

Particle-Hole Fluctuations in Superconductors

by

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*A thesis submitted in partial fulfillment of
the requirements for the degree of*

Master of Science

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Abstract

In this thesis we investigate how corrections originating from particle-hole interactions may be introduced into the Bardeen-Cooper-Schrieffer (BCS) theory of superconductivity using functional integral methods. The attractive Fermionic contact interaction is simultaneously decoupled in the Cooper and exchange channels, with the exchange-channel decoupling field treated as a small fluctuation about its zero mean-field value. Upon integrating out the exchange-channel fluctuation field, the system is described by a new effective action for the Cooper-channel decoupling field, which models the superconducting condensate. The saddle-point condition of this effective action generates the standard mean-field BCS equations with correction terms containing particle-hole polarization bubbles. The corrections obtained in this thesis are similar in spirit, albeit different in form, to those originally found in 1961 by Gor'kov and Melik-Barkhudarov (GMB). An advantage of the technique employed here, as opposed to the GMB approach, is the methodical manner in which fluctuations can be incorporated into superconductors.

“Entropy continually increases. We can, by isolating parts of the world and postulating rather idealised conditions in our problems, arrest the increase, but we cannot turn it into a decrease. That would involve something much worse than a violation of an ordinary law of Nature, namely, an improbable coincidence. The law that entropy always increases—the second law of thermodynamics—holds, I think, the supreme position among the laws of Nature. If someone points out to you that your pet theory of the universe is in disagreement with Maxwell’s equations—then so much the worse for Maxwell’s equations. If it is found to be contradicted by observation—well, these experimentalists do bungle things sometimes. But if your theory is found to be against the second law of thermodynamics I can give you no hope; there is nothing for it but to collapse in deepest humiliation.”

Eddington, A.S.

Acknowledgements

I would like to thank Dr. Rufus Boyack, my primary collaborator for the research presented here. My first exposure to the theory of superconducting fluctuations was in Dr. Boyack's lectures on the topic, and his notes were an invaluable reference. Over the course of this project Dr. Boyack gave countless hours of his time in the form of deep discussion, guidance, and checking my calculations for errors. That said, any errors which may remain in this thesis are entirely my own.

I thank Professor Frank Marsiglio, my supervisor, for his mentorship, patience, and insight over the course of my degree. I further thank my thesis committee members: Professors Frank Hegmann, Richard Sydora, Joseph Maciejko and the aforementioned Frank Marsiglio for their difficult questions and valuable perspectives.

Finally, I thank my close friend Russell McLellan and my fiancée Chantal Jonsson for their support and dedicated proofreading assistance.

This work was supported by the Canada Graduate Scholarships-Master's (CGS-M) scholarship from the Natural Sciences and Engineering Research Council of Canada (NSERC).

Contents

Abstract	ii
Acknowledgements	iv
1 Introduction	1
2 The functional integral formalism	3
2.1 Coherent state functional integral	3
2.1.1 The spatial continuum limit	8
2.2 Non-interacting systems: Gaussian integration	8
2.2.1 Real Bosonic fields	8
2.2.2 Complex Bosonic fields	9
2.2.3 Fermionic fields	9
2.3 Matsubara frequency summation	10
2.3.1 Bosonic Matsubara sums	10
2.3.2 Fermionic Matsubara sums	12
3 BCS theory of superconductivity	15
3.1 BCS as a saddle-point of the functional integral	15
3.1.1 BCS gap equation	20
3.1.2 BCS number equation	22
3.2 Superconducting fluctuations away from the BCS saddle-point	23
3.3 GMB correction	27
4 Exchange channel fluctuations about the BCS saddle-point	29
4.1 Decoupling in the Cooper and exchange channels	30
4.2 Gaussian fluctuations in the exchange channel	33
4.3 Modified saddle-point condition	36
4.3.1 Exchange channel fluctuation propagator: small-momentum expansion	39
4.4 Modified number equation	42
5 Conclusion	44
Bibliography	46

A	Grassmann numbers	48
A.1	Gaussian integration of Grassmann variables	51
B	Coherent states	52
B.1	Bosonic coherent states	52
B.2	Fermionic coherent states	56
C	Assorted Matsubara sums	59
C.1	Maki-Thompson style diagram	59
C.2	Density of states style diagram	62
C.3	Number equation correction	63

List of Figures

3.1	Superconducting fluctuation propagator above T_c . The divergence of this propagator signals the superconducting phase transition.	27
3.2	Critical Temperature equation with the GMB correction	28
4.1	Representation of interactions in the Cooper and exchange channels.	29
4.2	Fluctuation correction to the BCS T_c equation	38
4.3	Term appearing in both the GMB correction and exchange-channel fluctuation correction to the critical temperature.	39
C.1	Maki-Thompson style diagram arising in exchange channel fluctuation corrections to the BCS gap equation.	59
C.2	Density of states style diagram arising in exchange channel fluctuation corrections to the BCS gap equation.	62

List of Symbols

T	Temperature.
β	Inverse temperature $1/T$.
μ	Chemical potential.
N	Total number of particles.
\mathbf{v}	Vector with components v_i .
$\epsilon_{\mathbf{k}}$	Dispersion relation in terms of wavevector \mathbf{k} .
G_0	Free Fermionic Green's function
G	Dressed Fermionic Green's function
τ	Imaginary time.
$i\Omega_m$	Bosonic matsubara frequency.
$i\omega_n$	Fermionic matsubara frequency.
k	Composite Fermionic frequency and momentum $(i\omega_n \mathbf{k})$.
q	Composite Bosonic frequency and momentum $(i\Omega_m \mathbf{k})$.
Δ	Superconducting order parameter.
\bar{z}	Complex conjugate of z .
a^\dagger	Hermitian adjoint of a .
$ x\rangle$	Quantum state labelled by x .
$\langle x $	Quantum co-state labelled by x .
$\mathcal{F}[f]$	\mathcal{F} is a <i>functional</i> acting on the function $f(x)$.
$\mathcal{F}[f](x)$	The functional $\mathcal{F}[f]$ evaluated at x .
$\frac{\delta \mathcal{F}[f]}{\delta f(x)}$	Functional derivative of \mathcal{F} with respect to f at x .
$\mathcal{D}[f]$	Measure over a space of functions labelled f .
d	Integration measure with constants absorbed.
$\mathrm{d}^3\mathbf{k}$	Wavevector integration measure $(2\pi)^{-3}\mathrm{d}^3\mathbf{k}$.
d^4k	Fermionic Matsubara sum and wavevector integration measure $T \sum_n \mathrm{d}^3\mathbf{k}$.
d^4q	Bosonic Matsubara sum and wavevector integration measure $T \sum_m \mathrm{d}^3\mathbf{q}$.
tr	Trace over vector or Nambu indices
Tr	Trace over position or momentum indices as well as vector or Nambu indices
\det	Determinant over vector or Nambu indices
Det	Determinant over position or momentum indices as well as vector or Nambu indices

1 Introduction

A large body of work in the condensed matter physics literature is devoted to going beyond the Bardeen-Cooper-Schrieffer (BCS) theory of superconductivity, which is a mean-field description of superconductors from a first-principles microscopic point of view published in 1957 [1]. BCS theory performs admirably in describing a class of superconductors known as *conventional*, but there is a much larger class of *unconventional* superconductors for which the applicability of BCS is suspect. There is a widely held belief that the BCS theory contains certain unrealistic assumptions, ignoring physical effects which may be relevant to the description of unconventional superconductors.

One line of inquiry going beyond the BCS description, which was first explored by Gor'kov and Melik-Barkhudarov (GMB) in 1961 [2], holds that, due to the assumptions implicit in BCS theory, the effects of interactions between *particles* and *holes*, i.e. vacancies in the Fermi sea, are ignored in favour of the more dominant *particle-particle* interactions which drive the superconducting phase transition. GMB used a method to re-introduce the particle-hole interactions into the BCS theory and found that with their modification the critical temperature was reduced by a simple numerical factor of $(4e)^{1/3} \approx 2.22$.

This thesis began as a humble project to understand how the GMB correction was implemented and ended as an odyssey through the bountiful, yet treacherous, sea that is the functional integral formalism of quantum field theory. Dissatisfied with the exposition in the GMB paper, which is characteristically terse and relies heavily on the authors' keen physical insight, we set out to see if we would replicate the correction starting from first principles using functional integral methods. We chose the functional integral approach over the more common canonical approach in terms of operators on a Hilbert space because the functional integral formalism is more rigid than

most canonical methods, giving firm mathematical guidance where physical intuition may fail, and because it is a formalism especially well suited to studying *fluctuation* phenomena [3].

In this document, we chronicle our current understanding of how weak magnetization fluctuations in superconducting systems lead to a modified form of the BCS theory of superconductivity which accounts for particle-hole interaction effects. The modifications we derive differ from those of Gor'kov and Melik-Barkhudarov, and we cannot yet make quantitative comparisons between the predictions of our corrections and theirs. Instead, the central result of this thesis is a robust platform for understanding fluctuation corrections to superconductors which arise from interaction channels other than the dominant particle-particle channel.

2 The functional integral formalism

Any question about a many-body quantum mechanical system described by a Hamiltonian operator H at thermal equilibrium, or in the linear response regime, may be answered through manipulations of the partition function

$$\mathcal{Z} = \text{Tr} e^{-\beta H} . \quad (2.1)$$

By utilizing the coherent-state basis, the traditional approach to calculating the partition function, which is based on operators acting on Hilbert space vectors, may be recast into integrals over a relevant space of functions describing the physical system [3]. This reformulation leads to a different, but equivalent language for studying condensed matter systems that can have advantages over traditional formulations, especially in the context of studying controlled fluctuations about a *classical* configuration. We call this formalism the *coherent state functional integral* and it will play a central role in our work to go beyond the mean-field BCS theory of superconductivity.

2.1 Coherent state functional integral

In many-body physics, one must consider systems with Bosonic or Fermionic degrees of freedom distributed throughout a lattice. Hence, we generalize the standard notion of single-body coherent states introduced in Appendix B to many-body systems. Considering a Fock space spanned by a set of N Bosonic or Fermionic creation and annihilation operators a_i^\dagger and a_i and letting $\zeta = +1$ for Bosons or -1 for Fermions, a

many-body coherent state is the product of N independent single-body coherent states

$$|\varphi\rangle = \exp\left(\zeta \sum_i \varphi_i a_i^\dagger\right) |0\rangle \quad , \quad (2.2)$$

where φ_i is either a complex number for a Bosonic system or an anti-commuting Grassmann number for Fermionic systems in order to respect the commutation or anti-commutation relations of the field operators a_i^\dagger and a_i , as explained in Appendix B. These many-body coherent states have the properties

$$a_i |\varphi\rangle = \varphi_i |\varphi\rangle \quad , \quad (2.3)$$

$$\langle\varphi| a_i^\dagger = \langle\varphi| \bar{\varphi}_i \quad , \quad (2.4)$$

$$\langle\varphi'|\varphi\rangle = \exp\left(\sum_i \bar{\varphi}'_i \varphi_i\right) |\varphi\rangle \quad , \quad (2.5)$$

and

$$\mathbb{1} = \int d^N(\bar{\varphi} \varphi) \exp\left(-\sum_i \bar{\varphi}_i \varphi_i\right) |\varphi\rangle \langle\varphi| \quad , \quad (2.6)$$

where we have defined

$$d^N(\bar{\varphi} \varphi) \equiv \prod_i \frac{d(\bar{\varphi}_i \varphi_i)}{(2\pi i)^{(1+\zeta)/2}} \quad .$$

With these states, we are ready to construct the partition function for a Bosonic or Fermionic field theory in terms of functional integrals. Taking a normal ordered Hamiltonian $H[a^\dagger, a]$,¹ the partition function may be written as

$$\begin{aligned}
\mathcal{Z} &= \text{Tr} e^{-\beta H} \\
&= \sum_n \langle n | \exp\left(-\beta H[a^\dagger, a]\right) | n \rangle \\
&= \int \mathfrak{d}^N(\bar{\varphi}, \varphi) \exp\left(-\sum_i \bar{\varphi}_i \varphi_i\right) \sum_n \langle n | \varphi \rangle \langle \varphi | \exp\left(-\beta H[a^\dagger, a]\right) | n \rangle \\
&= \int \mathfrak{d}^N(\bar{\varphi}, \varphi) \exp\left(-\sum_i \bar{\varphi}_i \varphi_i\right) \zeta \langle \varphi | \exp\left(-\beta H[a^\dagger, a]\right) \sum_n | n \rangle \langle n | \varphi \rangle \\
&= \int \mathfrak{d}^N(\bar{\varphi}, \varphi) \exp\left(-\sum_i \bar{\varphi}_i \varphi_i\right) \zeta \langle \varphi | \exp\left(-\beta H[a^\dagger, a]\right) | \varphi \rangle . \tag{2.7}
\end{aligned}$$

Even though we took H to be normal ordered, $\exp(-\beta H)$ is *not* normal ordered. However, we can write the exponential of the Hamiltonian as an infinite product of normal ordered operators

$$\begin{aligned}
\lim_{M \rightarrow \infty} \exp\left(-\beta H[a^\dagger, a]\right) &= \lim_{M \rightarrow \infty} \exp\left(-\frac{\beta}{M} H[a^\dagger, a]\right)^M \\
&= \lim_{M \rightarrow \infty} \left(1 - \frac{\beta}{M} H[a^\dagger, a]\right)^M . \tag{2.8}
\end{aligned}$$

Defining $\Delta\tau \equiv \beta/M$, breaking apart the exponential of the Hamiltonian as shown, and inserting a coherent-state resolution of unity between each factor, we find

$$\begin{aligned}
\mathcal{Z} &= \lim_{\Delta\tau \rightarrow 0} \int \mathfrak{d}^N(\bar{\varphi}^1, \varphi^1) \exp\left(-\sum_i \bar{\varphi}_i^1 \varphi_i^1\right) \\
&\quad \times \zeta \langle \varphi^1 | \left(1 - \Delta\tau H[a^\dagger, a]\right) \mathbb{1}^N \left(1 - \Delta\tau H[a^\dagger, a]\right) \mathbb{1}^{N-1} \dots \mathbb{1}^2 \left(1 - \Delta\tau H[a^\dagger, a]\right) | \varphi^1 \rangle \\
&= \lim_{\Delta\tau \rightarrow 0} \prod_{n=1}^M \int \mathfrak{d}^N(\bar{\varphi}^n, \varphi^{n-1}) \exp\left(-\sum_i \bar{\varphi}_i^n \varphi_i^{n-1}\right) \langle \varphi^n | \left(1 - \Delta\tau H[a^\dagger, a]\right) | \varphi^{n-1} \rangle , \tag{2.9}
\end{aligned}$$

¹We remind the reader that an operator is *normal-ordered* if all creation operators appear to the left of annihilation operators. For a normal ordered operator $A[a^\dagger, a]$, $\langle \varphi | A[a^\dagger, a] | \varphi \rangle = \exp(\bar{\varphi} \varphi) A[\bar{\varphi}, \varphi]$.

where we have defined $\zeta\varphi^0 \equiv \varphi^N$. We now use

$$\begin{aligned} \lim_{\Delta\tau \rightarrow 0} \langle \varphi^n | (1 - \Delta\tau H[a^\dagger a]) | \varphi^{n-1} \rangle &= \lim_{\Delta\tau \rightarrow 0} \exp\left(\sum_i \bar{\varphi}_i^n \varphi_i^n\right) (1 - \Delta\tau H[\bar{\varphi}^n \varphi^{n-1}]) \\ &= \lim_{\Delta\tau \rightarrow 0} \exp\left(\sum_i \bar{\varphi}_i^n \varphi_i^n - \Delta\tau H[\bar{\varphi}^n \varphi^{n-1}]\right) \end{aligned}$$

to write

$$\mathcal{Z} = \lim_{\Delta\tau \rightarrow 0} \int \left(\prod_{n=1}^M d^N(\bar{\varphi}^n \varphi^n) \right) \exp \left[- \sum_{i,n} \Delta\tau \left(\bar{\varphi}_i^n \frac{\bar{\varphi}_i^n - \bar{\varphi}_i^{n-1}}{\Delta\tau} + H[\bar{\varphi}^n \varphi^{n-1}] \right) \right] . \quad (2.10)$$

With sufficient courage, we are now prepared to take the infinite limit. Just as in the construction of elementary integral calculus where one defines

$$\lim_{\Delta x \rightarrow 0} \sum_{i=1}^N F_i \Delta x \equiv \int F(x) dx , \quad (2.11)$$

we find that our indexed sets of variables $\{\bar{\varphi}\}$ and $\{\varphi\}$ become functions being integrated over in the exponential:²

$$\bar{\varphi}_i(\tau) \equiv \lim_{\Delta\tau \rightarrow 0} \bar{\varphi}_i^n , \quad (2.12)$$

$$\varphi_i(\tau) \equiv \lim_{\Delta\tau \rightarrow 0} \varphi_i^n , \quad (2.13)$$

and

$$\partial_\tau \varphi_i(\tau) \equiv \lim_{\Delta\tau \rightarrow 0} \frac{\varphi_i^n - \varphi_i^{n-1}}{\Delta\tau} . \quad (2.14)$$

With the above limits, we define

$$\begin{aligned} L[\bar{\phi} \phi](\tau) &\equiv \lim_{\Delta\tau \rightarrow 0} \sum_i \bar{\varphi}_i^n \frac{\varphi_i^n - \varphi_i^{n-1}}{\Delta\tau} + H(\bar{\varphi}^n \varphi^{n-1}) \\ &= \sum_i \bar{\varphi}_i(\tau) \partial_\tau \varphi_i(\tau) + H[\bar{\varphi} \phi](\tau) , \end{aligned} \quad (2.15)$$

²Note that the constraint from before that $\varphi^{N+1} = \zeta\varphi^1$ translates to $\varphi(\beta) = \zeta\varphi(0)$, meaning that (Fermionic) Bosonic fields must be (*anti*-)periodic functions in τ with a period β .

such that

$$\begin{aligned} S[\bar{\phi} \phi] &\equiv \lim_{\Delta\tau \rightarrow 0} \sum_{i,n} \Delta\tau \left(\bar{\varphi}_i^n \frac{\varphi_i^n - \varphi_i^{n-1}}{\Delta\tau} + H(\bar{\varphi}^n \varphi^{n-1}) \right) \\ &= \int_0^\beta d\tau L[\bar{\varphi} \varphi](\tau) . \end{aligned} \quad (2.16)$$

We call L and S the imaginary time Lagrangian and action, respectively, because if we were to take the analytic continuation of these quantities as $\tau \rightarrow it$, the above would be the familiar coherent-state Lagrangian and action. Upon performing such an analytic continuation, the partition function would become the generating functional for a real time quantum field theory. The variable τ is often known as *imaginary* time. By performing calculations with imaginary time and then analytically continuing to real time, we encode thermal effects into time dependent quantities.

