Approaching the Thermodynamic Limit in BCS Theory

by

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We investigate the problem of simulating infinite superfluid neutron matter using finite systems. With a view to guiding a Quantum Monte Carlo simulation, we study the effects of finite volume on calculations of quantities of finite superfluid systems such as the pairing Gap, the chemical potential and the energy. We present a review of the theory of BCS along with a review of the theories that have been formulated to extend BCS to finite systems, namely Projected BCS (PBCS) and Full BCS (FBCS). In the context of BCS and PBCS we perform calculations of the pairing Gap, the chemical potential and the energy of finite superfluid systems of neutrons at densities relevant to the inner crust of neutron stars. From those calculations we study the approach of a finite volume of superfluid neutrons to the Thermodynamic Limit (TL). Finally, ways to alleviate the Finite Size effects using Twisted Periodic Boundary Conditions are proposed.
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Chapter 1

Introduction

1.1 Neutron Matter

Neutron matter is a nuclear system with applications in many different areas of physics. The inner crust of neutron stars consists of a lattice of heavy nuclei filled with a sea of neutrons and a roughly uniform sea of electrons [1]. These neutrons, being at a density slightly before the nuclear saturation density \( n_0 = 0.16 \text{ fm}^{-3} \) where the neutron-neutron interaction is attractive through the \( ^1S_0 \) channel, they form a superfluid. In the physics of neutron-rich nuclei, density functionals are used to describe the extreme isospin imbalance limit. While, typically, these density functionals are constrained by heavy nuclei, in the extreme isospin imbalance region they are less constrained [2]. It has also been shown that the equation of state (EoS) of neutron matter can be used to eliminate unphysical density functionals [3]. The unitary regime of a Fermi gas is the regime where the s-wave scattering length \( a \) is large compared to the interparticle spacing [4]. In this regime all interaction length scales drop out of the problem and the gas experiences universal behaviour which depends only on the dimensionless parameter \( k_F a \). Feshbach resonances [5, 6] in ultra cold atom
experiments have the ability to probe the properties of those systems and indirectly the properties of a neutron gas in the same regime [7]. Moreover, critical properties of neutron stars such as the mass-radius relationship and the maximum mass of the star are closely related to the EoS of high-density, low-temperature neutron matter. At the same time, an EoS at the same densities can compare different approaches to the nuclear Hamiltonian since, in this regime several channels of the nucleon-nucleon interaction become relevant. Finally, recent gravitational signals have been observed from neutron star mergers. The efforts to theoretically interpret those signals have resulted in constraints on the EoS of dense matter [8, 9, 10, 11, 12, 13] which in turn, as outlined above, can update, validate or invalidate nuclear models.

It is evident that neutron matter is a deeply intriguing nuclear system that extends to multiple disciplines of physics, from condensed matter, to nuclear physics and astrophysics. As a fermionic system, one of its most important features is pairing which is responsible for interesting properties of nuclei and neutron stars alike. Neutron pairing increases the stability of nuclei with even particle number as well as it can reduce the moment of inertia of a nucleus. In neutron stars pairing is manifested in the inner crust where neutron pairs form a superfluid [14]. This superfluid is believed to be responsible for pulsar glitches [15] and it plays a role in the cooling of the star [16].

1.2 Periodic Boundary Conditions and Finite Size Effects

Neutron matter like the one found in the interior of neutron stars is, effectively, an infinite system and as such its simulation is not a trivial task. The most common
approach consists of one simulating a finite version of the system (e.g., a cubic box) to which they employ periodic boundary conditions (PBC). The PBC make the system “see” its self around it and eventually we end up with an infinite collection of identical copies of the initial finite system which serves as an approximation of the infinite system. Clearly the bigger the initial finite system the better the approximation of the infinite system. Therefore as the simulation volume increases all intensive quantities of the system tend to their Thermodynamic Limit (TL) value. However, the trend in the way that they do so is not trivial. This quasi-random error introduced by the volume of the simulation box is referred to as the Finite-Size (FS) effects. In Figure 1.1 we see such effects in the energy of a free Fermi gas. One can see that there are special $N$ values around which FS effects become minimum. That is happening near $N = 2, 14, 38, 54, 66, 114, \ldots$ where the free Fermi gas has enough particles to completely fill an energy level (shell closure). This effect comes from the fact that the wavefunction becomes ambiguous when the number of particles is not enough to completely fill an energy level (not a shell closure) since the particles in the unfilled level can be re-arranged to yield the same energy. In other words, due to the energy degeneracy, the wavefunction of a free Fermi gas not at shell closure is not well-defined. The unique existence of particle configurations at shell closure, along with its effect on the Finite-Size effects, motivates the study at those special $N$ values.

