = (\pi, \pi, \pi)$. The physical picture for this order is a checkboard - a spin singlet on site $i$, no atom on adjacent sites, a singlet on site $i + 2$ and so on so forth. Clearly, the bipartiteness of the lattice and the condition of half-filling are important for the formation of this order. Secondly, the CDW order at half-filling coexists with the superfluid order. This is highlighted by the fact that the condition for divergence of the charge susceptibility at $q = Q$ turns out to be the same as the one for pairing instability, namely the gap equation. However, the respective symmetries that are spontaneously broken are different in the two cases. While the superfluid order can be thought of as broken $U(1)$ gauge symmetry, the CDW order breaks the underlying $SU(2)$ symmetry of the Hubbard model. In order to see this we perform the Anderson pseudo-spin transformation:

$$
\begin{align*}
S_i^+ &= (-1)^i c_{i,1}^\dagger c_{i,1}^\dagger \\
S_i^- &= (-1)^i c_{i,1} c_{i,1}^\dagger \\
S_i^z &= \frac{1}{2} (c_{i,\sigma}^\dagger c_{i,\sigma} - 1)
\end{align*}
$$
Then in the limit $U/t \gg 1$, one can write the attractive Hubbard Hamiltonian (2.1) as

$$H_{eff} = J \sum_{<i,j>} S_i \cdot S_j - \mu \sum_i S_i^z$$  \hspace{1cm} \text{(G.9)}$$

with $J = t^2/U$. For $\mu = 0$, this Hamiltonian reduces to the pseudo-spin Heisenberg model and is manifestly $SU(2)$ invariant. A charge density wave order, which is essentially an ordering in the $z$ direction in (G.9) spontaneously breaks this $SU(2)$ symmetry. Hence, even though the CDW order appears to break only the discrete translational symmetry of the lattice, the correct broken symmetry is a continuous $SU(2)$ and hence according to Goldstone's theorem gives rise to two massless Goldstone bosons. These appear as "roton dip" in the collective excitation spectrum near half-filling (Burkov and Paramekanti, 2008).
Appendix H

Numerical evaluation of $\Omega_g$

The first step in the calculation of the Gaussian part of the thermodynamic potential is to solve the gap equation for a given chemical potential. Since we do not know the analytical form of the number equation once we include Gaussian fluctuations, we work in the grand canonical ensemble and obtain $\Delta(\mu)$ from equations (2.19). We next numerically compute $\Omega_g[\mu, \Delta(\mu)]$ using the formula in equation (2.27). All the 3 momenta sums are over the entire Brillouin zone for a $20 \times 20 \times 20$ lattice and have an implicit factor of total number of lattice sites in front. The Matsubara sum over the imaginary frequencies $i\omega_n$ is computed along the imaginary axis for each $q$ mode.

The integral in equation (2.27) is split as follows:

$$\int_0^\infty \ln(\text{Det} M)dy = \int_0^{y_c} \ln(\text{Det} M)dy + \int_{y_c}^\infty F(y)dy \quad (H.1)$$

where the first integral on the left hand side is computed numerically and the second integral is evaluated analytically using the large $y$ asymptote of the integrand. The function $F(y)$ is given by

$$F(y) = \frac{4U}{y^2} \sum_{ikn,k} (u^2v'^2 + v^2u'^2)(E + E') \quad (H.2)$$

Here one has to be careful about the integrable log-divergence at $q = (0,0,0)$, $y = 0$ coming from Goldstone’s Theorem. To take this into account we expand the integrand for $q = (0,0,0)$ and small $y$ and obtain $\ln(\text{Det} M(0,y)) \approx \ln(Ky^2)$, where $K$ =
\[ a^2 + b^2 - g^2 \] and

\[
\begin{align*}
a^2 &= 2U \left( 1 - U \sum_k \frac{u^4 + v^4}{2E} \right) \left( \sum_k \frac{u^4 + v^4}{8E^3} \right) \tag{H.3} \\
b^2 &= \left[ U \sum_k \frac{-u^4 + v^4}{4E^2} \right]^2 \\
g^2 &= -2U \sum_k \frac{u^2v^2}{4E^3}
\end{align*}
\]