Finally, we are left with the question of making sense of our infinite product of integrals outside of the exponential of the action. This object is best thought of as a functional integration measure

$$\lim_{M \rightarrow \infty} \left(\prod_{n=1}^M \int d^N(\bar{\varphi}^n \varphi^n) \right) \equiv \int \mathcal{D}[\bar{\varphi} \varphi] . \quad (2.17)$$

Restated, $\mathcal{D}[\bar{\varphi} \varphi]$ is the measure for an integral where each point in the integration domain is not a *number*, but rather a *function*, and this function is passed to the exponential of the action functional $S[\bar{\varphi} \varphi]$ in the evaluation of the partition function.

Putting all these definitions together, we have arrived at the coherent-state functional integral representation of the partition function, given by

$$\mathcal{Z} = \int \mathcal{D}[\bar{\varphi} \varphi] \exp \left(- S[\bar{\varphi} \varphi] \right) . \quad (2.18)$$

We call the transformation which replaced the *Hamiltonian* description with which we started with that of a *Lagrangian* description in terms of functional integrals, a *Legendre*

transformation, after the Legendre transformation familiar in classical mechanics,

$$H[a^\dagger a] \rightarrow L[\bar{\varphi} \varphi](\tau) = \bar{\varphi}(\tau) \partial_\tau \varphi(\tau) + H[\bar{\varphi} \varphi](\tau) . \quad (2.19)$$

2.1.1 The spatial continuum limit

The previously introduced formalism readily generalizes from lattice models with a quantum mechanical degree of freedom at every point in the lattice to field theories with a field at every point in space. One need only to replace the sums over the lattice index i with integrals over position variables x . Such continuum limits are often calculationally convenient but are liable to introduce unphysical effects into the theory which must be carefully excised in order to stay faithful to the underlying lattice model.

2.2 Non-interacting systems: Gaussian integration

Before considering more complicated systems, let us restrict our attention to a special class of condensed matter systems: those for which the action is a quadratic form. It will turn out that all such systems are *exactly solvable* via the laws of Gaussian integration. We will explore three examples of such actions.

2.2.1 Real Bosonic fields

A *real* field is one for which $\bar{\phi}(x) = \phi(x)$ or, equivalently, in momentum space $\bar{\phi}(k) = \phi(-k)$. Therefore, creating a particle travelling with momentum k is equivalent to annihilating a particle with momentum $-k$ ³.

By analogy to the Gaussian integration rule for sets of real numbers,

$$\begin{aligned} \int_{\mathbb{R}^n} \frac{d^n \mathbf{x}}{\sqrt{(2\pi)^n}} \exp\left(-\frac{1}{2} \mathbf{x}^T \cdot \mathbf{A} \cdot \mathbf{x}\right) &= \sqrt{\frac{1}{\det(\mathbf{A})}} \\ &= \exp\left(-\frac{1}{2} \text{tr} \log(\mathbf{A})\right) , \end{aligned} \quad (2.20)$$

³Because electrons in metals typically couple only to the real part of the phonon field $b^\dagger + b$, phonons are often treated as real Bosonic fields when their coupling to electrons is dominant [3].

we may define

$$\int \mathcal{D}[\phi] \exp \left[- \int_0^\beta d\tau \int d^3\mathbf{k} \phi(\tau \mathbf{k}) \hat{A} \phi(\tau - \mathbf{k}) \right] = \exp \left(-\frac{1}{2} \text{TrLog}[\hat{A}] \right) \quad (2.21)$$

for a linear differential operator \hat{A} .

2.2.2 Complex Bosonic fields

The law for *complex* Gaussian integrals holds that

$$\begin{aligned} \int_{\mathbb{C}^n} \frac{d^n(\bar{\mathbf{z}} \mathbf{z})}{(2\pi)^n} \exp \left(-\bar{\mathbf{z}}^\dagger \cdot \mathbf{A} \cdot \mathbf{z} \right) &= \frac{1}{\det(\mathbf{A})} \\ &= \exp \left(-\text{trlog}(\mathbf{A}) \right) \end{aligned} \quad (2.22)$$

and so we analogously define

$$\int \mathcal{D}[\bar{\phi} \phi] \exp \left[- \int_0^\beta d\tau \int d^3\mathbf{k} \bar{\phi}(\tau \mathbf{k}) \hat{A} \phi(\tau \mathbf{k}) \right] = \exp \left(-\text{TrLog}[\hat{A}] \right) . \quad (2.23)$$

2.2.3 Fermionic fields

Referring to the Appendix A.1, we see that for two vectors of n Grassmann variables $\bar{\eta}$ and η ,

$$\begin{aligned} \int d^n(\bar{\eta} \eta) \exp (\bar{\eta}^\text{T} \cdot \mathbf{A} \cdot \eta) &= \det(\mathbf{A}) \\ &= \exp \left(\text{trlog}(\mathbf{A}) \right) , \end{aligned} \quad (2.24)$$

where we note the all important difference of a minus sign from the Bosonic case.

Boldly generalizing to functional integration, we have

$$\int \mathcal{D}[\bar{\psi} \psi] \exp \left[- \int_0^\beta d\tau \int d^3\mathbf{k} \bar{\psi}(\tau \mathbf{k}) \hat{A} \psi(\tau \mathbf{k}) \right] = \exp \left(\text{TrLog}[\hat{A}] \right) . \quad (2.25)$$

2.3 Matsubara frequency summation

One may naively think that finite temperature many-body physics must be more difficult than zero temperature, but in practice, due to the formalism developed by Takeo Matsubara [4], finite temperature field theory calculations actually tend to be easier and more natural than their zero temperature counterparts. After doing calculations at a finite temperature, it is often straightforward to take the zero temperature limit.

2.3.1 Bosonic Matsubara sums

Consider the action for a system of free complex Bosons,

$$S[\bar{\phi} \phi] = \int_0^\beta d\tau \int d^3\mathbf{q} \bar{\phi}(\tau, \mathbf{q}) (\partial_\tau + \xi_{\mathbf{q}}) \phi(\tau, \mathbf{q}) , \quad (2.26)$$

where $\xi_{\mathbf{q}} = \epsilon_{\mathbf{q}} - \mu$, with $\epsilon_{\mathbf{q}}$ as the free particle dispersion relation and μ as the chemical potential. Recalling that the field ϕ must be periodic in β , i.e. $\phi(\tau + \beta) = \phi(\tau)$, we may then write ϕ in a Fourier series as

$$\phi(\tau, \mathbf{q}) = \frac{1}{\sqrt{\beta}} \sum_{m=-\infty}^{\infty} \phi(i\Omega_m, \mathbf{q}) e^{-i\Omega_m \tau} , \quad (2.27)$$

where

$$\phi(i\Omega_m, \mathbf{q}) \equiv \frac{1}{\sqrt{\beta}} \int_0^\beta d\tau \phi(\tau, \mathbf{q}) e^{i\Omega_m \tau} , \quad (2.28)$$

and we defined the Bosonic *Matsubara frequency* $i\Omega_m \equiv i 2m\pi/\beta$. We may now write the action as

$$\begin{aligned} S[\bar{\phi} \phi] &= \int_0^\beta d\tau \int d^3\mathbf{q} \bar{\phi}(\tau, \mathbf{q}) (\partial_\tau + \xi_{\mathbf{q}}) \phi(\tau, \mathbf{q}) \\ &= \frac{1}{\beta} \sum_m \int d^3\mathbf{q} \bar{\phi}(i\Omega_m, \mathbf{q}) (-i\Omega_m + \xi_{\mathbf{q}}) \phi(i\Omega_m, \mathbf{q}) \\ &\equiv - \int d^4q \bar{\phi}(q) D_0^{-1}(q) \phi(q) , \end{aligned} \quad (2.29)$$

where in the final line we defined

$$q \equiv (i\Omega_m \mathbf{q}) \ , \quad (2.30)$$

$$\int \mathrm{d}^4 q \equiv \frac{1}{\beta} \sum_m \int \mathrm{d}^3 \mathbf{q} \ , \quad (2.31)$$

and

$$D_0(q) = \frac{1}{i\Omega_m - \xi_{\mathbf{q}}} \ . \quad (2.32)$$

We call D_0 the *thermal* Green's function for the Bosonic field ϕ since it is the inverse of its differential operator. In moving to the Matsubara representation, we have diagonalized the action, and the fields may be integrated out to find

$$\begin{aligned} \mathcal{Z} &= \int \mathcal{D}[\bar{\phi} \phi] \exp \left[\int \mathrm{d}^4 q \bar{\phi}(q) D_0^{-1}(q) \phi(q) \right] \\ &= \exp \left[- \mathrm{Tr} \mathrm{Log} (- \beta D_0^{-1}) \right] \\ &= \exp \left[- \beta V \int \mathrm{d}^4 q \log (- \beta D_0^{-1}(q)) \right] \ . \end{aligned} \quad (2.33)$$

The particle number density is then

$$\begin{aligned} n &= \frac{1}{\beta V} \left(\frac{\partial \log \mathcal{Z}}{\partial \mu} \right)_{T,V} \\ &= - \int \mathrm{d}^4 q \frac{\partial \log D_0^{-1}(q)}{\partial \mu} \\ &= - \int \mathrm{d}^4 q D_0(q) \frac{\partial D_0^{-1}(q)}{\partial \mu} \\ &= - \frac{1}{\beta} \sum_m \int \mathrm{d}^3 \mathbf{q} \frac{1}{i\Omega_m - \xi_{\mathbf{q}}} \ . \end{aligned} \quad (2.34)$$

We call the m summation a Matsubara sum. The Matsubara frequency sum may be computed analytically by noticing that each point in the Matsubara sum is a point in the complex plane coinciding with the poles of the Bose-Einstein distribution, defined

as

$$b(z) = \frac{1}{e^{\beta z} - 1} , \quad (2.35)$$

such that $b(i\Omega_m)$ is a *simple* pole of weight +1 for all m . Hence,

$$\frac{1}{\beta} \sum_m \frac{1}{i\Omega_m - \xi_q} = \frac{1}{2\pi i} \oint_C dz \frac{b(z)}{i\Omega_m - \xi_q} , \quad (2.36)$$

where the integration contour C encloses all the poles of $b(z)$ *counter-clockwise*. Replacing the integration contour C with C' , where C' wraps *clockwise* around the pole at ξ_q ,⁴ we find

$$\frac{1}{\beta} \sum_m \frac{1}{i\Omega_m - \xi_q} = -b(\xi_q) , \quad (2.37)$$

such that

$$n = \int d^3\mathbf{q} b(\xi_q) . \quad (2.38)$$

2.3.2 Fermionic Matsubara sums

Matsubara frequency summation for Fermions is nearly identical to that for Bosons with the key difference that the fields must be *anti-periodic* in β , i.e. $\psi(\tau + \beta) = -\psi(\tau)$.

For this reason, their Fourier series representation uses the *odd* frequencies

$$\psi(\tau \mathbf{k}) = \frac{1}{\sqrt{\beta}} \sum_n \psi(i\omega_n \mathbf{k}) e^{-i\omega_n \tau} , \quad (2.39)$$

where

$$\psi(i\omega_n \mathbf{k}) \equiv \frac{1}{\sqrt{\beta}} \int_0^\beta d\tau \psi(\tau \mathbf{k}) e^{i\omega_n \tau} , \quad (2.40)$$

⁴There are of course also semicircular contributions to C' at infinity but these will be exponentially small provided the summand is properly regularized [3].

and we call $i\omega_n \equiv i(2n+1)\pi/\beta$ a *Fermionic Matsubara frequency*.

Studying a free action analogous to Eq. 2.26, we observe

$$\begin{aligned}
\mathcal{Z} &= \int \mathcal{D}[\bar{\psi} \psi] \exp \left[- \int_0^\beta d\tau \int d^3\mathbf{k} \bar{\psi}(\tau, \mathbf{k}) (\partial_\tau + \xi_{\mathbf{k}}) \psi(\tau, \mathbf{k}) \right] \\
&= \int \mathcal{D}[\bar{\psi} \psi] \exp \left[- \frac{1}{\beta} \sum_m \int d^3\mathbf{k} \bar{\psi}(i\omega_m, \mathbf{k}) (-i\omega_m + \xi_{\mathbf{k}}) \psi(i\omega_m, \mathbf{k}) \right] \\
&= \int \mathcal{D}[\bar{\psi} \psi] \exp \left[\int d^4k \bar{\psi}(k) G_0^{-1}(k) \psi(k) \right] \\
&= \exp \left[\beta V \int d^4k \log \left(-\beta G_0^{-1}(k) \right) \right] , \tag{2.41}
\end{aligned}$$

so that the particle number is given by

$$\begin{aligned}
n &= \frac{1}{\beta V} \left(\frac{\partial \log \mathcal{Z}}{\partial \mu} \right)_{T,V} \\
&= \int d^4q \frac{\partial \log G_0^{-1}(k)}{\partial \mu} \\
&= \int d^4k G_0(k) \\
&= \frac{1}{\beta} \sum_n \int d^3\mathbf{k} \frac{1}{i\omega_n - \xi_{\mathbf{k}}} . \tag{2.42}
\end{aligned}$$

We now observe that the sum over the Fermionic Matsubara frequencies coincides with the poles of the *Fermi-Dirac* distribution, defined as

$$f(z) = \frac{1}{e^{\beta z} + 1} , \tag{2.43}$$

such that $f(i\omega_n)$ is a simple pole of weight -1 for any n . Thus, we may write

$$\frac{1}{\beta} \sum_n \frac{1}{i\omega_n - \xi_{\mathbf{k}}} = \frac{1}{2\pi i} \oint_C dz \frac{f(z)}{i\omega_n - \xi_{\mathbf{k}}} , \tag{2.44}$$

where C is now a *clockwise* oriented contour enclosing the poles of $f(z)$. The contour C

may then be replaced by a new contour C' , enclosing the simple pole at $z = \xi_{\mathbf{k}}$ *counter-clockwise* so that

$$n = \int d^3\mathbf{k} f(\xi_{\mathbf{k}}) . \quad (2.45)$$

3 BCS theory of superconductivity

John Bardeen, Leon Cooper, and John Robert Schrieffer (BCS) published a paper in 1957 on their Nobel prize winning microscopic theory of superconductivity [1]. In their paper, BCS argue that interactions between electrons and phonons lead to an effective interaction between electrons which is attractive near the Fermi surface. It was shown that even though the effective attraction may be incredibly weak, it can lead to bound-states between two electrons, known as Cooper pairs, and there is a critical temperature T_c below which the Fermi surface develops an instability towards the proliferation and condensation of Cooper pairs. This instability is the hallmark of the superconducting phase transition [3, 5–9].

In this chapter, we introduce the BCS theory of superconductivity using functional integral methods to serve as an introduction to using the coherent state functional integral to study interacting systems. Then, in the next chapter, we will follow this same derivation but include additional effects which we will show result in particle-hole corrections to the BCS theory.

3.1 BCS as a saddle-point of the functional integral

The simplest route to derive the BCS theory of superconductivity in the functional integral formalism comes from considering a neutral gas of Fermions with an attractive contact interaction. Such a system can be described by the continuum Hamiltonian

$$\begin{aligned}
 H[c^\dagger, c] &= \int d^3\mathbf{x} c_\sigma^\dagger(\mathbf{x}) \frac{\hat{\mathbf{p}}^2}{2m} c_\sigma(\mathbf{x}) - g \int d^3\mathbf{x} c_\uparrow^\dagger(\mathbf{x}) c_\downarrow^\dagger(\mathbf{x}) c_\downarrow(\mathbf{x}) c_\uparrow(\mathbf{x}) \\
 &= \int d^3\mathbf{k} c_{\mathbf{k}\sigma}^\dagger \frac{\mathbf{k}^2}{2m} c_{\mathbf{k}\sigma} - g \int d^3(\mathbf{k}_1 \dots \mathbf{k}_4) c_{\mathbf{k}_1\uparrow}^\dagger c_{\mathbf{k}_3\downarrow}^\dagger c_{\mathbf{k}_4\downarrow} c_{\mathbf{k}_2\uparrow} \delta_{\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3 - \mathbf{k}_4} \quad , \quad (3.1)
 \end{aligned}$$

where $g > 0$ is the coupling for an attractive s -wave pairing interaction. The physical justification for studying such an interaction is that in electron-phonon systems, the effective interaction potential between electrons takes the approximate form

$$\frac{g \omega_D^2}{(\xi_{\mathbf{k}} - \xi_{\mathbf{k}'})^2 - \omega_D^2}, \quad (3.2)$$

where ω_D is the *Debye* frequency. Hence, for $|\xi_{\mathbf{k}} - \xi_{\mathbf{k}'}| < \omega_D$, the effective potential between electrons is attractive. This is then *further* approximated as saying that we only consider interactions for which the electrons *separately* satisfy $|\xi_{\mathbf{k}}| < \omega_D$ and $|\xi_{\mathbf{k}'}| < \omega_D$ [5]. We will treat the attractive interaction potential as a simple constant $-g$. When needed, we will impose the constraint that interactions involving g be restricted to a window of width ω_D about the Fermi surface [3, 6].