We do not always have the luxury of large simulation volumes. Quantum Monte Carlo (QMC) techniques, which have been used extensively to extract properties of neutron matter, scale unfavorably with the number of particles and, therefore, one is usually restricted to simulations of a few hundreds of particles. A technique that has been used [17] to alleviate the Finite Size effects is that of the Twisted Boundary Conditions (TBC) or the Twisted Averaged Boundary (TABC) Conditions. In this
Figure 1.1: FS dependence of the non-interacting free-Fermi gas. FS effects go to zero in the TL. The minimum at $N = 67$ motivates a study at the closed shell $N = 66$. the inset shows the same relationship on a linear scale.

technique one observes that the periodic boundary conditions require from the moduli of the wavefunction to be equal on opposite sides of the simulation volume leaving room for an arbitrary phase difference (referred to as a twist) between the actual values of the wavefunction. For a cubic box:

$$\psi(x + L\hat{x}, y, z) = e^{i\theta x}\psi(x, y, z)$$

This twist ends up in the quantization condition for the momenta:

$$k = \frac{2\pi}{L} n + \frac{\theta_i}{L}, \quad \text{where} \quad -\pi \leq \theta_i \leq \pi, \quad i = x, y, z$$  (1.1)
We can see that by taking the limit of $L \to \infty$ and making the cubic box an infinite system, this twist drops out of the problem showing explicitly that it is not an observable of the infinite system. The method of the TBC or TABC relies on manipulating this twist to reduce finite size effects. Especially, for TABC, one observes from Eq. 1.1 that every given $k$ can be reached by a unique combination of $(n, \theta$. This means that by averaging over all possible $\theta$ the $k$-lattice, that we would have with PBCS, turns into a ”solid volume” bounded by a Fermi surface. The volume inside the Fermi surface would be $\Omega = (2\pi)^3 \frac{B}{L^3} = (2\pi)^3 \rho$ equal to the one corresponding to the system in the TL. Therefore, by twist-averaging our wave functions we expect to minimize the FS effects that arise from the quantization of the momenta by PBC.

There are a other ways that one can manipulate this twist

- special values of this twist can be used
- the twist can be a dynamical variable which leads to the dynamical twist averaged boundary conditions (DTBC)

None of these methods is the right one in general. The right choice is problem dependent.
Chapter 2

The BCS Theory of Superconductivity

2.1 The BCS Ground State

The Ground State A system of unpolarized fermions can become unstable under the formation of Cooper pairs. That is, given an infinitesimally small attractive interaction the fermions condensate forming a ground state of energy lower than that of the ground state of the non-interacting system. This ground state is called the BCS ground state after Bardeen, Cooper and Schrieffer who proposed it in 1957 and is expressed mathematically as:

$$|\psi_{BCS}\rangle = \prod_k (u_k + v_k \hat{c}_{k\uparrow}^{\dagger} \hat{c}_{-k\downarrow}^{\dagger}) |0\rangle$$

(2.1)

where $|0\rangle$ is the vacuum state and $\hat{c}_{k\sigma}^{\dagger}, \hat{c}_{k\sigma}$ are Fermi operators which create or annihilate, respectively, a fermion with momentum $k$ and $\sigma$. These operators follow the Fermi anti-commutation relations:
\[ \{ \hat{c}_{k\sigma}, \hat{c}^\dagger_{k'\sigma'} \} = \delta_{kk'} \delta_{\sigma\sigma'} \]

\[ \{ \hat{c}_{k\sigma}, \hat{c}_{k'\sigma'} \} = 0 \quad (\text{Com I}) \]

The quantities \( v_k \) and \( u_k \) are the probability amplitudes to find the pair state \( k \) occupied and unoccupied respectively. As such they are, in principle, complex numbers that obey the constraint:

\[ |u_k|^2 + |v_k|^2 = 1 \tag{2.2} \]

This constraint expresses a conservation of probability: “the pair state \( k \) can be found either occupied or unoccupied”.