We note that the terms independent of \( y \) in the expressions for \( a, b \) and \( g \) cancel due to Goldstone’s theorem and the term linear in \( y \) cancel due to symmetry. The integrand \( \ln(\text{Det} M(0, y)) \) for \( q = 0 \) is then integrated between limits 0 and a small value of \( y = y_s \). The rest of the integral for \( q = 0 \) is evaluated numerically between \( y_s \) and \( y_c \), and analytically between limits \( y_c \) and \( \infty \) using the asymptotic form \( F(y) \).
Appendix I

Comparison of our $1/N$ expansion at $T = 0$ with Veillette et al. (2007) (VSR)

In this appendix we show the equivalence of our method for obtaining the $1/N$ correction to the chemical potential at $T = 0$ with the one obtained by Veillette et al. (2007) (VSR). We start with equation (2.35) and write the numerator as

$$\frac{d\Omega_g}{d\mu} = \frac{\partial \Omega_g}{\partial \mu} + \frac{\partial \Omega_g}{\partial \Delta} \frac{d\Delta}{d\mu} \quad (I.1)$$

We next evaluate the denominator of equation (2.35)

$$\frac{d^2\Omega_g}{d\mu^2} = \frac{\partial^2 \Omega_g}{\partial \mu^2} + \left( \frac{\partial^2 \Omega_g}{\partial \Delta \partial \mu} \right) \frac{d\Delta}{d\mu} \quad (I.2)$$

Putting equations (I.1, I.2) in equation (2.35) we obtain

$$\delta \mu = -\frac{\left( \frac{\partial \Omega_g}{\partial \mu} \right) \left( \frac{\partial^2 \Omega_g}{\partial \Delta^2} \right) - \left( \frac{\partial \Omega_g}{\partial \Delta} \right) \left( \frac{\partial^2 \Omega_g}{\partial \Delta \partial \mu} \right)}{\left( \frac{\partial^2 \Omega_g}{\partial \mu^2} \right) \left( \frac{\partial^2 \Omega_g}{\partial \Delta^2} \right) - \left( \frac{\partial^2 \Omega_g}{\partial \Delta \partial \mu} \right)} \quad (I.3)$$

which is the same as equation (3.31) of Veillette et al. (2007). However, it should be emphasized that the respective $1/N$ corrections to the gap parameter within our theory and within VSR are nevertheless different and can be traced back to the question of feedback discussed earlier.
Appendix J

Landau critical velocity

One of the predictions of Landau’s two-fluid model is that if the superfluid component of a liquid flows relative to the walls of the container at a velocity smaller than the Landau critical velocity $v_c$, then it may be able to do so without dissipation. Otherwise, the flow will be unstable against creation of quasiparticles. The quantity we calculate in this appendix is the Landau critical velocity $v_c$ away from half-filling. We use the Landau criterion to calculate an upper bound on $v_c$. In equation form it states: $v_c = \min\{E(k)/k\}$, where $E(k)$ is the energy of an excitation carrying momentum $k$. It has been pointed out in the literature (Burkov and Paramekanti, 2008) that the onset of CDW order close to half-filling triggers dynamical instability in the superflow. Consequently, the estimation of critical velocity using Landau criterion in presence of such dynamical instabilities turns out to be wrong. Here we restrict ourselves to low filling fractions and give a qualitative idea about the different physics that sets the critical velocity in the two different regimes in absence of dynamical instabilities. In the BCS limit, the single particle excitations $E_k = \sqrt{(\epsilon_k - \mu)^2 + \Delta^2}$ sets the energy scale $E(k)$. On the other hand, in the BEC limit, the critical velocity (away from half-filling) is simply given by the slope of the $\omega(k)$ curve at $k = 0$ and is thus equal to the sound velocity. Figure (2.7) shows how the Landau criterion then leads to a non-monotonicity of the critical velocity with a peak near unitarity conforming to the fact that the system is most robust near unitarity.
Appendix K

Calculation of the Mean Field thermodynamic potential in presence of a phase twist