We can move to a functional integral representation through the Legendre transform

$$\begin{aligned} S[\bar{\psi} \psi] &= \int_0^\beta d\tau \left[\int d^3\mathbf{k} \bar{\psi}_{\mathbf{k}\sigma}(\tau) (\partial_\tau - \mu) \psi_{\mathbf{k}\sigma}(\tau) + H[\bar{\psi} \psi](\tau) \right] \\ &= \int_0^\beta d\tau \left[\int d^3\mathbf{k} \bar{\psi}_\sigma(x) \left(\partial_\tau + \frac{\mathbf{k}^2}{2m} - \mu \right) \psi_\sigma(x) \right. \\ &\quad \left. - g \int d^3(\mathbf{k}_1 \dots \mathbf{k}_4) \bar{\psi}_{\mathbf{k}_1\uparrow}(\tau) \bar{\psi}_{\mathbf{k}_3\downarrow}(\tau) \psi_{\mathbf{k}_4\downarrow}(\tau) \psi_{\mathbf{k}_2\uparrow}(\tau) \delta_{\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3 - \mathbf{k}_4} \right]. \end{aligned} \quad (3.3)$$

Switching the imaginary time dependence to Matsubara frequencies and taking $k = (i\omega_n \mathbf{k})$, the action becomes

$$S[\bar{\psi} \psi] = - \int d^4k \bar{\psi}_{\mathbf{k}\sigma} G_0^{-1}(k) \psi_{\mathbf{k}\sigma} - g \int d^4(k \mathbf{k}' q) (\bar{\psi}_{\mathbf{k}\uparrow} \bar{\psi}_{\mathbf{k}'+q\downarrow}) (\psi_{\mathbf{k}'\downarrow} \psi_{\mathbf{k}+q\uparrow}), \quad (3.4)$$

where $G_0^{-1}(k) \equiv i\omega_n - \xi_{\mathbf{k}}$. In writing the interaction integrand as $(\bar{\psi}_{\mathbf{k}\uparrow} \bar{\psi}_{\mathbf{k}'+q\downarrow}) (\psi_{\mathbf{k}'\downarrow} \psi_{\mathbf{k}+q\uparrow})$ we are expressing the interaction solely in the Cooper channel. That is, we write the interaction in a form suggestive of a coupling between two composite operators $\bar{\psi}_{\mathbf{k}\uparrow} \bar{\psi}_{\mathbf{k}'+q\downarrow}$ and $\psi_{\mathbf{k}'\downarrow} \psi_{\mathbf{k}+q\uparrow}$ instead of Fermion density or spin operators which would correspond to the *direct* and *exchange* channels, respectively. The partition function for this system

as a coherent state path integral takes the form

$$\mathcal{Z} = \int \mathcal{D}[\bar{\psi} \psi] e^{-S[\bar{\psi} \psi]} . \quad (3.5)$$

We introduce a complex scalar auxiliary field through a resolution of unity

$$1 = \int \mathcal{D}[\bar{\Delta} \Delta] \exp \left[- \int \mathrm{d}^4 q \frac{|\Delta(q)|^2}{g} \right] , \quad (3.6)$$

where a factor of $(\text{Det } g)^{-1}$ has been absorbed into the integration measure to make sure the integral is unity. If we now shift the auxiliary fields as

$$\bar{\Delta}(q) \rightarrow \bar{\Delta}(q) - g \int \mathrm{d}^4 k \bar{\psi}_{k\uparrow} \bar{\psi}_{-k+q\downarrow} , \quad (3.7)$$

and

$$\Delta(q) \rightarrow \Delta(q) - g \int \mathrm{d}^4 k \psi_{-k+q\downarrow} \psi_{k\uparrow} , \quad (3.8)$$

then we obtain

$$\begin{aligned} 1 &= \int \mathcal{D}[\bar{\Delta} \Delta] \exp \left[- \int \mathrm{d}^4 q \frac{|\Delta(q)|^2}{g} \right] \\ &= \int \mathcal{D}[\bar{\Delta} \Delta] \exp \left[- \int \mathrm{d}^4 q \frac{|\Delta(q)|^2}{g} + \int \mathrm{d}^4(k \ q) \Delta(q) \bar{\psi}_{k\uparrow} \bar{\psi}_{-k+q\downarrow} + \int \mathrm{d}^4(k \ q) \bar{\Delta}(q) \psi_{-k+q\downarrow} \psi_{k\uparrow} \right. \\ &\quad \left. - g \int \mathrm{d}^4(k \ k' \ q) \bar{\psi}_{k\uparrow} \bar{\psi}_{k'+q\downarrow} \psi_{k'\downarrow} \psi_{k+q\uparrow} \right] . \end{aligned} \quad (3.9)$$

Therefore, the Cooper channel contact interaction may be expressed as

$$\begin{aligned} &\exp \left[g \int \mathrm{d}^4(k \ k' \ q) (\bar{\psi}_{k\uparrow} \bar{\psi}_{k'+q\downarrow}) (\psi_{k'\downarrow} \psi_{k+q\uparrow}) \right] \\ &= \int \mathcal{D}[\bar{\Delta} \Delta] \exp \left[- \int \mathrm{d}^4 q \frac{|\Delta(q)|^2}{g} + \int \mathrm{d}^4(k \ q) \Delta(q) \bar{\psi}_{k\uparrow} \bar{\psi}_{-k+q\downarrow} \right. \\ &\quad \left. + \int \mathrm{d}^4(k \ q) \bar{\Delta}(q) \psi_{-k+q\downarrow} \psi_{k\uparrow} \right] , \end{aligned} \quad (3.10)$$

such that the action may be written as

$$S[\bar{\psi} \psi \bar{\Delta} \Delta] = - \int d^4k \bar{\psi}_{k\sigma} G_0^{-1}(k) \psi_{k\sigma} + \int d^4q \frac{|\Delta(q)|^2}{g} + \int d^4(q, k) \left[\bar{\Delta}(q) \psi_{-k+q\downarrow} \psi_{k\uparrow} + \Delta(q) \bar{\psi}_{k\uparrow} \bar{\psi}_{-k+q\downarrow} \right]. \quad (3.11)$$

Hence, we have managed to remove the four-Fermi interaction at the cost of introducing a Bosonic field Δ coupled to the Fermions. Such a replacement is known as the Hubbard-Stratonovich transformation [10, 11].

Looking closer at the newly generated interactions, we notice that Δ couples to $\bar{\psi}\bar{\psi}$ and $\bar{\Delta}$ couples to $\psi\psi$, meaning that the Boson Δ must carry charge $-2e$ and breaks Fermion number conservation. This object may thus be interpreted as a bound-state of two electrons which we call a Cooper pair [5].

This action is a quadratic form in the fields $\bar{\psi}$ and ψ , but not in a form to which our established rules of Gaussian integration apply. However, with a change of basis we can put the action in a more familiar form. Defining a *Nambu* spinor

$$\Psi^\dagger(k, q) = \begin{pmatrix} \bar{\psi}_{k+q\uparrow} & \psi_{-k+q\downarrow} \end{pmatrix} \quad (3.12)$$

and the inverse of a Nambu Green's function

$$\mathcal{G}^{-1}(k, q) = \begin{pmatrix} G_0^{-1}(k) \delta_q & \Delta(q) \\ \bar{\Delta}(-q) & -G_0^{-1}(-k) \delta_q \end{pmatrix}, \quad (3.13)$$

we find that the action may be succinctly written as

$$S[\bar{\Psi} \Psi \bar{\Delta} \Delta] = \int d^4q \frac{|\Delta(q)|^2}{g} - \int d^4(k, q) \bar{\Psi}^\dagger(k, 0) \mathcal{G}^{-1}(k, q) \Psi(k, q). \quad (3.14)$$

In this form, the Fermionic integral in the partition function may be computed to be

$$\begin{aligned}
\mathcal{Z} &= \int \mathcal{D}[\bar{\Psi} \Psi \bar{\Delta} \Delta] e^{-S[\bar{\Psi} \Psi \bar{\Delta} \Delta]} \\
&= \int \mathcal{D}[\bar{\Delta} \Delta] \exp \left[- \int d^4q \frac{|\Delta(q)|^2}{g} + \text{TrLog} \left(-\beta \mathcal{G}^{-1} \right) \right] \\
&= \int \mathcal{D}[\bar{\Delta} \Delta] \exp \left[-S_{\text{BCS}}[\bar{\Delta} \Delta] \right] , \tag{3.15}
\end{aligned}$$

where

$$S_{\text{BCS}}[\bar{\Delta} \Delta] \equiv \int d^4q \frac{|\Delta(q)|^2}{g} - \text{TrLog} \left(-\beta \mathcal{G}^{-1} \right) . \tag{3.16}$$

Taking a moment to compare the action we started with in Eq. 3.4 to our new effective action Eq. 3.16, little seems to have been gained. We traded a Fermionic action with a quadratic term and a quartic interaction for a Bosonic action with a quadratic term and a logarithmic term whose power series expansion would include interactions of every order involving $|\Delta|^2$ and mediated by electron Green's functions. However, the situation is better than it may seem. While $\bar{\psi}$ and ψ describe the *microscopic* physics of the system, we may think of Δ as a collective mode which we can use to understand the *macroscopic* physics more readily. In particular, if the expectation value of $\Delta(q=0)$ were to take on a large value, that would suggest a homogeneous distribution of Cooper pairs throughout the system and indicate the onset of superconductivity.

Note that while we have reframed the physics of this system in terms of a collective mode Δ , we have not yet made an approximation. One would find that all the physics contained in our original action 3.4 is preserved in 3.16 if only it were possible to compute the functional integral exactly. However, the advantage of this redefinition is that it has brought the physics relevant to superconductivity to the forefront.

The fact that the small q physics of Δ is of primary interest to us indicates that we should be able to study this action at the *mean-field level*.

3.1.1 BCS gap equation

A natural first approximation one can make to study the action in Eq. 3.16 is known as the saddle-point approximation, and it turns out to be the path integral equivalent of mean-field theory. The logic behind the saddle-point approximation is that for some partition function

$$\mathcal{Z} = \int \mathcal{D}[\bar{\Delta} \Delta] \exp \left[- S_{BCS}[\bar{\Delta} \Delta] \right] , \quad (3.17)$$

if there is a region in the integration domain where the action is a saddle-point, i.e.

$$\frac{\delta S_{BCS}[\bar{\Delta} \Delta]}{\delta \bar{\Delta}(q)} = 0 = \frac{\delta S_{BCS}[\bar{\Delta} \Delta]}{\delta \Delta(q)} , \quad (3.18)$$

then there should be *large* contributions to the partition function \mathcal{Z} since in these regions, the contribution to the partition function would amount to (functional) integrals over a constant.¹

At this point we make the customary assumption of BCS theory, that $\Delta(q) = \Delta \delta(q)$. This assumption implies we expect that if there are Cooper pairs, they are homogeneously distributed throughout the system with no spatial or temporal variation. Hence, we find that the saddle-point condition for the BCS action implies

$$\begin{aligned} 0 &= \int \mathrm{d}^4 q' \frac{\delta |\Delta(q')|^2}{\delta \bar{\Delta}(q)} - \frac{\delta}{\delta \bar{\Delta}(q)} \mathrm{Tr} \mathrm{Log}(\mathcal{G}^{-1}) \\ &= \frac{\Delta \delta(0)}{g} - \mathrm{Tr} \left[\mathcal{G} \frac{\delta}{\delta \bar{\Delta}(q)} \mathcal{G}^{-1} \right] \\ &= \frac{\Delta \delta(0)}{g} - \beta V \int \mathrm{d}^4(k q') \mathrm{tr} \left[\mathcal{G}(k q') \frac{\delta}{\delta \bar{\Delta}(q)} \mathcal{G}^{-1}(-k q') \right] \\ &= \frac{\Delta}{g} - \int \mathrm{d}^4 k \mathrm{tr} \left[\mathcal{G}(k 0) \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \right] , \end{aligned} \quad (3.19)$$

¹Note that the condition that the action be stationary is exactly the condition which generates the equations of motion in classical mechanics [12].

and a corresponding conjugate equation. Inverting \mathcal{G}^{-1} , we find

$$\begin{aligned} \mathcal{G}(k) &= \frac{1}{G_0^{-1}(k)G_0^{-1}(-k) + |\Delta|^2} \begin{pmatrix} G_0^{-1}(-k) & \Delta \\ \bar{\Delta} & G_0^{-1}(k) \end{pmatrix} \\ &\equiv \begin{pmatrix} G(k) & F(k) \\ \bar{F}(k) & -G(-k) \end{pmatrix} . \end{aligned} \quad (3.20)$$

Noticing that $F(k) = \Delta G(k)G_0(-k)$, we see that the saddle-point equation Eq. 3.19 reads

$$\frac{\Delta}{g} = \int d^4k \Delta G(k)G_0(-k) . \quad (3.21)$$

Defining $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta|^2}$, we perform the Matsubara summation to find

$$\begin{aligned} \Delta &= g \int d^4k \frac{-\Delta}{(i\omega_n)^2 - E_{\mathbf{k}}^2} \\ &= g \int_{|\xi_{\mathbf{k}}| < \omega_D} d^3\mathbf{k} \frac{1}{\beta} \sum_n \frac{-\Delta}{(i\omega_n)^2 - E_{\mathbf{k}}^2} \\ &= g \int_{|\xi_{\mathbf{k}}| < \omega_D} d^3\mathbf{k} \oint_C \frac{dz}{2\pi i} \frac{-f(z)}{z^2 - E_{\mathbf{k}}^2} \Delta \\ &= g \int_{|\xi_{\mathbf{k}}| < \omega_D} d^3\mathbf{k} \oint_{C'} \frac{dz}{2\pi i} \frac{-f(z)}{(z - E_{\mathbf{k}})(z + E_{\mathbf{k}})} \Delta \\ &= g \int_{|\xi_{\mathbf{k}}| < \omega_D} d^3\mathbf{k} \frac{f(-E_{\mathbf{k}}) - f(E_{\mathbf{k}})}{2E_{\mathbf{k}}} \Delta , \end{aligned} \quad (3.22)$$

where the contour C encloses the poles of the Fermi function $f(z)$ clockwise and C' encloses the poles at $\pm E_{\mathbf{k}}$ counter-clockwise. The presence of g in front of the \mathbf{k} integral should remind us that we only integrate over energies in a window of width $2\omega_D$ of the Fermi surface, otherwise this integral would *diverge* in 3 spatial dimensions due to the continuum approximation. Realizing that $1 - 2f(z) = \tanh(\frac{1}{2}\beta z)$, we find the famous BCS gap equation

$$\Delta = g \int_{|\xi_{\mathbf{k}}| < \omega_D} d^3\mathbf{k} \frac{\tanh(\frac{1}{2}\beta E_{\mathbf{k}})}{2E_{\mathbf{k}}} \Delta . \quad (3.23)$$

Studies of this equation show that at high temperatures, the only solutions are $\Delta = 0$ but then at a critical temperature T_c , the derivative of $\Delta(T)$ discontinuously jumps and Δ

takes on a finite value [6, 7]. Finite Δ will open a gap in the excitation spectrum $\pm E_{\mathbf{k}}$, leading us to call Δ the gap or order-parameter because its presence indicates a phase transition.

We can look for the temperature at which the phase transition occurs by discarding the trivial solution $\Delta = 0$ and ignoring terms of order $|\Delta|^2$ or greater:

$$\begin{aligned} 1 &= g \int d^4k G_0(k)G_0(-k) \\ &= g \int_{|\xi_{\mathbf{k}}| < \omega_D} d^3\mathbf{k} \frac{\tanh\left(\frac{1}{2}\beta\xi_{\mathbf{k}}\right)}{2\xi_{\mathbf{k}}} . \end{aligned} \quad (3.24)$$

Finding a β for which the above relation holds will yield the critical temperature. We call Eq. 3.24 the T_c equation.

3.1.2 BCS number equation

The gap and T_c equations derived above take the chemical potential μ as a parameter, but often we are not interested in systems with a given chemical potential and instead a given particle number density. In such a case, we must use our knowledge of the grand canonical ensemble to generate an equation which determines the chemical potential given a number density. Taking the mean-field approximation, whereby we may take $\mathcal{Z} \approx \exp(-S_{\text{BCS}})$, we see

$$\begin{aligned} n_{mf} &= \frac{1}{\beta V} \left(\frac{\partial \log \mathcal{Z}}{\partial \mu} \right)_{T,V} \\ &= -\frac{1}{\beta V} \left(\left(\frac{\partial S_{\text{BCS}}}{\partial \mu} \right)_{\Delta=\Delta_{mf}} + \frac{\delta S_{\text{BCS}}}{\delta \Delta} \left(\frac{\partial \Delta}{\partial \mu} \right)_{\Delta=\Delta_{mf}} \right)_{T,V} . \end{aligned} \quad (3.25)$$

Using the fact that the second term must vanish by definition at the saddle-point, we have²

$$\begin{aligned}
n_{mf} &= \frac{1}{\beta V} \frac{\partial}{\partial \mu} \text{TrLog}(-\beta \mathcal{G}^{-1}) \\
&= \int d^4 k \text{tr} \left(\mathcal{G} \frac{\partial \mathcal{G}^{-1}}{\partial \mu} \right) \\
&= \int d^4 k \text{tr} \left[\mathcal{G} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right] \\
&= 2 \int d^4 k G(k) .
\end{aligned} \tag{3.26}$$

The above Matsubara sum may be computed such that

$$n_{mf} = \int d^3 \mathbf{k} \left[1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} (1 - 2f(E_{\mathbf{k}})) \right] . \tag{3.27}$$

Eq. 3.27 is often known as the BCS number equation.