These two complex functions of \( k \) uniquely define the BCS ground state and can be determined by minimizing the Free Energy of the system:

\[ F_{BCS} = \langle \hat{H} - \mu_{ch} \hat{N} \rangle_{BCS} = \langle \psi_{BCS} | \hat{H} - \mu_{ch} \hat{N} | \psi_{BCS} \rangle \tag{2.3} \]

where \( \mu_{ch} \) is the chemical potential, \( \hat{N} \) is the number operator and \( \hat{H} \) is the Hamiltonian of the system. It is hinted at this point, by the existence of \( \mu_{ch} \), that the BCS ground state is defined in a grand canonical ensemble. In other words, \( |\psi_{BCS}\rangle \) is not an eigenstate of the number operator \( \hat{N} \). However, one can expand \( |\psi_{BCS}\rangle \) in eigenstates of \( \hat{N} \):

\[ |\psi_{BCS}\rangle = \sum_N \lambda_N |\psi_N\rangle \]
where for each of those eigenstates [18]

$$|\psi_N\rangle = \hat{P}_N |\psi_{BCS}\rangle = \oint dz z^{-\frac{N}{2}} \prod_{k} \left( u_k + z v_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger \right) |0\rangle$$

The derivation of the above expression as well as properties and further analysis of those states can be found in chapter 3.

2.1.1 Single Particle Energy, Hamiltonian & Interaction

In order to minimize the Free Energy (2.3) one has to write the Hamiltonian of the System. We will only consider the pairing Hamiltonian:

$$\hat{H} = \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{kl} V_{kl} c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger c_{-l\downarrow} c_{l\uparrow}$$

where:

- $\epsilon_k$ is the single particle kinetic energy $\frac{\hbar^2}{2m} |k|^2$. The momentum $k$ will be, in principle, quantized in a manner dependent on the boundary conditions except for the case of an infinite system (see chapter 4). Following the analysis of section 1.2 we employ periodic boundary conditions leading to the following quantization of the momenta:

$$k = \frac{2\pi}{L} \left( n + \frac{\theta}{2\pi} \right)$$

where $\theta$ is the Twist that was introduced in section 1.2. Finally:
\[ \epsilon_k = \frac{\hbar}{2m} \left| \frac{2\pi}{L} (n + \frac{\theta}{2\pi}) \right|^2 = \frac{2\pi^2 \hbar}{mL^2} \left| n + \frac{\theta}{2\pi} \right|^2 \]

- \( V_{kl} \) is the matrix element of the pairing potential:

\[ V_{kl} = (k, -k| \hat{V} | l, -l) \]

For convenience we can also define the pair annihilation and creation operators:

\[ \hat{p}_k \equiv \hat{c}_{-k\downarrow}^\dagger \hat{c}_{k\uparrow} \]
\[ \hat{p}_k^\dagger \equiv \hat{c}_{k\uparrow}^\dagger \hat{c}_{-k\downarrow} \]

where \( \hat{p}_k \) annihilates a pair of particles on state \( k \) while \( \hat{p}_k^\dagger \) creates a pair of particles on state \( k \). These operators have the following \textit{quasi-bosonic} commutation relations:

\[ [\hat{p}_k^\dagger, \hat{p}_l^\dagger] = M_k \delta_{kl} \]
\[ [\hat{p}_k^\dagger, \hat{p}_l] = [\hat{p}_k, \hat{p}_l^\dagger] = 0 \quad \text{(Com I)} \]

where \( \delta_{kl} \) is the Kronecker Delta function which is 1 for \( k = l \) and 0 otherwise.

Using these new operators, the BCS ground state is written as:

\[ |\psi_{BCS}\rangle = \prod_k (u_k + v_k \hat{p}_k^\dagger) |0\rangle \quad (2.4) \]

while the Hamiltonian is written as:
\[ \hat{H} = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{kl} V_{kl} \hat{p}^\dagger_k \hat{p}_l \]

With this Hamiltonian the Energy is:

\[ \langle \mathcal{H} \rangle_{BCS} = \langle \psi_{BCS} | \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{kl} V_{kl} \hat{p}^\dagger_k \hat{p}_l | \psi_{BCS} \rangle = \sum_{k\sigma} \epsilon_k v_k^2 + \sum_{kl} V_{kl} u_k^* v_k^* v_l = (2.5) \]
\[ = \sum_{k\sigma} \epsilon_k v_k^2 + \sum_{kl} V_{kl} u_k v_k u_l v_l = (2.6) \]
\[ = \sum_{k\sigma} \epsilon_k v_k^2 + \sum_{kl} V_{kl} u_k v_k u_l v_l = (2.7) \]

The derivation can be found in Appendix A. We have taken \( v_k \) and \( u_k \) to be real functions of \( k \) ignoring a phase difference between them. It will be seen in chapter 3 that introducing this phase difference is important only to the use of projection operators.