The mean field thermodynamic potential at $T = 0$ is given by

$$\tilde{\Omega}_0 = \frac{\Delta_0^2}{U} - \frac{1}{\beta} \sum_{i\tilde{k}_n, k} \text{Tr} \ln \tilde{G}_0^{-1}(k)$$  \hspace{1cm} (K.1)

where

$$\tilde{G}_0^{-1} = \begin{pmatrix} (i\tilde{k}_n - \tilde{\xi}_k)e^{-ik_0^+} & \Delta_0 \\ \Delta_0 & (i\tilde{k}_n + \tilde{\xi}_k)e^{+ik_0^+} \end{pmatrix}$$  \hspace{1cm} (K.2)

and $i\tilde{k}_n = ik_n - \frac{kQ}{2m}$ and $\tilde{\xi}_k = \xi_k + Q^2/2m$. We would like to show how to evaluate the Matsubara sum in $-1/\beta \sum_{i\tilde{k}_n, k} \text{Tr} \ln \tilde{G}_0^{-1}$. To proceed, we shall use the identity $\text{Tr} \ln \tilde{G}_0^{-1} = \ln \text{Det} \tilde{G}_0^{-1}$. Then,

$$-1/\beta \sum_{i\tilde{k}_n, k} \text{Tr} \ln \tilde{G}_0^{-1}$$

$$= -\frac{1}{2\pi i} \sum_{i\tilde{k}_n, k} \int_c dz f(z) \left[ \ln(z - \tilde{\xi} + \frac{kQ}{2m})e^{-z0^+} + \ln(z + \tilde{\xi} - \frac{kQ}{2m})e^{+z0^+} \\
+ \ln(1 - \frac{\Delta_0^2}{(z+\tilde{\xi} - \frac{kQ}{2m})(z-\tilde{\xi} + \frac{kQ}{2m})}) \right]$$

$$= -(I_1 + I_2 + I_3)$$  \hspace{1cm} (K.3)
Now at $T = 0$, the Fermi distribution $f(z) = \frac{1}{e^{\beta z} + 1} = 0$ for $z > 0$ and $f(z) = 1$ for $z < 0$. We next evaluate,

\begin{equation}
I = \int dz \ln\left(z - \frac{k\cdot Q}{2m} + \bar{E}\right) \quad (\text{here } \bar{E} = (\xi^2 + \Delta_0^2)^{1/2})
\end{equation}

\begin{align*}
&= \int_{-\bar{E} + \frac{k\cdot Q}{2m}}^{0} \frac{d\omega}{2\pi i} \left[ \ln(\omega - \frac{k\cdot Q}{2m} + \bar{E} + i\eta) - \ln(\omega - \frac{k\cdot Q}{2m} + \bar{E} - i\eta) \right] \\
&= \int_{-\bar{E}}^{0} \frac{d\omega}{2\pi i} \left[ \ln(|\omega + \bar{E}|e^{i\delta}) - \ln(|\omega + \bar{E}|e^{i2\pi}) \right] \\
&= \frac{1}{2\pi i} (\Theta(\bar{E})|\omega + \bar{E}|^0_{\bar{E}} - \Theta(-\bar{E})|\omega - \bar{E}|^0_{-\bar{E}})
\end{align*}

To evaluate $I_3$ we use the same procedure as before. For $\xi - \frac{k\cdot Q}{2m} > 0$, the branch cut extending from $-\bar{E}$ to $-\xi$ contributes and gives $I_3 = \bar{E}\Theta(\bar{E} - \frac{k\cdot Q}{2m}) - |\xi|$. For $\xi - \frac{k\cdot Q}{2m} < 0$, the branch cut extending from $-\bar{E}$ to $0$ contributes and gives $I_3 = \bar{E}\Theta(\bar{E} - \frac{k\cdot Q}{2m})$.

Combining, we get $I_3 = \bar{E}\Theta(\bar{E} - \frac{k\cdot Q}{2m}) - |\xi|\Theta(\xi)$.