3.2 Superconducting fluctuations away from the BCS saddle-point

So far we have explored a mean-field description of superconducting systems, but one advantage of the path integral formalism is that it is a very natural setting for the study of fluctuations about a given mean-field configuration. To do this study, we write our Cooper channel decoupling field as

$$\Delta(q) = \Delta_{sp} \delta(q) + \eta(q) , \tag{3.28}$$

where Δ_{sp} is the saddle-point configuration and η is to be thought of as a perturbation away from the mean-field. If we assume that the mean-field theory is a fairly good description of the macroscopic physics, then we should expect that η is small and so we will only keep terms in the action up to order $|\eta|^2$. Keeping only these terms will

²From now on, we implicitly take Δ, T and V to be constant.

allow us to perform the functional integral exactly, which will produce a new term in the action modifying the mean-field BCS gap equation.

The Nambu-Gorkov Green's function is written in terms of η as

$$\begin{aligned}\mathcal{G}^{-1} &= \mathcal{G}_{sp}^{-1} - \Sigma_\eta \\ &= \mathcal{G}_{sp}^{-1} \left(1 - \mathcal{G}_{sp} \Sigma_\eta \right) ,\end{aligned}\tag{3.29}$$

where

$$\Sigma_\eta(q) = \begin{pmatrix} 0 & -\eta(q) \\ -\bar{\eta}(-q) & 0 \end{pmatrix} ,\tag{3.30}$$

so the action becomes

$$\begin{aligned}S[\bar{\eta} \eta] &= \int d^4q \frac{|\Delta_{sp} \delta_q + \eta(q)|^2}{g} - \text{TrLog} \left[\mathcal{G}_{sp}^{-1} \left(1 - \mathcal{G}_{sp} \Sigma_\eta \right) \right] \\ &\approx \beta V \frac{|\Delta_{sp}|^2}{g} - \text{TrLog} \left[\mathcal{G}_{sp}^{-1} \right] + \frac{\Delta_{sp} \bar{\eta}(0) + \eta(0) \bar{\Delta}_{sp}}{g} + \text{Tr} \left[\mathcal{G}_{sp} \Sigma_\eta \right] \\ &\quad + \int d^4q \frac{|\eta(q)|^2}{g} + \frac{1}{2} \text{Tr} \left[\mathcal{G}_{sp} \Sigma_\eta \mathcal{G}_{mf} \Sigma_\eta \right] \\ &= \beta V \frac{|\Delta_{sp}|^2}{g} - \text{TrLog} \left[\mathcal{G}_{sp}^{-1} \right] + \int d^4q \frac{|\eta(q)|^2}{g} + \frac{1}{2} \text{Tr} \left[\mathcal{G}_{sp} \Sigma_\eta \mathcal{G}_{mf} \Sigma_\eta \right] \\ &\equiv S_{\text{BCS}} + S_{\text{Fluc}}[\bar{\eta} \eta] .\end{aligned}\tag{3.31}$$

In the final line we used the fact that the saddle-point condition Eq. 3.18 implies that the terms linear in η and $\bar{\eta}$ vanish. Resolving the quartic trace in position space and

then taking the Fourier transform, we find

$$\begin{aligned}
\text{Tr} \left[\mathcal{G}_{sp} \Sigma_\eta \mathcal{G}_{sp} \Sigma_\eta \right] &= \text{tr} \int \mathbb{d}^4(x, y) \mathcal{G}_{sp}(x, y) \Sigma_\eta(y) \mathcal{G}_{sp}(y, x) \Sigma_\eta(x) \\
&= \text{tr} \int \mathbb{d}^4(k, q) \mathcal{G}_{sp}(k) \Sigma_\eta(q) \mathcal{G}_{sp}(k - q) \Sigma_\eta(-q) \\
&= \text{tr} \int \mathbb{d}^4(k, q) \begin{pmatrix} G(k) & F(k) \\ \bar{F}(k) & -G(-k) \end{pmatrix} \begin{pmatrix} 0 & \eta(q) \\ \bar{\eta}(-q) & 0 \end{pmatrix} \\
&\quad \times \begin{pmatrix} G(k - q) & F(k - q) \\ \bar{F}(k - q) & -G(-k + q) \end{pmatrix} \begin{pmatrix} 0 & \eta(-q) \\ \bar{\eta}(q) & 0 \end{pmatrix} \\
&= - \int \mathbb{d}^4(k, q) \left[G(k) \eta(q) G(q - k) \bar{\eta}(q) + G(-k) \bar{\eta}(-q) G(k - q) \eta(-q) \right. \\
&\quad \left. - F(k) \bar{\eta}(q) F(k - q) \bar{\eta}(-q) - \bar{F}(k) \eta(q) \bar{F}(k - q) \eta(-q) \right] , \tag{3.32}
\end{aligned}$$

such that

$$\begin{aligned}
S_{\text{Fluc}}[\bar{\eta}, \eta] &= \int \mathbb{d}^4 q \bar{\eta}(q) \left[\frac{1}{g} - \int \mathbb{d}^4 k G(k) G(q - k) \right] \eta(q) \\
&\quad + \frac{1}{2} \int \mathbb{d}^4(k, q) \left[\bar{\eta}(q) F(k) F(k - q) \bar{\eta}(-q) + \eta(q) \bar{F}(k) \bar{F}(k - q) \eta(-q) \right] \\
&= - \int \mathbb{d}^4 q \left[\Phi(q) |\eta(q)|^2 - \frac{1}{2} \left(\Xi(q) \bar{\eta}(q) \bar{\eta}(-q) + \bar{\Xi}(q) \eta(q) \eta(-q) \right) \right] , \tag{3.33}
\end{aligned}$$

where we have defined

$$\Phi(q) \equiv \int \mathbb{d}^4 k G(k) G(q - k) - \frac{1}{g} , \tag{3.34}$$

and

$$\Xi(q) \equiv \int \mathbb{d}^4 k F(k) F(k - q) . \tag{3.35}$$

To perform the η and $\bar{\eta}$ integrals we can perform a trick analogous to the one we used to integrate out the Fermion fields coupled to Δ . Defining

$$\Lambda(q) = \begin{pmatrix} \eta(q) \\ \bar{\eta}(-q) \end{pmatrix}, \quad (3.36)$$

and

$$\mathcal{L}^{-1}(q) = \begin{pmatrix} \Phi(q) & -\bar{\Xi}(q) \\ -\Xi(q) & \Phi(-q) \end{pmatrix}, \quad (3.37)$$

the fluctuation action becomes

$$S_{\text{Fluc}}[H] = - \int d^4q \frac{1}{2} \Lambda^\dagger(q) \mathcal{L}^{-1}(q) \Lambda(q).$$

We note that $\Lambda^\dagger(q) = (\tau_x \Lambda(-q))^T$, so the two fields are not independent degrees of freedom. Hence, we must treat Λ as a *real* Bosonic field so that we do not over-count degrees of freedom. Performing the functional integral over the fluctuation field, we find that

$$\begin{aligned} \mathcal{Z} &\approx \int \mathcal{D}[\Lambda] \exp \left[-S_{\text{BCS}}[\bar{\Delta}, \Delta] + \int d^4q \frac{1}{2} \Lambda^T(-q) (\tau_x \mathcal{L}^{-1}(q)) \Lambda(q) \right] \\ &= \text{Det} \left(-g \tau_x \mathcal{L}^{-1} \right)^{-1/2} \exp \left[-S_{\text{BCS}}[\bar{\Delta}, \Delta] \right] \\ &= \text{Det} \left(g^2 (|\Phi|^2 - |\Xi|^2) \right)^{-1/2} \exp \left[-S_{\text{BCS}}[\bar{\Delta}, \Delta] \right] \\ &= \exp \left[-S_{\text{BCS}}[\bar{\Delta}, \Delta] - \frac{1}{2} \text{TrLog} \left(g^2 (|\Phi|^2 - |\Xi|^2) \right) \right], \end{aligned} \quad (3.38)$$

where we have used that the $-G(-k) = \bar{G}(k)$, i.e. the complex conjugate of G , the to write $\Phi(q)\Phi(-q) = |\Phi(q)|^2$. In the limit where $\Delta \rightarrow 0$, we have that

$$\frac{1}{2} \text{TrLog} (-g \mathcal{L}^{-1}) \rightarrow \text{TrLog} \left(1 - g \int d^4k G_0(k) G_0(q-k) \right) \equiv \text{TrLog}(-gL^{-1}) \quad (3.39)$$

and we notice that the condition $L^{-1}(q=0) = 0$ is the BCS T_c equation, Eq. 3.24. This equality makes sense if we think of $L(q)$ as the propagator for superconducting pair fluctuations above T_c . At the critical temperature, the propagator $L(q)$ diverges for

$q = 0$ causing a proliferation of Cooper pairs, signalling a phase transition.

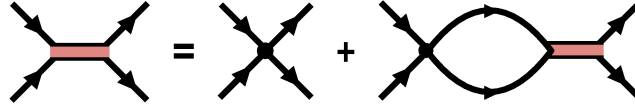


FIGURE 3.1: Superconducting fluctuation propagator above T_c . The divergence of this propagator signals the superconducting phase transition.

3.3 GMB correction

In 1961, Gor'kov and Melik-Barkhudarov published a paper detailing a modification to the BCS theory of superconductivity [2]. GMB recognized that in probing only the mean-field physics of *particle-particle* pairing in the Cooper channel, the BCS theory is made insensitive to contributions which may arise from *particle-hole* interactions. One may envisage that if particle-hole pairs are fluctuating near the Fermi surface, then the density of states available for *particle-particle* pairing will be reduced, resulting in a weaker superconducting condensate than would have been predicted by the BCS theory.

In aiming to account for the neglected particle-hole effects, GMB inserted a particle-hole polarization bubble into a vertex in the standard Cooper fluctuation propagator, so that the $q = 0$ critical temperature equation becomes

$$1 = g \int d^4k G_0(k)G_0(-k) + \Sigma_{\text{GMB}}(0) \quad (3.40)$$

where

$$\Sigma_{\text{GMB}}(Q) = \int d^4(k p q) \left(G_0(p - q + Q)G_0(k - p)G_0(p_q - k + Q)G_0(k) \right. \\ \left. \times G_0(q - k + Q)G_0(k - q)L(p + Q)L(q + Q) \right) , \quad (3.41)$$

as visualized in Fig. 3.2 [13, 14].

$$1 = \text{Diagram 1} + \text{Diagram 2}$$

FIGURE 3.2: Critical Temperature equation with the GMB correction

GMB found that their particle-hole correction term resulted in a dramatic reduction of T_c in the weak-coupling BCS regime by a factor of $(4e)^{1/3}$. This reduction in T_c is indistinguishable from rescaling the interaction strength g . Further study has been conducted by various authors [13–16] who have shown that the GMB correction has much more pronounced effects on the predictions of T_c when considering the strongly interacting Bose-Einstein condensate (BEC) regime. In the BEC regime, effects due to the GMB correction cannot be accounted for by rescaling BCS parameters.

4 Exchange channel fluctuations about the BCS saddle-point

We now come to the purpose of this thesis: using functional integral methods to implement a GMB-like correction to the BCS theory in a systematic and well-defined fashion. Instead of pulling a particle-hole susceptibility out of a sea of ignored diagrams and inserting it into the Cooper pair fluctuation propagator, our tactic will instead be to start with the four-Fermi interaction as with BCS, but this time focus our attention simultaneously on *both* particle-particle and particle-hole interactions. In this approach, the particle-hole interactions are never ignored and do not need to be reintroduced. We accomplish this analysis through simultaneously decoupling the interaction in the Cooper and exchange channels, though such an analysis could also include the density channel for an action where it plays a larger role.

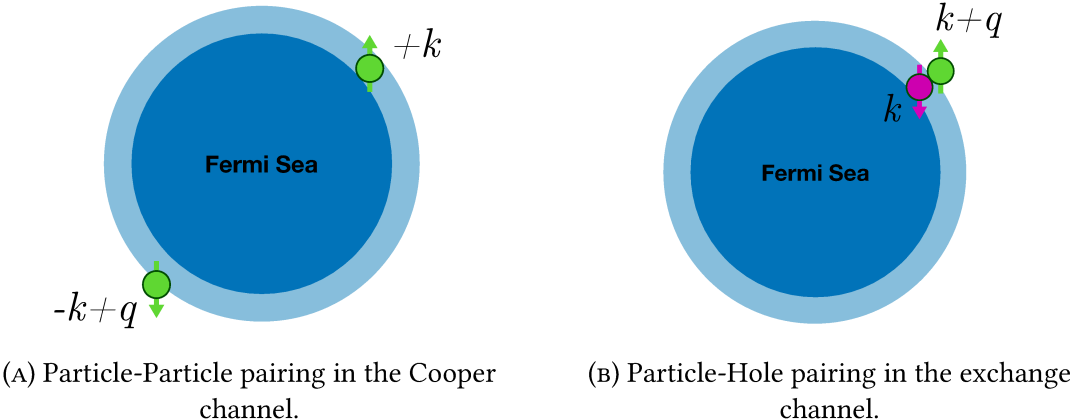


FIGURE 4.1: Representation of interactions in the Cooper and exchange channels.

4.1 Decoupling in the Cooper and exchange channels

We again start with the action of a neutral Fermi gas with an attractive contact interaction,

$$\begin{aligned}
S_F[\bar{\psi} \psi] &= S_0[\bar{\psi} \psi] + S_I[\bar{\psi} \psi] \\
&= - \int \mathrm{d}^4 k \bar{\psi}_{\sigma k} G_0^{-1}(k) \psi_{\sigma k} - g \int \mathrm{d}^4(k_1 k_2 k_3 k_4) \bar{\psi}_{\uparrow k_1} \bar{\psi}_{\downarrow k_3} \psi_{\downarrow k_4} \psi_{\uparrow k_2} \delta_{k_1 - k_2 + k_3 - k_4} \quad ,
\end{aligned} \tag{4.1}$$

but instead of writing this interaction solely in the *Cooper channel* as was done in the previous chapter, we will simultaneously decompose the interaction into both the Cooper and exchange channels,

$$\begin{aligned}
S_I[\bar{\psi} \psi] \approx - \int_{q \ll k_F} \mathrm{d}^4(k k' q) \left[g(\bar{\psi}_{\uparrow k} \bar{\psi}_{\downarrow -k+q})(\psi_{\downarrow -k'+q} \psi_{\uparrow k'}) \right. \\
\left. - \frac{g}{6}(\bar{\psi}_{\alpha k} \boldsymbol{\sigma}_{\alpha\beta} \psi_{\beta k-q}) \cdot (\bar{\psi}_{\alpha' k'} \boldsymbol{\sigma}_{\alpha'\beta'} \psi_{\beta' k'+q}) \right] \quad .
\end{aligned} \tag{4.2}$$

The decomposition in Eq. 4.2 may initially seem inappropriate, since for unbounded q the two terms are separately equal to the original interaction. However, because we are interested in probing only the saddle-point physics of the Cooper channel, modulo small fluctuations, a Hubbard-Stratonovich transformation solely in the Cooper channel makes our analysis insensitive to the physics we would see for small q in the exchange channel term.¹

In order to simultaneously analyze the effects of the Cooper and exchange contributions to the interactions, we introduce *two* resolutions of unity into the generating functional

$$1 = \int \mathcal{D}[\bar{\Delta} \Delta] \exp \left[- \int \mathrm{d}^4 q \frac{\bar{\Delta}(q) \Delta(q)}{g} \right] \tag{4.3}$$

¹A more detailed discussion of decomposing interactions into multiple channels may be found in [3].

and

$$1 = \int \mathcal{D}[\mathbf{m}] \exp \left[- \int \mathrm{d}^4 q \frac{\mathbf{m}(q) \cdot \mathbf{m}(-q)}{2\tilde{g}} \right] , \quad (4.4)$$

where $\tilde{g} \equiv g/3$, $\bar{\Delta}$ and Δ form a complex scalar field, and \mathbf{m} is a real vector field with three components because we wish to couple it to the Fermion spin operator.

Performing field redefinitions on Δ

$$\Delta_q \rightarrow \Delta_q - g \int \mathrm{d}^4 k \psi_{-k+q\downarrow} \psi_{k\uparrow} , \quad (4.5)$$

and on $\bar{\Delta}$

$$\bar{\Delta}_q \rightarrow \bar{\Delta}_q - g \int \mathrm{d}^4 k \bar{\psi}_{k\uparrow} \bar{\psi}_{-k+q\downarrow} , \quad (4.6)$$

we find that

$$\begin{aligned} 1 &= \int \mathcal{D}[\bar{\Delta} \Delta] \exp \left[- \int \mathrm{d}^4 q \frac{\bar{\Delta}(q) \Delta(q)}{g} \right] \\ &= \int \mathcal{D}[\bar{\Delta} \Delta] \exp \left[- \int \mathrm{d}^4 q \frac{\bar{\Delta}(q) \Delta(q)}{g} + \int \mathrm{d}^4(k \ q) (\Delta_q \bar{\psi}_{k\uparrow} \bar{\psi}_{-k+q\downarrow} + \bar{\Delta}_q \psi_{-k+q\downarrow} \psi_{k\uparrow}) \right. \\ &\quad \left. - g \int \mathrm{d}^4(k \ k' \ q) (\bar{\psi}_{k\uparrow} \bar{\psi}_{-k+q\downarrow}) (\psi_{-k'+q\downarrow} \psi_{k'\uparrow}) \right] , \quad (4.7) \end{aligned}$$

and hence, the Cooper channel contribution from the interaction may be expressed as

$$\begin{aligned} &\exp \left[g \int \mathrm{d}^4(k \ k' \ q) (\bar{\psi}_{\uparrow k} \bar{\psi}_{\downarrow -k+q}) (\psi_{\downarrow -k'+q} \psi_{\uparrow k'}) \right] \\ &= \int \mathcal{D}[\bar{\Delta} \Delta] \exp \left[- \int \mathrm{d}^4 q \frac{\bar{\Delta}(q) \Delta(q)}{g} + \int \mathrm{d}^4(k \ q) (\Delta_q \bar{\psi}_{k\uparrow} \bar{\psi}_{-k+q\downarrow} + \bar{\Delta}_q \psi_{-k+q\downarrow} \psi_{k\uparrow}) \right] . \quad (4.8) \end{aligned}$$

Likewise, we perform shifts on \mathbf{m}

$$\mathbf{m}_q \rightarrow \mathbf{m}_q - i\tilde{g} \int \mathrm{d}^4 k (\bar{\psi}_{k\alpha} \boldsymbol{\sigma}_{\alpha\beta} \psi_{k-q\beta}) , \quad (4.9)$$

such that

$$\begin{aligned}
1 &= \int \mathcal{D}[\mathbf{m}] \exp \left[- \int \mathrm{d}^4 q \frac{\mathbf{m}(q) \cdot \mathbf{m}(-q)}{2\tilde{g}} \right] \\
&= \int \mathcal{D}[\mathbf{m}] \exp \left[- \int \mathrm{d}^4 q \frac{\mathbf{m}(q) \cdot \mathbf{m}(-q)}{2\tilde{g}} + i \int \mathrm{d}^4(k, q) \mathbf{m}_q \cdot (\bar{\psi}_{k\alpha} \boldsymbol{\sigma}_{\alpha\beta} \psi_{k+q\beta}) \right. \\
&\quad \left. + \frac{g}{6} \int \mathrm{d}^4(k, k', q) (\bar{\psi}_{\alpha k} \boldsymbol{\sigma}_{\alpha\beta} \psi_{\beta k+q}) \cdot (\bar{\psi}_{\alpha' k'} \boldsymbol{\sigma}_{\alpha'\beta'} \psi_{\beta' k'-q}) \right] ,
\end{aligned} \tag{4.10}$$

so that the exchange channel contribution from the interaction becomes

$$\begin{aligned}
&\exp \left[-\tilde{g} \int \mathrm{d}^4(k, k', q) (\bar{\psi}_{\alpha k} \boldsymbol{\sigma}_{\alpha\beta} \psi_{\beta k+q}) \cdot (\bar{\psi}_{\alpha' k'} \boldsymbol{\sigma}_{\alpha'\beta'} \psi_{\beta' k'-q}) \right] \\
&= \int \mathcal{D}[\mathbf{m}] \exp \left[- \int \mathrm{d}^4 q \frac{\mathbf{m}(q) \cdot \mathbf{m}(-q)}{2\tilde{g}} + i \int \mathrm{d}^4(k, q) \mathbf{m}_q \cdot (\bar{\psi}_{k\alpha} \boldsymbol{\sigma}_{\alpha\beta} \psi_{k+q\beta}) \right] .
\end{aligned} \tag{4.11}$$

Hence, these shifts couple \mathbf{m} to the Fermion spin operator $S = \bar{\psi}_\alpha \boldsymbol{\sigma}_{\alpha\beta} \psi_\beta$, so we can think of \mathbf{m} as a magnetization field.

With these shifts, we now write the generating functional as

$$\begin{aligned}
\mathcal{Z} &= \int \mathcal{D}[\bar{\psi}, \psi] e^{-S_F[\bar{\psi}, \psi]} \\
&= \int \mathcal{D}[\bar{\psi}, \psi, \bar{\Delta}, \Delta, \mathbf{m}] e^{-S_{F+HS}[\bar{\psi}, \psi, \bar{\Delta}, \Delta, \mathbf{m}]} ,
\end{aligned} \tag{4.12}$$

where

$$\begin{aligned}
S[\bar{\psi}, \psi, \bar{\Delta}, \Delta, \mathbf{m}] &= - \int \mathrm{d}^4 k \bar{\psi}_{k\sigma} G_0^{-1}(k) \psi_{k\sigma} + \int \mathrm{d}^4 q \left(\frac{\bar{\Delta}_q \Delta_q}{g} + \frac{\mathbf{m}_q \cdot \mathbf{m}_{-q}}{2\tilde{g}} \right) \\
&\quad - \int \mathrm{d}^4(k, q) \left(\Delta_q \bar{\psi}_{k\uparrow} \bar{\psi}_{-k+q\downarrow} + \bar{\Delta}_q \psi_{-k+q\downarrow} \psi_{k\uparrow} + i \mathbf{m}_q \cdot (\bar{\psi}_{k\alpha} \boldsymbol{\sigma}_{\alpha\beta} \psi_{k+q\beta}) \right) \\
&= - \int \mathrm{d}^4(k, q) \frac{1}{2} \Psi^\dagger(k, 0) \mathcal{G}_{kq}^{-1} \Psi(k, q) + \int \mathrm{d}^4 q \left(\frac{\bar{\Delta}_q \Delta_q}{g} + \frac{\mathbf{m}_q \cdot \mathbf{m}_{-q}}{2\tilde{g}} \right) ,
\end{aligned} \tag{4.13}$$

and where

$$\Psi^\dagger(k, 0) = \begin{pmatrix} \bar{\psi}_k & \psi_{-k}^T \end{pmatrix} , \quad \Psi(k, q) = \begin{pmatrix} \psi_{k+q} \\ \bar{\psi}_{-k+q}^T \end{pmatrix} , \tag{4.14}$$

$$\bar{\psi}_k = \begin{pmatrix} \bar{\psi}_{k\uparrow} & \bar{\psi}_{k\downarrow} \end{pmatrix}, \quad \psi_k = \begin{pmatrix} \psi_{k\uparrow} \\ \psi_{k\downarrow} \end{pmatrix}, \quad (4.15)$$

and

$$\mathcal{G}^{-1}(k, q) = \begin{pmatrix} G_0^{-1}(k)\delta_q + i\boldsymbol{\sigma} \cdot \mathbf{m}(q) & \Delta(q)i\sigma_y \\ \bar{\Delta}(-q)i\sigma_y^T & -G_0^{-1}(-k)\delta_q - i\boldsymbol{\sigma}^T \cdot \mathbf{m}(q) \end{pmatrix}. \quad (4.16)$$

However, Ψ^\dagger and Ψ are *not* independent degrees of freedom because

$$\Psi^\dagger(k) = (\tau_x \Psi(k))^T = \Psi(k)^T \tau_x. \quad (4.17)$$

Therefore, we integrate only over Ψ as a *real Nambu* field to avoid over-counting degrees of freedom:

$$\begin{aligned} \mathcal{Z} &= \int \mathcal{D}[\Psi, \bar{\Delta}, \Delta, \mathbf{m}] \exp \left[\frac{1}{2} \int \mathrm{d}^4(k, q) \Psi^T(k) (\mathcal{G}(k, q) \tau_x)^{-1} \Psi(k, q) \right. \\ &\quad \left. - \int \mathrm{d}^4 q \left(\frac{\bar{\Delta}_q \Delta_q}{g} + \frac{\mathbf{m}_q \cdot \mathbf{m}_{-q}}{2\tilde{g}} \right) \right] \\ &= \int \mathcal{D}[\bar{\Delta}, \Delta, \mathbf{m}] \exp \left[- \int \mathrm{d}^4 q \left(\frac{\bar{\Delta}_q \Delta_q}{g} + \frac{\mathbf{m}_q \cdot \mathbf{m}_{-q}}{2\tilde{g}} \right) + \frac{1}{2} \mathrm{Tr} \mathrm{Log} \left(-\beta \mathcal{G}^{-1} \right) \right]. \quad (4.18) \end{aligned}$$

4.2 Gaussian fluctuations in the exchange channel

At this point we will make two simplifying assumptions:

- The Cooper channel collective mode is homogeneous in both space and imaginary time, i.e., $\Delta_q = \Delta \delta_q$.
- The exchange channel collective mode is sufficiently weak that we can expand it to Gaussian order about zero net magnetization.

With the second assumption, we can give \mathbf{m} a similar treatment to that given to the superconducting fluctuations η in the previous chapter. This will allow us to understand how the presence of exchange channel fluctuations effect the superconducting

state rather than studying Cooper channel fluctuations. Considering both channels at the same time would be preferable, but also more technically difficult due to coupling between them, so we leave it to future work.

Finally, it should be noted that when we studied superconducting fluctuations, the fluctuations η were defined only *after* identifying a saddle point to fluctuate about, since the fluctuation was in the same variable Δ as the saddle-point condition. By contrast, we are here considering fluctuations in a separate variable m , and so for the purposes of these fluctuations, Δ is not fixed at its saddle-point value as was the case with the superconducting fluctuations. These magnetization fluctuations will introduce new terms into the saddle point equation for Δ .

Before expanding the logarithm in powers of m , we write

$$\begin{aligned}\mathcal{G}^{-1}(k, q) &= \mathcal{G}_{\Delta}^{-1}(k) + i\Sigma_m(q) \\ &= \mathcal{G}_{\Delta}^{-1}(k) \left(1 + i\mathcal{G}_{\Delta}(k)\Sigma_m(q) \right),\end{aligned}\quad (4.19)$$

where

$$\begin{aligned}\mathcal{G}_{\Delta}^{-1}(k) &= \begin{pmatrix} G_0^{-1}(k) & \Delta i\sigma_y \\ \bar{\Delta} i\sigma_y^T & -G_0^{-1}(-k) \end{pmatrix}, \\ \Sigma_m(q) &= \begin{pmatrix} \boldsymbol{\sigma} \cdot \mathbf{m}(q) & 0 \\ 0 & -\boldsymbol{\sigma}^T \cdot \mathbf{m}(q) \end{pmatrix},\end{aligned}\quad (4.20)$$

and

$$\begin{aligned}\mathcal{G}(k) &= \frac{1}{G_0^{-1}(k)G_0^{-1}(-k) + \bar{\Delta}\Delta} \begin{pmatrix} G_0^{-1}(-k) & \Delta i\sigma_y \\ \bar{\Delta} i\sigma_y^T & -G_0^{-1}(k) \end{pmatrix} \\ &\equiv \begin{pmatrix} G(k) & F(k) i\sigma_y \\ \bar{F}(k) i\sigma_y^T & -G(-k) \end{pmatrix}.\end{aligned}\quad (4.21)$$

With these definitions, we expand the logarithm in the effective action to Gaussian order,

$$\begin{aligned} \text{TrLog}(\mathcal{G}^{-1}) &= \text{TrLog}\left[\mathcal{G}_\Delta^{-1}\left(1 + i\mathcal{G}_\Delta(k)\Sigma_m(q)\right)\right] \\ &= \text{TrLog}(\mathcal{G}_\Delta^{-1}) + i\text{Tr}(\mathcal{G}_\Delta\Sigma_m) + \frac{1}{2}\text{Tr}(\mathcal{G}_\Delta\Sigma_m\mathcal{G}_\Delta\Sigma_m) + \mathcal{O}(m^3) . \end{aligned} \quad (4.22)$$

The term linear in m will vanish by the saddle-point condition, so we focus on the quadratic term,

$$\begin{aligned} \text{Tr}(\mathcal{G}_\Delta\Sigma_m\mathcal{G}_\Delta\Sigma_m) &= \text{tr} \int d^4(x_1 x_1)\mathcal{G}_\Delta(x_1 x_2)\Sigma_m(x_2)\mathcal{G}_\Delta(x_2 x_1)\Sigma_m(x_1) \\ &= \text{tr} \int d^4(k q)\mathcal{G}_\Delta(k)\Sigma_m(q)\mathcal{G}_\Delta(k-q)\Sigma_m(-q) \\ &= \text{tr} \int d^4(k q) \begin{pmatrix} G(k)(\boldsymbol{\sigma} \cdot \mathbf{m}(q)) & -iF(k)\sigma_y(\boldsymbol{\sigma}^T \cdot \mathbf{m}_q) \\ -i\bar{F}(k)\sigma_y(\boldsymbol{\sigma} \cdot \mathbf{m}_q) & G(-k)(\boldsymbol{\sigma}^T \cdot \mathbf{m}_q) \end{pmatrix} \\ &\quad \times \begin{pmatrix} G(k-q)(\boldsymbol{\sigma} \cdot \mathbf{m}_{-q}) & -iF(k-q)\sigma_y(\boldsymbol{\sigma}^T \cdot \mathbf{m}_{-q}) \\ -i\bar{F}(k-q)\sigma_y(\boldsymbol{\sigma} \cdot \mathbf{m}_{-q}) & G(q-k)(\boldsymbol{\sigma}^T \cdot \mathbf{m}_{-q}) \end{pmatrix} . \end{aligned} \quad (4.23)$$

Using the identities

$$\begin{aligned} (\boldsymbol{\sigma} \cdot \mathbf{m}_q)(\boldsymbol{\sigma} \cdot \mathbf{m}_{-q}) &= (\boldsymbol{\sigma}^T \cdot \mathbf{m}_q)(\boldsymbol{\sigma}^T \cdot \mathbf{m}_{-q}) \\ &= \mathbf{m}_q \cdot \mathbf{m}_{-q} \mathbb{1} \end{aligned}$$

and

$$\begin{aligned} \sigma_y(\boldsymbol{\sigma}^T \cdot \mathbf{m}_q)\sigma_y(\boldsymbol{\sigma} \cdot \mathbf{m}_{-q}) &= \sigma_y(\boldsymbol{\sigma} \cdot \mathbf{m}_q)\sigma_y(\boldsymbol{\sigma}^T \cdot \mathbf{m}_{-q}) \\ &= -\mathbf{m}_q \cdot \mathbf{m}_{-q} \mathbb{1} , \end{aligned}$$

we find

$$\frac{1}{2}\text{Tr}(\mathcal{G}_\Delta\Sigma_m\mathcal{G}_\Delta\Sigma_m) = 2 \int d^4(k q) \left(G(k)G(k-q) + \bar{F}(k)F(k-q) \right) \mathbf{m}_q \cdot \mathbf{m}_{-q} . \quad (4.24)$$

Hence, the generating functional to Gaussian order in m becomes

$$\begin{aligned}
\mathcal{Z} &= \int \mathcal{D}[\bar{\Delta} \Delta \mathbf{m}] \exp \left[-\beta V \frac{\bar{\Delta} \Delta}{g} - \int \mathrm{d}^4 q \frac{\mathbf{m}_q \cdot \mathbf{m}_{-q}}{2\tilde{g}} + \frac{1}{2} \mathrm{Tr} \mathrm{Log} \left(-\beta \mathcal{G}^{-1} \right) \right] \\
&\approx \int \mathcal{D}[\bar{\Delta} \Delta \mathbf{m}] \exp \left[-\beta V \frac{\bar{\Delta} \Delta}{g} + \frac{1}{2} \mathrm{Tr} \mathrm{Log} \left(-\beta \mathcal{G}_{\Delta}^{-1} \right) + \frac{1}{2} \int \mathrm{d}^4 q \mathbf{m}_q \cdot D^{-1}(q) \mathbf{m}_{-q} \right] \\
&= \int \mathcal{D}[\bar{\Delta} \Delta] \exp \left[-\beta V \frac{\bar{\Delta} \Delta}{g} + \frac{1}{2} \mathrm{Tr} \mathrm{Log} \left(-\beta \mathcal{G}_{\Delta}^{-1} \right) - \frac{3}{2} \mathrm{Tr} \mathrm{Log} \left(-\tilde{g} D^{-1} \right) \right] \\
&= \int \mathcal{D}[\bar{\Delta} \Delta] \exp \left(-S_{\mathrm{Eff}}[\bar{\Delta} \Delta] \right), \tag{4.25}
\end{aligned}$$

where

$$D^{-1}(q) = 2 \int \mathrm{d}^4 k \left(G(k)G(k-q) + \bar{F}(k)F(k-q) \right) - \frac{1}{\tilde{g}} \tag{4.26}$$

is the effective propagator for magnetization fluctuations.

4.3 Modified saddle-point condition

We expect dominant contributions to the generating functional when

$$\begin{aligned}
0 &= \frac{\delta}{\delta \bar{\Delta}} S_{\mathrm{Fluc}}[\bar{\Delta} \Delta] \\
&= \frac{\Delta}{g} - \int \mathrm{d}^4 k \Delta G(k)G_0(q-k) + \frac{3}{2} \int \mathrm{d}^4 q D(q) \frac{\delta D^{-1}(-q)}{\delta \bar{\Delta}}, \tag{4.27}
\end{aligned}$$

where

$$\frac{\delta D^{-1}(q)}{\delta \bar{\Delta}} = 2 \int \mathrm{d}^4 k \frac{\delta}{\delta \bar{\Delta}} \left(G(k)G(k-q) - F(k)\bar{F}(k-q) \right). \tag{4.28}$$

In order to calculate this functional derivative, we note that

$$\begin{aligned}
\frac{\delta G(k)}{\delta \bar{\Delta}} &= G_0^{-1}(-k) \frac{\delta}{\delta \bar{\Delta}} \left(G_0^{-1}(k) G_0^{-1}(-k) + \bar{\Delta} \Delta \right)^{-1} \\
&= - \frac{G_0^{-1}(-k) \Delta}{\left(G_0^{-1}(k) G_0^{-1}(-k) + \bar{\Delta} \Delta \right)^2} \\
&= -\Delta G(k) G_0(-k) G(k) \ , \tag{4.29}
\end{aligned}$$

and so

$$\frac{\delta G(k) G(k-q)}{\delta \bar{\Delta}} = -\Delta \left(G(k) G_0(-k) G(k) G(k-q) + G(k) G(k-q) G_0(q-k) G(k-q) \right) \ . \tag{4.30}$$

Likewise,

$$\begin{aligned}
\frac{\delta}{\delta \bar{\Delta}} \bar{F}(k) F(k-q) &= \frac{\delta}{\delta \bar{\Delta}} \left(\bar{\Delta} \Delta G(k) G_0(-k) G(k-q) G_0(q-k) \right) \\
&= \Delta \left[G(k) G_0(-k) G(k-q) G_0(q-k) \right. \\
&\quad \left. - \Delta \bar{\Delta} \left(G^3(k) G_0^2(-k) G(k-q) G_0(q-k) + G(k) G_0(-k) G^3(k-q) G_0^2(q-k) \right) \right] \ . \tag{4.31}
\end{aligned}$$

We may now write the modified saddle-point equation as

$$\begin{aligned}
\frac{1}{g} &= \int \mathbb{d}^4 k \ G(k) G_0(-k) - 3 \int \mathbb{d}^4(k, q) \ D(q) \left[2G^2(k) G_0(-k) G(k-q) \right. \\
&\quad \left. + G(k) G_0(-k) G(k-q) G_0(q-k) \right. \\
&\quad \left. - 2\Delta \bar{\Delta} G^3(k) G_0^2(-k) G(k-q) G_0(q-k) \right] \ , \tag{4.32}
\end{aligned}$$

which gives way to the modified T_c equation

$$\begin{aligned}
\frac{1}{g} &= \int \mathbb{d}^4 k \ G_0(k) G_0(-k) - 3 \int \mathbb{d}^4(k, q) \ D_0(q) \left[G_0(k) G_0(-k) G_0(k-q) G_0(q-k) \right. \\
&\quad \left. + 2G_0(k) G_0(-k) G_0(k) G_0(k-q) \right] \ , \tag{4.33}
\end{aligned}$$

where we have defined

$$\begin{aligned} D_0^{-1}(q) &\equiv \lim_{\Delta \rightarrow 0} D^{-1}(q) \\ &= 2 \int d^4 k G_0(k) G_0(k-q) - \frac{1}{\tilde{g}}. \end{aligned} \quad (4.34)$$

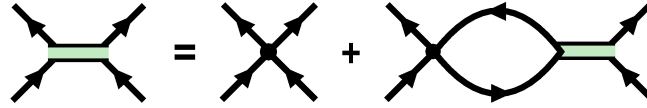
We call the fluctuation correction terms

$$\int d^4(k, q) D_0(q) G_0(k) G_0(-k) G_0(k-q) G_0(q-k) \quad (4.35)$$

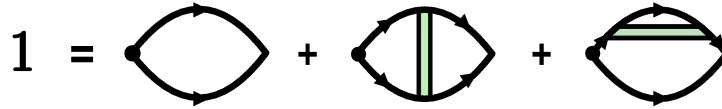
and

$$\int d^4(k, q) D_0(q) G_0(k) G_0(-k) G_0(k) G_0(k-q) \quad (4.36)$$

Maki-Thompson and Density of States (DoS) style diagrams respectively after the analogous diagrams from the superconducting fluctuation literature [17].