For $I_1 + I_2$, $\xi - \frac{k\cdot Q}{2m} > 0$ gives zero contribution at $T = 0$. For $\xi - \frac{k\cdot Q}{2m} < 0$, $I_1 + I_2 = \Theta(-\xi + \frac{k\cdot Q}{2m})|\omega - \frac{k\cdot Q}{2m} + \xi|^0_{-\xi + \frac{k\cdot Q}{2m}} = -\xi\Theta(-\xi)$ Combining $I_1 + I_2$ with $I_3$ we obtain:

\begin{equation}
-\frac{1}{\beta} \sum_{\text{Tr ln } \hat{G}_0^{-1}} = - \sum_k \left[ (\bar{E}_k - \frac{k\cdot Q}{2m})\Theta(\bar{E}_k - \frac{k\cdot Q}{2m}) - (\xi_k - \frac{k\cdot Q}{2m}) \right]
\end{equation}

Putting this back in equation (K.1) and taking the limit $Q \to 0$, we obtain the mean field thermodynamic potential in equation (2.64).
Appendix L

Calculation of the Mean Field thermodynamic potential for $T \geq T_c$

The mean field thermodynamic potential at $T = T_c$ is given by

$$\Omega_0 = -\frac{1}{\beta} \sum_{i_k,k} \text{Tr} \ln G_0^{-1}(k)$$  \hspace{1cm} (L.1)

where

$$G_0^{-1} = \begin{pmatrix} (ik_l - \xi_k)e^{-i\phi_0^+} & 0 \\ 0 & (ik_l + \xi_k)e^{+i\phi_0^+} \end{pmatrix}$$  \hspace{1cm} (L.2)

To proceed, we shall use the identity $\text{Tr} \ln G_0^{-1} = \ln \text{Det} G_0^{-1}$. Then,

$$-\sum_{k,i_k} \text{Tr} \ln G_0^{-1} = -\sum_{k,i_k} \ln \left[ (ik_l - \xi_k)e^{-i\phi_0^+}(ik_l + \xi_k)e^{+i\phi_0^+} \right]$$

$$= -\frac{1}{2\pi i} \sum_k \int_c dz f(z) \left[ \ln(z - \xi)e^{-z\phi_0^+} + \ln(z + \xi)e^{+z\phi_0^+} \right] = I_1 + I_2$$  \hspace{1cm} (L.3)

where the Fermi distribution $f(z) = \frac{1}{e^{\alpha z} + 1}$. We evaluate the first integral $I_1$ along the real axis by choosing the branch cut to run from $+\infty$ to $+\xi$ and similarly $I_2$ from $-\infty$ to $-\xi$. The divergence of the log at $\pm\infty$ is taken care of by the convergence factors. Then

$$-\frac{1}{2\pi i} \int_c dz \ln(z - \xi)e^{-z\phi_0^+} = \int_\xi^\infty \frac{d\omega}{2\pi i} \left[ \frac{\ln(\omega + i\eta - \xi)}{1 + \exp(\beta\omega)} - \frac{\ln(\omega - i\eta - \xi)}{1 + \exp(\beta\omega)} \right] e^{-\omega\phi_0^+}$$

$$= \int_\xi^\infty \frac{d\omega}{2\pi i} (-2\pi i) \frac{1}{1 + \exp(\beta\omega)} e^{-\omega\phi_0^+}$$

$$= \ln\left( \frac{1}{1 + \exp(-\beta\xi)} e^{-\xi\phi_0^+} \right) = \ln(f(-\xi))$$  \hspace{1cm} (L.4)
Similarly, $I_2 = \ln(f(-\xi))$ and hence

$$\Omega_0 = \frac{2}{\beta} \sum_k \ln(f(-\xi_k))$$  \hspace{1cm} (L.5)
Bibliography


Author’s Biography

Parag Ghosh was born on December 12th, 1977 in Kharagpur, India. He received his high school and college education in his hometown. He earned a Bachelor of Science degree in Physics and a Master of Science degree in Physics from Indian Institute of Technology, Kharagpur. In August 2001, he joined the graduate studies program in the University of Illinois at Urbana-Champaign.