(A) Exchange channel fluctuation propagator built from particle-hole polarization bubbles.



(B) Superconducting T_c equation with exchange channel fluctuation corrections. The first correction is called a Maki-Thompson style diagram and the second, a Density of States (DoS) style diagram.

FIGURE 4.2: Fluctuation correction to the BCS T_c equation

We emphasize that our T_c equation, Eq. 4.33, is *not* the same as the GMB T_c equation Eq. 3.40, however both corrected T_c equations contain the term

$$\int d^4(k' q) G_0(k)G_0(-k)G_0(k'+q)G_0(k')G_0(k-q)G_0(q-k) \quad (4.37)$$

in their diagrammatic expansions.

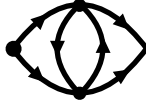


FIGURE 4.3: Term appearing in both the GMB correction and exchange-channel fluctuation correction to the critical temperature.

4.3.1 Exchange channel fluctuation propagator: small-momentum expansion

In practice, computing the Matsubara sums of the fluctuation terms Eq. 4.33 would prove difficult due to the presence of a $D_0(q)$ which contains the inverse of a constant added to a polarization bubble,

$$\begin{aligned} \Pi_0(q) &= 2 \int d^4k G_0(k)G_0(k-q) \\ &= \int d^3\mathbf{k} \frac{f(\xi_{\mathbf{k}}) - f(\xi_{\mathbf{k}-\mathbf{q}})}{i\Omega_m + \xi_{\mathbf{k}} - \xi_{\mathbf{k}-\mathbf{q}}} . \end{aligned} \quad (4.38)$$

In the regime where $k \approx k_F$ and $q < \omega_D \ll k_F$ we may write

$$\xi_{\mathbf{k}} - \xi_{\mathbf{k}-\mathbf{q}} = \frac{\mathbf{k} \cdot \mathbf{q}}{m} + \mathcal{O}(q^2) \quad (4.39)$$

and likewise

$$\begin{aligned} f(\xi_{\mathbf{k}}) - f(\xi_{\mathbf{k}-\mathbf{q}}) &= \left[\partial_{\xi_{\mathbf{k}}} f(\xi_{\mathbf{k}}) \right] \frac{\mathbf{k} \cdot \mathbf{q}}{m} + \mathcal{O}(q^2) \\ &\approx -\delta(\xi_{\mathbf{k}}) \frac{\mathbf{k} \cdot \mathbf{q}}{m} + \mathcal{O}(q^2) , \end{aligned} \quad (4.40)$$

where the final approximation holds for $T \ll T_F \sim 10000 K$ which is nearly exact for any superconducting system. Hence,

$$\begin{aligned}
\Pi_0(\mathbf{q}, i\Omega_m) &= -2 \int d^3\mathbf{k} \delta(\epsilon_{\mathbf{k}} - \mu) \frac{\frac{1}{m}\mathbf{q} \cdot \mathbf{k}}{i\Omega_m + \frac{1}{m}\mathbf{q} \cdot \mathbf{k}} \\
&= -\frac{2}{(2\pi)^3} \int k^2 dk d\Omega \delta(\epsilon_{\mathbf{k}} - \mu) \frac{\frac{1}{m}\mathbf{q} \cdot \mathbf{k}}{i\Omega_m + \frac{1}{m}\mathbf{q} \cdot \mathbf{k}} \\
&= -\frac{\nu(\mu)}{\int d\Omega} \int d\Omega \frac{v_F \mathbf{n} \cdot \mathbf{q}}{i\Omega_m + v_F \mathbf{n} \cdot \mathbf{q}} , \tag{4.41}
\end{aligned}$$

where \mathbf{n} is a unit vector integrated over the solid angle, v_F is the Fermi velocity and ν is the density of states function. Thus,

$$\begin{aligned}
\Pi_0(\mathbf{q}, i\Omega_m) &= -\frac{\nu(\mu)}{2} \int_{-1}^1 dx \frac{v_F |\mathbf{q}| x}{i\Omega_m + v_F |\mathbf{q}| x} \\
&= -\nu(\mu) \left[1 - \frac{i\Omega_m}{2v_F |\mathbf{q}|} \ln \left(\frac{i\Omega_m + v_F |\mathbf{q}|}{i\Omega_m - v_F |\mathbf{q}|} \right) \right] \tag{4.42}
\end{aligned}$$

such that

$$\begin{aligned}
D_0(\mathbf{q}, i\Omega_m) &= -\frac{\tilde{g}}{1 + \frac{\tilde{g}\nu(\mu)}{3} \left(\frac{\mathbf{q}v_F}{i\Omega_m} \right)^2 + \mathcal{O}(q^4)} \\
&= -\frac{\tilde{g} (i\Omega_m)^2}{(i\Omega_m)^2 - (c_e |\mathbf{q}|)^2} + \mathcal{O}(q^4) \\
&= -\frac{\tilde{g}}{2} \left(2 + \frac{c_e q}{i\Omega_m - c_e |\mathbf{q}|} - \frac{c_e q}{i\Omega_m + c_e |\mathbf{q}|} \right) + \mathcal{O}(q^4) , \tag{4.43}
\end{aligned}$$

where

$$c_e = \sqrt{\frac{\tilde{g}\nu(\mu)}{3}} v_F . \tag{4.44}$$

Hence, this particle-hole fluctuation propagator behaves like a constant added to a phonon propagator whose speed of sound is given by c_e . This constant term should be concerning if we were interested in high momenta, but for momenta q appreciably greater than ω_D we know that g would cease to be a constant interaction and would take on the form of the real phonon propagator and would have the correct high frequency and momentum behaviour.

Using this form of the normal-state fluctuation propagator, the Matsubara sums in the fluctuation terms of Eq. 4.33 may be computed using the methods in Appendix C.1 and C.2 in order to find

$$I(\mathbf{k} \mathbf{q}) = \frac{\tilde{g}}{4\xi_{\mathbf{k}}\xi_{\mathbf{k}-\mathbf{q}}} \left[\left(f(\xi_{\mathbf{k}}) - f(\xi_{\mathbf{k}-\mathbf{q}}) \right) \frac{\coth\left(\frac{1}{2}\beta c_e q\right) c_e q x - \coth\left(\frac{1}{2}\beta x\right) x^2}{x^2 - (c_e q)^2} \right. \\ \left. - \left(f(\xi_{\mathbf{k}}) + f(\xi_{\mathbf{k}-\mathbf{q}}) - 1 \right) \frac{\coth\left(\frac{1}{2}\beta c_e q\right) c_e q y - \coth\left(\frac{1}{2}\beta y\right) y^2}{y^2 - (c_e q)^2} \right], \quad (4.45)$$

and

$$J(\mathbf{k} \mathbf{q}) = T^2 \sum_{m,n} D_0(\mathbf{q}, i\Omega_m) G_0^2(\mathbf{k}, i\omega_n) G_0(-\mathbf{k}, -i\omega_m) G_0(\mathbf{k} - \mathbf{q}, i\omega_n - i\Omega_m) \\ = \frac{f(\xi_{\mathbf{k}})}{(2\xi_{\mathbf{k}})^2} J_1 + \left(\frac{f(\xi_{\mathbf{k}})}{(2\xi_{\mathbf{k}})^2} - \frac{f'(\xi_{\mathbf{k}})}{2\xi_{\mathbf{k}}} \right) J_2 + \frac{(1 - f(\xi_{\mathbf{k}}))}{2\xi_{\mathbf{k}}} J_3 - f(\xi_{\mathbf{k}-\mathbf{q}}) J_4, \quad (4.46)$$

where $x = \xi_{\mathbf{k}} - \xi_{\mathbf{k}-\mathbf{q}}$, $y = \xi_{\mathbf{k}} + \xi_{\mathbf{k}-\mathbf{q}}$, and

$$\frac{2J_1}{\tilde{g}} = \frac{2c_e q (x^2 + (c_e q)^2) b(c_e q) - 4(c_e q)^2 x b(x) + c_e q (x - c_e q)^2 + 2x^2 (x^2 - (c_e q)^2) b'(x)}{(x^2 - (c_e q)^2)^2} \quad (4.47)$$

$$\frac{2J_2}{\tilde{g}} = \frac{c_e q (x + 2xb(cq) - c_e q) - 2x^2 b(x)}{x^2 - (c_e q)^2} \quad (4.48)$$

$$\frac{2J_3}{\tilde{g}} = \frac{c_e q (y + 2yb(cq) + c_e q) - 2y^2 (1 + b(y))}{y^2 - (c_e q)^2} \quad (4.49)$$

$$\frac{2J_4}{\tilde{g}} = \frac{c_e q b(c_e q)}{(x - c_e q)^2 (y + c_e q)} + \frac{c_e q (1 + b(c_e q))}{(x + c_e q)^2 (y - c_e q)} - \frac{2y^2 (1 + b(y))}{(y^2 - (c_e q)^2) (2\xi_{\mathbf{k}})^2} \\ - \frac{2x \left((x^3 + (c_e q)^2 (x + 2y)) b(x) - x (x^2 - (c_e q)^2) (2\xi_{\mathbf{k}}) b'(x) \right)}{(x - c_e q)^2 (x + c_e q)^2 (2\xi_{\mathbf{k}})^2}, \quad (4.50)$$

such that the T_c equation becomes

$$1 = \int_{-\omega_D}^{\omega_D} d\xi \nu(\xi + \mu) \left[g \frac{\tanh\left(\frac{\beta\xi}{2}\right)}{\xi} - \int_{|\mathbf{q}| < \omega_D} \frac{d^3 \mathbf{q}}{(2\pi)^3} \left(I(\xi \mathbf{q}) + 2J(\xi \mathbf{q}) \right) \right]. \quad (4.51)$$

4.4 Modified number equation

Accounting for particle-hole fluctuation corrections, the mean-field number equation becomes

$$\begin{aligned}
n_{mf} &= \frac{1}{\beta V} \left(\frac{\partial S_{\text{EFF}}}{\partial \mu} \right)_{T,V} \\
&= \frac{1}{\beta V} \left(\left(\frac{\partial S_{\text{EFF}}}{\partial \mu} \right)_{\Delta=\Delta_{sp}} + \frac{\delta S_{\text{EFF}}}{\delta \Delta} \left(\frac{\partial \Delta}{\partial \mu} \right)_{\Delta=\Delta_{mf}} \right)_{T,V} \\
&= \frac{1}{\beta V} \left(\frac{\partial S_{\text{EFF}}}{\partial \mu} \right)_{\Delta,T,V} \\
&= \frac{1}{\beta V} \frac{\partial}{\partial \mu} \left(S_{\text{BCS}} + \frac{3}{2} \text{TrLog}(\tilde{g}D^{-1}) \right)_{\Delta,T,V} \\
&= 2 \int \mathbb{d}k G(k) + \frac{3}{2} \int \mathbb{d}q D(q) \left(\frac{\partial D^{-1}(-q)}{\partial \mu} \right)_{\Delta,T,V} . \tag{4.52}
\end{aligned}$$

Since we know that ²

$$\frac{\partial D^{-1}(q)}{\partial \mu} = 2 \int \mathbb{d}(k q) \frac{\partial}{\partial \mu} \left(G(k)G(k-q) - F(k)\bar{F}(k-q) \right) , \tag{4.53}$$

we first calculate

$$\begin{aligned}
\frac{\partial G(k)}{\partial \mu} &= -G(k) \left(\frac{\partial G^{-1}(k)}{\partial \mu} \right) G(k) \\
&= -G(k) \left(1 + |\Delta|^2 \frac{\partial G_0(-k)}{\partial \mu} \right) G(k) \\
&= -G(k) \left(1 - |\Delta|^2 G_0(-k)G_0(-k) \right) G(k) , \tag{4.54}
\end{aligned}$$

and

$$\begin{aligned}
\frac{\partial F(k)}{\partial \mu} &= \Delta \frac{\partial G(k)G_0(-k)}{\partial \mu} \\
&= -\Delta G(k)G_0(-k)G_0(-k) - \Delta G(k) \left(1 - |\Delta|^2 G_0(-k)G_0(-k) \right) G(k)G_0(-k) \\
&= -F(k)G_0(-k) - \Delta G(k) \left(1 - |\Delta|^2 G_0(-k)G_0(-k) \right) F(k) \tag{4.55}
\end{aligned}$$

²From now on, we will let the fact that the Δ , T and V are held constant be implicit.

such that

$$\begin{aligned}
n_{mf} &= 2 \int \mathrm{d}k G(k) - 3 \int \mathrm{d}^4(k, q) D(q) \left[G(k) \left(1 - |\Delta| G_0(k) G_0(-k) \right) G(k) G(k-q) - G_0(-k) \bar{F}(k) F(k-q) \right. \\
&\quad \left. - G(k) \left(1 - |\Delta|^2 G_0(k) G_0(-k) \right) \bar{F}(k) F(k-q) \right] \\
&= 2 \int \mathrm{d}k G(k) - 3 \int \mathrm{d}^4(k, q) D(q) \left(G(k) G(k-q) - F(k) \bar{F}(k-q) \right) G(k) \left(1 - |\Delta|^2 G_0(k) G_0(-k) \right) \\
&\quad + 3 \int \mathrm{d}^4(k, q) D(q) F(k) \bar{F}(k-q) G_0(-k) . \tag{4.56}
\end{aligned}$$

Near T_c , where we neglect terms of order $|\Delta|^2$ or higher, the equation becomes

$$n_{mf} = 2 \int \mathrm{d}^4 k G_0(k) - 3 \int \mathrm{d}^4(k, q) D_0(q) G_0(k) G_0(k-q) G_0(k) . \tag{4.57}$$

We show in Appendix C.3 how to compute the Matsubara sums in the fluctuation correction so that the number equation near T_c becomes

$$n_{mf} = 2 \int \mathrm{d}^3 \mathbf{k} f(\xi_{\mathbf{k}}) - 3 \int \mathrm{d}^3(\mathbf{k}, \mathbf{q}) \left(f'(\xi_{\mathbf{k}}) K_1(\mathbf{k}, \mathbf{q}) + \left(f(\xi_{\mathbf{k}}) - f(\xi_{\mathbf{k}-\mathbf{q}}) \right) K_2(\mathbf{k}, \mathbf{q}) \right) , \tag{4.58}$$

where

$$K_1(\mathbf{k}, \mathbf{q}) = \frac{\tilde{g}}{2} \left[\frac{2x^2 b(x) + (c_e q)^2 - x c_e q (1 - 2b(c_e q))}{x^2 - (c_e q)^2} \right] , \tag{4.59}$$

$$K_2(\mathbf{k}, \mathbf{q}) = \frac{\tilde{g}}{2} \left[\frac{2x, b'(x)}{x^2 - (c_e q)^2} + \frac{c_e q \left((x - c_e q)^2 + 2(x^2 + (c_e q)^2) b(c_e q) - 4c_e q b(x) \right)}{(x^2 - (c_e q)^2)^2} \right] , \tag{4.60}$$

and $x = \xi_{\mathbf{k}} - \xi_{\mathbf{k}-\mathbf{q}}$.

5 Conclusion

In this thesis we have provided a functional-integral based approach to incorporating particle-hole interactions into a model of superconductivity. The first step requires decoupling the Fermionic contact interaction into the Cooper and exchange channels, using Hubbard-Stratonovich transformations to represent the Cooper channel as a superconducting interaction and the exchange channel as an effective magnetization field. It was assumed that the system exhibits no net magnetization at the mean-field level, and small fluctuations in the magnetization field were studied at the Gaussian order. It was found that these fluctuations give rise to a particle-hole fluctuation propagator which introduces new terms into the BCS gap, T_c , and number equations. In the regime where the order parameter is small enough to be linearized, we have calculated the Matsubara sums in the new terms but we have left the momentum integrals to future work, and hence, do not yet know what quantitative effects this correction will have on the critical temperature, though we expect that the effects of fluctuations near T_c will be manifest in many observables [17].

The GMB correction and our exchange channel fluctuation correction are not the same, though it is possible that numerical studies will reveal that in certain regions of the parameter space they give similar predictions.

While it is too early to say whether our modification of the BCS theory of superconductivity should be regarded as more or less correct than that of Gor'kov and Melik-Barkhudarov, we can say that first, we are comforted by the fact that our corrections do not require us to recognize which diagrams were excluded from the BCS gap equation and to correctly reinsert them. Second, the diagrammatic form of our corrections show that the particle-hole effects enter as a new effective interaction vertex which transfers momentum between the Fermion lines in the Maki-Thompson style diagram and as a

self energy dressing of the Fermion Green's function in the DoS style diagram. These corrections are consistent with the form of diagrams that appear in the fluctuation literature, unlike the GMB correction.

Finally, we believe it is conceptually, pedagogically and practically advantageous that our corrections are implemented as fluctuation corrections to the BCS action because once implemented in that way, all calculations involving the corrected BCS action will naturally include particle-hole fluctuation effects without requiring any further guesswork or claims about how to properly re-insert neglected diagrams.

Future work

Looking towards the future, there is much left for us to explore using the formalism developed in this thesis. The obvious next step is to pursue a numerical strategy for calculating the momentum integral in the modified T_c equation, Eq. 4.51. We are interested in applying this formalism to a one dimensional lattice system to see if our corrections improve the agreement to known exact solutions relative to BCS [18]. Furthermore, we are interested in studying the effects of our *exchange* channel fluctuations simultaneously with the *Cooper* channel fluctuations seen in section 3.2 to see the relative importance of these fluctuation channels on transport quantities.

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A Grassmann numbers

The construction of Grassmann numbers can be thought of as similar to that of complex numbers. Consider an algebraic context where one decides it would be desirable to express the roots of the polynomial $x^2 + 1$. One could *suppose* the existence of a number i such that $i^2 = -1$ and so be led to discover the incredibly rich complex plane.

Similarly, we posit the existence of numbers η and θ such that $\eta\theta = -\theta\eta$ and hence, $\eta^2 = \theta^2 = 0$. We say η and $\theta \in \mathbb{G}$ where \mathbb{G} is known as the *Exterior algebra*. For some function f with a well defined Taylor expansion

$$f(x) = f_{(0)} + f_{(1)} x + \frac{1}{2} f_{(2)} x^2 + \dots \quad , \quad (\text{A.1})$$

we have

$$f(\eta) = f_{(0)} + f_{(1)} \eta \quad . \quad (\text{A.2})$$

Similarly, a Taylor expandable function g of two variables would take the following form with Grassmann valued inputs:

$$\begin{aligned} g(\eta \theta) &= g_{(0,0)} + g_{(1,0)} \eta + g_{(0,1)} \theta + g_{(1,1)} \eta\theta \\ &= g_{(0,0)} + g_{(1,0)} \eta + g_{(0,1)} \theta - g_{(1,1)} \theta\eta \quad , \end{aligned} \quad (\text{A.3})$$

so that we may formally define a Grassmann derivative operator $\partial/\partial\eta$ where

$$\frac{\partial}{\partial\eta} g(\eta \theta) \equiv g_{(1,0)} + g_{(1,1)} \theta \quad (\text{A.4})$$

and

$$\frac{\partial}{\partial \theta} g(\eta \theta) \equiv g_{(1,0)} - g_{(1,1)} \eta . \quad (\text{A.5})$$

For consistency with the anti-commutation of Grassmann numbers, the Grassmann derivative operator must also anti-commute with Grassmann numbers such that

$$\begin{aligned} \frac{\partial}{\partial \theta} \eta \theta &= -\eta \frac{\partial}{\partial \theta} \theta \\ &= -\theta . \end{aligned} \quad (\text{A.6})$$

We define a Grassmann integral operator $\int d\eta$ in analogy with the definite integral over all real numbers $\int_{\mathbb{R}} dx$. The integral operator $\int_{\mathbb{R}} dx$ has the property

$$\int_{\mathbb{R}} dx f(x+c) = \int_{\mathbb{R}} dx f(x) \quad (\text{A.7})$$

for any $c \in \mathbb{R}$. Similarly, we desire the property

$$\int d\eta f(\eta+c) = \int d\eta f(\eta) \quad (\text{A.8})$$

for any non-Grassmann valued c . Taylor expanding both sides, we find

$$\int d\eta (f_{(0)} + c) + \int d\eta f_{(1)} \eta = \int d\eta f_{(0)} + \int d\eta f_{(1)} \eta \quad (\text{A.9})$$

or

$$\int d\eta c = 0 . \quad (\text{A.10})$$

We next notice that because of the anti-commutation of Grassmann numbers, if we wish for the Grassmann integral operator $\int d\eta$ to act trivially on a Grassmann number

$\theta \neq \eta$, we see that

$$\int d\eta \theta \eta = - \int d\eta \eta \theta = - \left(\int d\eta \eta \right) \theta , \quad (\text{A.11})$$

and so $\int d\eta$ must anti-commute with θ .

Since all Grassmann valued functions are of the form $f(\eta) = f_{(0)} + f_{(1)} \eta$, we now need only define

$$\int d\eta \eta \quad (\text{A.12})$$

before we have fully specified the properties of Grassmann valued integration. Noticing that since $\int d\eta$ anti-commutes with θ for $\eta \neq \theta$, we think of $\int d\eta$ as a Grassmann valued quantity. The product of two Grassmann valued quantities may be thought of as non-Grassmann valued since

$$(\eta\theta)\chi = \chi(\eta\theta) . \quad (\text{A.13})$$

for any χ if η and $\theta \in \mathbb{G}$. Hence, we should have that $\int d\eta \eta$ evaluates to a non-Grassmann valued quantity. We may freely choose it to be normalized to unity such that

$$\int d\eta \eta \equiv 1 . \quad (\text{A.14})$$

Given the way we defined Grassmann numbers, it may rightly feel uncomfortable to write $\partial/\partial\eta$ or $\int d\eta$ since one would not write the analogous $\partial/\partial i$ and $\int di$. In this light, it is best to think of Grassmann derivatives and integrals as linear operators with properties loosely analogous to that of standard derivatives and integrals.

A.1 Gaussian integration of Grassmann variables

Here, we construct the equivalent of Gaussian integration of Grassmann numbers.

First, notice that for two vectors of n Grassmann numbers $\bar{\eta}$ and η ,

$$\begin{aligned} \int d^n(\bar{\eta} \eta) \exp(\bar{\eta}^T \eta) &\equiv \int d\bar{\eta}_1 d\eta_1 \dots d\bar{\eta}_n d\eta_n \exp\left(\sum_{i=1}^n \bar{\eta}_i \eta_i\right) \\ &= \int d\bar{\eta}_1 d\eta_1 \dots d\bar{\eta}_n d\eta_n \prod_{i=1}^n (1 - \bar{\eta}_i \eta_i) . \end{aligned} \quad (\text{A.15})$$

We now notice that since we integrate *every* $\bar{\eta}_i$ and η_i , any term in the integrand which does *not* contain a power of $\bar{\eta}_i$ or η_i for all $i \in (1 \dots n)$ will vanish. Hence,

$$\begin{aligned} \int d^n(\bar{\eta} \eta) \exp(\bar{\eta}^T \eta) &= (-1)^n \int d\bar{\eta}_1 d\eta_1 \dots d\bar{\eta}_n d\eta_n (\bar{\eta}_1 \eta_1 \dots \bar{\eta}_{n-1} \eta_{n-1} \bar{\eta}_n \eta_n) \\ &= (-1)^n (-1) \int d\bar{\eta}_1 d\eta_1 \dots d\bar{\eta}_{n-1} d\eta_{n-1} (\bar{\eta}_1 \eta_1 \dots \bar{\eta}_{n-1} \eta_{n-1}) \\ &= (-1)^n (-1) (-1) \int d\bar{\eta}_1 d\eta_1 \dots d\bar{\eta}_{n-2} d\eta_{n-2} (\bar{\eta}_1 \eta_1 \dots \bar{\eta}_{n-2} \eta_{n-2}) \\ &= \dots \\ &= (-1)^n (-1)^n \\ &= 1 . \end{aligned} \quad (\text{A.16})$$

Now consider the change of basis $\eta = M\psi$ and $\bar{\eta} = N\bar{\psi}$ for some matrices M and N .

In order to have $\int d^n \bar{\psi} \psi = \int d^n \bar{\eta} \eta$, we must have $d^n \eta = (\det M)^{-1} d^n \psi$ and

so

$$(\det MN)^{-1} \int d^n(\bar{\psi} \psi) \exp(\bar{\psi}^T N^T M \psi) = 1 .$$

Defining $A \equiv N^T M$, we arrive at the general Gaussian integral identity for Grassmann numbers:

$$\int d^n(\bar{\psi} \psi) \exp(\bar{\psi}^T A \psi) = \det A .$$

B Coherent states

B.1 Bosonic coherent states

Consider a Bosonic system whose Hilbert space may be constructed from a vacuum state, $|0\rangle$, and a set of creation and annihilation operators b^\dagger and b . A Bosonic *coherent state* $|\phi\rangle$ is defined as the right eigenstate of the annihilation operator ¹

$$b|\phi\rangle \equiv \phi|\phi\rangle, \quad (\text{B.1})$$

where $\phi \in \mathbb{C}$. Such a state can be constructed from an exponential ²

$$\begin{aligned} |\phi\rangle &\equiv \sum_{n=0}^{\infty} \frac{\phi^n}{\sqrt{n!}} |n\rangle \\ &= \sum_{n=0}^{\infty} \frac{(\phi b^\dagger)^n}{n!} |0\rangle \\ &= e^{\phi b^\dagger} |0\rangle, \end{aligned}$$

¹We specify that the coherent state is the *right* eigenstate of b because the operator b is not Hermitian.

²Note that coherent states *cannot* have a definite particle number since they are a superposition of *all* occupation numbers by construction.

where $|n\rangle$ is the n^{th} eigenstate of the number operator $b^\dagger b$. With this definition

$$\begin{aligned}
 b|\phi\rangle &= b \sum_{n=0}^{\infty} \frac{\phi^n (b^\dagger)^n}{n!} |0\rangle \\
 &= \sum_{n=0}^{\infty} \frac{\phi^n}{n!} \left((b^\dagger)^n b + [b, (b^\dagger)^n] \right) |0\rangle \\
 &= \sum_{n=0}^{\infty} \frac{\phi^n}{n!} [b, (b^\dagger)^n] |0\rangle \\
 &= \sum_{n=0}^{\infty} \frac{\phi^n}{n!} n (b^\dagger)^{n-1} |0\rangle \\
 &= \phi e^{\phi b^\dagger} |0\rangle \quad , \tag{B.2}
 \end{aligned}$$

and hence

$$b|\phi\rangle \equiv \phi|\phi\rangle .$$

Similarly, a Bosonic coherent co-state is simply the adjoint of the coherent state

$$\langle\phi| = \langle 0| e^{\bar{\phi} b}$$

such that ³

$$\langle\phi| b^\dagger = \langle\phi| \bar{\phi} . \tag{B.3}$$

³We define $\bar{\phi}$ as the complex conjugate of ϕ .

Similarly, the action of the creation (annihilation) operator on Bosonic coherent (co)states is that of the partial derivative operator

$$\begin{aligned}
 b^\dagger |\phi\rangle &= \sum_{n=0}^{\infty} \frac{\phi^n (b^\dagger)^{n+1}}{n!} |0\rangle \\
 &= \sum_{n=1}^{\infty} \frac{n \phi^{n-1} (b^\dagger)^n}{n!} |0\rangle \\
 &= \partial_\phi |\phi\rangle \quad .
 \end{aligned} \tag{B.4}$$

The inner product between two Bosonic coherent states is given by

$$\begin{aligned}
 \langle\phi|\phi'\rangle &= \langle 0|e^{\bar{\phi}b} e^{\phi'b^\dagger} |0\rangle \\
 &= \langle 0|e^{\phi'b^\dagger} e^{\bar{\phi}b} e^{\bar{\phi}\phi'} [b^\dagger, b] |0\rangle \\
 &= e^{\bar{\phi}\phi'} \langle 0|e^{\phi'b^\dagger} e^{\bar{\phi}b} |0\rangle \\
 &= e^{\bar{\phi}\phi'} \quad .
 \end{aligned} \tag{B.5}$$

The property $\langle\phi|\phi'\rangle = e^{\bar{\phi}\phi'}$ implies that the set of Bosonic coherent states form an *over-complete* basis in the physical Hilbert space, since a coherent state $|\phi\rangle$ has finite overlap with any other coherent state $|\phi'\rangle$ for non infinite $\phi, \phi' \in \mathbb{C}$.

Due to the properties that creation and annihilation operators have when acting on coherent states, any *normal-ordered* operator constructed from the creation and annihilation operators $A[b^\dagger b] = :A[b^\dagger b]:$ has the property

$$\langle\phi'|A[b^\dagger b]|\phi\rangle = A(\bar{\phi}' \phi) e^{\bar{\phi}'\phi} \quad , \tag{B.6}$$

where $A(\bar{\phi}' \phi)$ is the regular expression for the normal ordered operator A with all instances of b^\dagger replaced by the complex number $\bar{\phi}'$ and all instances of b replaced by ϕ .

The projection of an arbitrary state $|\Psi\rangle$ onto a Bosonic coherent state $|\phi\rangle$ is given by

$$\begin{aligned}
\langle\phi|\Psi\rangle &= \langle\phi|\sum_n\frac{\Psi_n}{\sqrt{n!}}|n\rangle \\
&= \sum_n\frac{\Psi_n}{n!}\langle\phi|(b^\dagger)^n|0\rangle \\
&= \sum_n\frac{\Psi_n}{n!}\langle\phi|(b^\dagger)^n|0\rangle \\
&= \sum_n\frac{\Psi_n}{n!}\langle\phi|(\bar{\phi})^n|0\rangle \\
&= \sum_n\frac{\Psi_n\bar{\phi}^n}{n!}.
\end{aligned} \tag{B.7}$$

If we interpret Ψ_n as the n^{th} derivative of a function Ψ with respect to $\bar{\phi}$, we are led to interpret $\langle\phi|\Psi\rangle$ as the Taylor expansion of an *anti-analytic* function $\Psi(\bar{\phi})$ such that

$$\langle\phi|\Psi\rangle = \Psi(\bar{\phi}). \tag{B.8}$$

Likewise, we have $\langle\Psi|\phi\rangle = \bar{\Psi}(\phi)$, i.e. the conjugate of an *anti-analytic* function.

To perform calculations with Bosonic coherent states we will need the resolution of unity in the coherent state basis, the form of which we will verify is given by

$$\mathbb{1} = \int\frac{d(\bar{\phi}\phi)}{2\pi i}e^{-\bar{\phi}\phi}|\phi\rangle\langle\phi|. \tag{B.9}$$

In order to prove the above equality, we show that the right hand side is equivalent to the Fock space identity element⁴

$$\begin{aligned}
\int \frac{d(\bar{\phi} \phi)}{2\pi i} e^{-\bar{\phi}\phi} |\phi\rangle \langle\phi| &= \sum_{nm} \int \frac{d(\bar{\phi} \phi)}{2\pi i} e^{-\bar{\phi}\phi} \frac{\bar{\phi}^n \phi^m}{\sqrt{n! m!}} |m\rangle \langle n| \\
&= \sum_{nm} \frac{1}{\sqrt{n! m!}} \int_0^\infty r dr \int_0^{2\pi} \frac{d\theta}{\pi} (re^{i\theta})^n (re^{-i\theta})^m e^{-r^2} |m\rangle \langle n| \\
&= \sum_{nm} \frac{1}{\sqrt{n! m!}} \int_0^\infty 2r dr r^{n+m} e^{-r^2} \int_0^{2\pi} \frac{d\theta}{2\pi} e^{i(n-m)\theta} |m\rangle \langle n| \\
&= \delta_{nm} \sum_n \frac{1}{n!} \int_0^\infty dr^2 (r^2)^n e^{-r^2} |n\rangle \langle n| \\
&= \delta_{nm} \sum_n |n\rangle \langle n| .
\end{aligned} \tag{B.10}$$

B.2 Fermionic coherent states

We now generalize the concept of coherent states to Fermionic systems. Consider an eigenstate $|\psi\rangle$ of the Fermionic annihilation operator c , then the anti-commutation relations would force these states to have the property

$$c c |\psi\rangle = 0 = \psi^2 |\psi\rangle ,$$

where ψ is the eigenvalue of the operator c . Hence,

$$\psi\psi = 0 . \tag{B.11}$$

Complex numbers do not have this property. Rather, we will need to use a type of number first considered by Hermann Grassmann known eponymously as Grassmann numbers [3]. We introduce the properties of Grassmann numbers and define a simple calculus on them in Appendix A. Defining ψ to be Grassmann valued, we may write

⁴We define the measure $d(\bar{\phi} \phi) \equiv d\bar{\phi} \wedge d\phi$ which may be shown to equal $2i d\text{Re}(\phi) d\text{Im}(\phi)$

the Fermionic coherent state as

$$|\psi\rangle = \exp[-\psi c^\dagger] |0\rangle = (1 - \psi c^\dagger) |0\rangle , \quad (\text{B.12})$$

where we used the fact that $\psi^2 = 0$. Demanding that $c\psi = -\psi c$ and $c^\dagger\psi = -\psi c^\dagger$ then we find

$$\begin{aligned} c|\psi\rangle &= c(1 - \psi c^\dagger) |0\rangle \\ &= -\psi c c^\dagger |0\rangle \\ &= \psi |0\rangle \\ &= (1 - \psi c^\dagger) |0\rangle \\ &= \psi |\psi\rangle . \end{aligned} \quad (\text{B.13})$$

Defining $\bar{\psi}$ to be an independent Grassmann number for ψ , we can compute

$$\begin{aligned} \langle\psi|c^\dagger &= \langle 0| (1 - c\bar{\psi}) c^\dagger \\ &= \langle 0|\bar{\psi} \\ &= \langle 0| (1 - c\bar{\psi}) \bar{\psi} \\ &= \langle\psi|\bar{\psi} . \end{aligned} \quad (\text{B.14})$$

The inner product between Fermionic coherent states is then the same as for Bosons:

$$\begin{aligned} \langle\eta|\psi\rangle &= \langle 0|(1 - c\bar{\eta})(1 - \psi c^\dagger)|0\rangle \\ &= \langle 0|(1 - c\bar{\eta})(1 - \psi c^\dagger)|0\rangle \\ &= 1 + \bar{\eta}\psi \\ &= e^{\bar{\eta}\psi} . \end{aligned} \quad (\text{B.15})$$

The Fermionic coherent-state resolution of unity is given by

$$\begin{aligned}
\mathbb{1} &= \int d(\bar{\psi} \ \psi) e^{-\bar{\psi}\psi} |\psi\rangle \langle\psi| \\
&= \int d(\bar{\psi} \ \psi) (1 - \bar{\psi}\psi) \left[|0\rangle \langle 0| - \psi |1\rangle \langle 0| - \bar{\psi} |0\rangle \langle 1| + |1\rangle \langle 1| \right] \\
&= \int d\bar{\psi} \left[\bar{\psi} |0\rangle \langle 0| - |1\rangle \langle 0| + \bar{\psi} |1\rangle \langle 1| \right] \\
&= |0\rangle \langle 0| + |1\rangle \langle 1| \quad , \tag{B.16}
\end{aligned}$$

and we note that the integration measure is not divided by a factor of $2\pi i$ as was the case with Bosonic coherent-states.

C Assorted Matsubara sums

C.1 Maki-Thompson style diagram

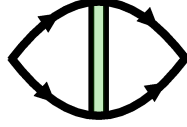


FIGURE C.1: Maki-Thompson style diagram arising in exchange channel fluctuation corrections to the BCS gap equation.

We wish to evaluate the Matsubara sum

$$I = T^2 \sum_{m,n} D_0(\mathbf{q}, i\Omega_m) G_0(\mathbf{k}, i\omega_n) G_0(-\mathbf{k}, -i\omega_n) G_0(\mathbf{k} - \mathbf{q}, i\Omega_m - i\omega_n) G_0(\mathbf{q} - \mathbf{k}, i\omega_n - i\Omega_m) , \quad (\text{C.1})$$

and as such we start with calculating

$$\begin{aligned} \tilde{I}(i\Omega_m) &= T \sum_n G_0(\mathbf{k}, i\omega_n) G_0(-\mathbf{k}, -i\omega_n) G_0(\mathbf{k} - \mathbf{q}, i\Omega_m - i\omega_n) G_0(\mathbf{q} - \mathbf{k}, i\omega_n - i\Omega_m) \\ &= T \sum_n \frac{1}{i\omega_n - \xi_{\mathbf{k}}} \frac{1}{i\omega_n + \xi_{\mathbf{k}}} \frac{1}{i\omega_n - i\Omega_m - \xi_{\mathbf{k}-\mathbf{q}}} \frac{1}{i\omega_n - i\Omega_m + \xi_{\mathbf{k}-\mathbf{q}}} \\ &= \frac{1}{2\pi i} \oint_{C'} dz \frac{1}{\exp(\beta z) + 1} \frac{1}{z - \xi_{\mathbf{k}}} \frac{1}{z + \xi_{\mathbf{k}}} \frac{1}{z - i\Omega_m - \xi_{\mathbf{k}-\mathbf{q}}} \frac{1}{z - i\Omega_m + \xi_{\mathbf{k}-\mathbf{q}}} , \quad (\text{C.2}) \end{aligned}$$

where C' is a clockwise oriented closed contour enclosing the poles of the Fermi function,

$$f(z) = \frac{1}{\exp(\beta z) + 1} ,$$

which are of weight -1 . With appropriate regularization of semicircular contributions at infinity, the integration contour may be reversed so that we now integrate around the contour C which is a set of closed, counterclockwise contours around the poles at ξ_k , $-\xi_k$, $i\Omega_m + \xi_{k-q}$ and $i\Omega_m - \xi_{k-q}$. Hence,

$$\begin{aligned} \tilde{I}(i\Omega_m) &= \frac{f(\xi_k)}{(2\xi_k)(\xi_k - \xi_{k-q} - i\Omega_m)(\xi_k + \xi_{k-q} - i\Omega_m)} \\ &+ \frac{f(-\xi_k)}{(-2\xi_k)(-\xi_k - \xi_{k-q} - i\Omega_m)(-\xi_k + \xi_{k-q} - i\Omega_m)} \\ &+ \frac{f(i\Omega_m + \xi_{k-q})}{(i\Omega_m + \xi_{k-q} - \xi_k)(i\Omega_m + \xi_{k-q} + \xi_k)(2\xi_{k-q})} \\ &+ \frac{f(i\Omega_m - \xi_{k-q})}{(i\Omega_m - \xi_{k-q} - \xi_k)(i\Omega_m - \xi_{k-q} + \xi_k)(-2\xi_{k-q})}, \end{aligned} \quad (\text{C.3})$$

which, after some manipulations, may be cast in the form

$$\begin{aligned} \tilde{I}(i\Omega_m) &= \frac{1}{4\xi_k\xi_{k-q}} \left(\frac{f(\xi_k) - f(\xi_{k-q})}{\xi_k - \xi_{k-q} - i\Omega_m} - \frac{f(\xi_k) + f(\xi_{k-q} - 1)}{\xi_k + \xi_{k-q} - i\Omega_m} \right) \\ &+ \frac{1}{4\xi_k\xi_{k-q}} \left(\frac{f(\xi_k) - f(\xi_{k-q})}{\xi_k - \xi_{k-q} + i\Omega_m} - \frac{f(\xi_k) + f(\xi_{k-q} - 1)}{\xi_k + \xi_{k-q} + i\Omega_m} \right). \end{aligned} \quad (\text{C.4})$$

Next, in order to calculate the full sum I_1 , we consider the sums

$$I_1 = T \sum_m D_0(\mathbf{q}, i\Omega_m) \left(\frac{1}{i\Omega_m + x} - \frac{1}{i\Omega_m - x} \right),$$

and

$$I_2 = T \sum_m D_0(\mathbf{q}, i\Omega_m) \left(\frac{1}{i\Omega_m + y} - \frac{1}{i\Omega_m - y} \right), \quad (\text{C.5})$$

where we have defined $x = \xi_k - \xi_{k-q}$ and $y = \xi_k + \xi_{k-q}$ such that

$$I = \frac{(f(\xi_k) - f(\xi_{k-q}))I_1 - (f(\xi_k) + f(\xi_{k-q} - 1))I_2}{4\xi_k\xi_{k-q}}. \quad (\text{C.6})$$

We will work in the regime where

$$D_0(\mathbf{q}, i\Omega_m) \approx -\frac{\tilde{g}}{2} \left(\frac{i\Omega_m}{i\Omega_m - c_e q} + \frac{i\Omega_m}{i\Omega_m + c_e q} \right), \quad (\text{C.7})$$

i.e. $|\mathbf{q}| \ll k_F$ and $T \ll T_F$. Hence,

$$\begin{aligned} \frac{2I_1}{\tilde{g}} &= -T \sum_m \left(\frac{i\Omega_m}{i\Omega_m - c_e q} + \frac{i\Omega_m}{i\Omega_m + c_e q} \right) \left(\frac{1}{i\Omega_m + x} - \frac{1}{i\Omega_m - x} \right) \\ &= \frac{1}{2\pi i} \oint_{C'_1} dz b(z) \left(\frac{z}{z - c_e q} + \frac{z}{z + c_e q} \right) \left(\frac{1}{z + x} - \frac{1}{z - x} \right), \end{aligned} \quad (\text{C.8})$$

where C'_1 is the contour enclosing the poles of the Bose function $b(z)$ counter-clockwise. Since the poles of $b(z)$ have weight -1 , the contour C'_1 can be replaced by the contour C_{11} which is clockwise oriented and encloses the first order poles at $c_e q$, $-c_e q$ and $\xi_k - \xi_{k-q}$. Hence, by the residue theorem we have

$$\begin{aligned} \frac{2I_1}{\tilde{g}} &= b(c_e q) c_e q \left(\frac{1}{c_e q + x} - \frac{1}{c_e q - x} \right) + (1 + b(c_e q)) c_e q \left(\frac{1}{-c_e q + x} - \frac{1}{-c_e q - x} \right) \\ &\quad - (1 + b(x)) x \left(\frac{1}{x + c_e q} + \frac{1}{x - c_e q} \right) - b(x) x \left(\frac{1}{x - c_e q} + \frac{1}{x + c_e q} \right) \\ &= \left[c_e q (1 + 2b(c_e q)) - x (1 + 2b(x)) \right] \frac{2x}{x^2 - (c_e q)^2} \\ &= 2 \frac{\coth(\frac{1}{2}\beta c_e q) c_e q x - \coth(\frac{1}{2}\beta x) x^2}{x^2 - (c_e q)^2}. \end{aligned} \quad (\text{C.9})$$

Similarly,

$$\frac{2I_2}{\tilde{g}} = 2 \frac{\coth(\frac{1}{2}\beta c_e q) c_e q y - \coth(\frac{1}{2}\beta y) y^2}{y^2 - (c_e q)^2}, \quad (\text{C.10})$$

which allows us to write

$$\begin{aligned} I &= \frac{\tilde{g}}{4\xi_k \xi_{k-q}} \left[\left(f(\xi_k) - f(\xi_{k-q}) \right) \frac{\coth(\frac{1}{2}\beta c_e q) c_e q x - \coth(\frac{1}{2}\beta x) x^2}{x^2 - (c_e q)^2} \right. \\ &\quad \left. - \left(f(\xi_k) + f(\xi_{k-q}) - 1 \right) \frac{\coth(\frac{1}{2}\beta c_e q) c_e q y - \coth(\frac{1}{2}\beta y) y^2}{y^2 - (c_e q)^2} \right]. \end{aligned} \quad (\text{C.11})$$

C.2 Density of states style diagram

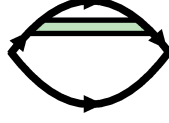


FIGURE C.2: Density of states style diagram arising in exchange channel fluctuation corrections to the BCS gap equation.

We wish to evaluate the Matsubara sum

$$J = T^2 \sum_{m,n} D_0(\mathbf{q}, i\Omega_m) G_0^2(\mathbf{k}, i\omega_n) G_0(\mathbf{k}, i\omega_m) G_0(\mathbf{k} - \mathbf{q}, i\omega_n - i\Omega_m) , \quad (\text{C.12})$$

so we first determine

$$\begin{aligned} \tilde{J}(i\Omega_m) &= T \sum_n G_0^2(\mathbf{k}, i\omega_n) G_0(\mathbf{k}, i\omega_m) G_0(\mathbf{k} - \mathbf{q}, i\omega_n - i\Omega_m) \\ &= \frac{f(\xi_{\mathbf{k}})}{(2\xi_{\mathbf{k}})(\xi_{\mathbf{k}} - \xi_{\mathbf{k}-\mathbf{q}} - i\Omega_m)^2} + \frac{f(\xi_{\mathbf{k}})}{(2\xi_{\mathbf{k}})^2(\xi_{\mathbf{k}} - \xi_{\mathbf{k}-\mathbf{q}} - i\Omega_m)} - \frac{f'(\xi_{\mathbf{k}})}{(2\xi_{\mathbf{k}})(\xi_{\mathbf{k}} - \xi_{\mathbf{k}-\mathbf{q}} - i\Omega_m)} \\ &\quad + \frac{1 - f(\xi_{\mathbf{k}})}{(2\xi_{\mathbf{k}})^2(\xi_{\mathbf{k}} + \xi_{\mathbf{k}-\mathbf{q}} + i\Omega_m)} - \frac{f(\xi_{\mathbf{k}-\mathbf{q}})}{(\xi_{\mathbf{k}} - \xi_{\mathbf{k}-\mathbf{q}} - i\Omega_m)^2(\xi_{\mathbf{k}} + \xi_{\mathbf{k}-\mathbf{q}} + i\Omega_m)} , \end{aligned} \quad (\text{C.13})$$

so that

$$J = \frac{f(\xi_{\mathbf{k}})}{2\xi_{\mathbf{k}}} J_1 + \left(\frac{f(\xi_{\mathbf{k}})}{(2\xi_{\mathbf{k}})^2} - \frac{f'(\xi_{\mathbf{k}})}{2\xi_{\mathbf{k}}} \right) J_2 + \frac{(1 - f(\xi_{\mathbf{k}}))}{(2\xi_{\mathbf{k}})^2} J_3 - f(\xi_{\mathbf{k}-\mathbf{q}}) J_4 , \quad (\text{C.14})$$

where

$$J_1 = T \sum_m D_0(\mathbf{q}, i\Omega_m) \frac{1}{(x - i\Omega_m)^2} \quad (\text{C.15})$$

$$J_2 = T \sum_m D_0(\mathbf{q}, i\Omega_m) \frac{1}{x - i\Omega_m} \quad (\text{C.16})$$

$$J_3 = T \sum_m D_0(\mathbf{q}, i\Omega_m) \frac{1}{y + i\Omega_m} \quad (\text{C.17})$$

$$J_4 = T \sum_m D_0(\mathbf{q}, i\Omega_m) \frac{1}{(x - i\Omega_m)^2 (y + i\Omega_m)} . \quad (\text{C.18})$$

Again, using

$$D_0(\mathbf{q}, i\Omega_m) = -\frac{\tilde{g}}{2} \left(\frac{i\Omega_m}{i\Omega_m - c_q q} + \frac{i\Omega_m}{i\Omega_m + c_q q} \right) \quad (\text{C.19})$$

we determine

$$\frac{2J_1}{\tilde{g}} = \frac{2c_e q (x^2 + (c_e q)^2) b(c_e q) - 4(c_e q)^2 x b(x) + c_e q (x - c_e q)^2 + 2x^2 (x^2 - (c_e q)^2) b'(x)}{(x^2 - (c_e q)^2)^2} \quad (\text{C.20})$$

$$\frac{2J_2}{\tilde{g}} = \frac{c_e q (x + 2xb(cq) - c_e q) - 2x^2 b(x)}{x^2 - (c_e q)^2} \quad (\text{C.21})$$

$$\frac{2J_3}{\tilde{g}} = \frac{c_e q (y + 2yb(cq) + c_e q) - 2y^2 (1 + b(y))}{y^2 - (c_e q)^2} \quad (\text{C.22})$$

$$\begin{aligned} \frac{2J_4}{\tilde{g}} = & \frac{c_e q b(c_e q)}{(x - c_e q)^2 (y + c_e q)} + \frac{c_e q (1 + b(c_e q))}{(x + c_e q)^2 (y - c_e q)} - \frac{2y^2 (1 + b(y))}{(y^2 - (c_e q)^2) (2\xi_{\mathbf{k}})^2} \\ & - \frac{2x \left((x^3 + (c_e q)^2 (x + 2y)) b(x) - x (x^2 - (c_e q)^2) (2\xi_{\mathbf{k}}) b'(x) \right)}{(x - c_e q)^2 (x + c_e q)^2 (2\xi_{\mathbf{k}})^2} . \end{aligned} \quad (\text{C.23})$$

C.3 Number equation correction

We wish to evaluate the Matsurbara sum

$$K = T^2 \sum_n D_0(\mathbf{q}, i\Omega_m) G_0^2(\mathbf{k}, i\omega_n) G_0(\mathbf{k} - \mathbf{q}, i\omega_n - i\Omega_m) , \quad (\text{C.24})$$

so we first calculate

$$\begin{aligned} \tilde{K}(i\Omega_m) &= I \sum_n G_0^2(\mathbf{k}, i\omega_n) G_0(\mathbf{k} - \mathbf{q}, i\omega_n - i\Omega_m) \\ &= \frac{1}{2\pi i} \oint_C dz \frac{f(z)}{(z - \xi_{\mathbf{k}})(z - i\Omega_m - \xi_{\mathbf{k} - \mathbf{q}})} \\ &= \frac{f'(\xi_{\mathbf{k}})}{i\Omega_m - x} - \frac{f(\xi_{\mathbf{k}}) - \xi_{\mathbf{k} - \mathbf{q}}}{(i\Omega_m - x)^2} , \end{aligned} \quad (\text{C.25})$$

where C is counter-clockwise oriented around the poles at $\xi_{\mathbf{k}}$ and $i\Omega_m + \xi_{\mathbf{k}}$. We now have

$$\begin{aligned} K &= T \sum_m \int dz D_0(\mathbf{q}, i\Omega_m) \left(\frac{f'(\xi_{\mathbf{k}})}{i\Omega_m - x} - \frac{f(\xi_{\mathbf{k}}) - f(\xi_{\mathbf{k}-\mathbf{q}})}{(i\Omega_m - x)^2} \right) \\ &= f'(\xi_{\mathbf{k}})K_1 + \left(f(\xi_{\mathbf{k}}) - f(\xi_{\mathbf{k}-\mathbf{q}}) \right) K_2, \end{aligned} \quad (\text{C.26})$$

where

$$\begin{aligned} \frac{2K_1}{\tilde{g}} &= T \sum_m D_0(\mathbf{q}, i\Omega_m) \frac{1}{i\Omega_m - x} \\ &= \frac{2x^2 b(x) + (c_e q)^2 - x c_e q (1 - 2b(c_e q))}{x^2 - (c_e q)^2}, \end{aligned} \quad (\text{C.27})$$

and

$$\begin{aligned} \frac{2K_2}{\tilde{g}} &= -T \sum_m D_0(\mathbf{q}, i\Omega_m) \frac{1}{(i\Omega_m - x)^2} \\ &= \frac{2x b'(x)}{x^2 - (c_e q)^2} + \frac{c_e q \left((x - c_e q)^2 + 2(x^2 + (c_e q)^2) b(c_e q) - 4c_e q b(x) \right)}{(x^2 - (c_e q)^2)^2}. \end{aligned} \quad (\text{C.28})$$