### 2.1.2 The Variational Method and The BCS Gap Equations

Having chosen the interaction, the parameters \( v_k \) and \( u_k \) of the ground state are found by minimizing the quantity (2.3) under the constraint (2.2). We will use the variational method where we define an angle \( \theta_k \) so that:

\[ u_k = \sin \theta_k \]
\[ v_k = \cos \theta_k \]

Now the constraint (2.2) is automatically satisfied and the energy can be written in terms of \( \theta_k \) by direct substitution in Eq. (2.7):
\[ \langle \mathcal{H} \rangle_{BCS} = \sum_{k\sigma} \epsilon_k \cos^2 \theta_k + \sum_{kl} V_{kl} \sin \theta_k \cos \theta_l \cos \theta_l + \sum_{kl} V_{kl} \sin \theta_k \cos \theta_l \sin \theta_l \cos \theta_l \]

and the Free Energy:

\[ \mathcal{F} = \langle \mathcal{H} - \mu_{ch} \hat{N} \rangle_{BCS} = \langle \psi_{BCS} | \mathcal{H} - \mu_{ch} \hat{N} | \psi_{BCS} \rangle = \]

\[ = \langle \psi_{BCS} | \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{kl} V_{kl} \hat{c}_{k\uparrow}^\dagger \hat{c}_{-k\downarrow}^\dagger \hat{c}_{-k\downarrow} \hat{c}_{k\uparrow} - \mu_{ch} \sum_{k\sigma} \hat{n}_{k\sigma} | \psi_{BCS} \rangle = \]

\[ = \langle \psi_{BCS} | \sum_{k\sigma} (\epsilon_k - \mu_{ch}) \hat{n}_{k\sigma} + \sum_{kl} V_{kl} \hat{c}_{k\uparrow}^\dagger \hat{c}_{-k\downarrow}^\dagger \hat{c}_{-k\downarrow} \hat{c}_{k\uparrow} | \psi_{BCS} \rangle = \]

\[ = \langle \psi_{BCS} | \sum_{k\sigma} \xi_k \hat{n}_{k\sigma} + \sum_{kl} V_{kl} \hat{c}_{k\uparrow}^\dagger \hat{c}_{-k\downarrow}^\dagger \hat{c}_{-k\downarrow} \hat{c}_{k\uparrow} | \psi_{BCS} \rangle = \]

\[ = \sum_{k\sigma} \xi_k v_k^2 + \sum_{kl} V_{kl} u_k v_k u_l v_l = \sum_{k\sigma} \xi_k \cos^2 \theta_k + \sum_{kl} V_{kl} \sin \theta_k \cos \theta_k \sin \theta_l \cos \theta_l \]

where we have defined \( \xi_k \equiv \epsilon_k - \mu_{ch} \). We see that the Free Energy of the state is equal to the energy of the system where the single particle kinetic energies are measured from the chemical potential \( \mu_{ch} \). Minimizing the Free Energy with respect to \( \theta_k \):

\[ \frac{\partial}{\partial \theta_k} \mathcal{F} = 0 \quad \forall k \Rightarrow \]

\[ \tan 2\theta_k = \frac{2 \sum_1 V_{kl} \sin 2\theta_l}{2\xi_k} \]

or

\[ \Delta_k = -\frac{1}{2} \sum_1 V_{kl} \Delta_l \frac{\Delta_l}{E_l} \]

where we have defined the quantities:
∆_k ≡ −ξ_k \tan 2θ_k = − \sum_1 V_{kl} u_l v_l = − \frac{1}{2} \sum_1 V_{kl} \sin 2θ_l

E_k ≡ \sqrt{ξ_k^2 + ∆_k^2}

∆_k is called the Gap Function while E_k is called the quasi-particle excitation energy and it is equal to the energy required to destroy a pair in the state k. Using those and trigonometric identities we can write:

\[ \sin 2θ_k = 2v_k u_k = \frac{∆_k}{E_k} \]
\[ \cos 2θ_k = v_k^2 - u_k^2 = -\frac{ξ_k}{E_k} \]

The first equation (along with the definition of ∆_k above) chooses a sign for the product v_k u_k since \( \frac{∆_k}{E_k} > 0 \). Alternatively, we could have defined ∆_k = − tan 2θ_k which would have led to a minus sign on the right hand side of the first equation above. The last of the equations above combined with the constraint (2.2) gives v_k and u_k as a function of the quasi-particle excitation energy and, therefore, the Gap:

\[ v_k = \left[ \frac{1}{2} \left( 1 - \frac{ξ_k}{E_k} \right) \right]^{1/2} \]
\[ u_k = \left[ \frac{1}{2} \left( 1 + \frac{ξ_k}{E_k} \right) \right]^{1/2} \]

However, as mentioned before, the BCS ground state is defined in a grand canonical ensemble which means that the above Gap equation has to be solved simultaneously with the constraint:
\[
\langle N \rangle = \sum_k 2v_k^2 = \sum_k \left( 1 - \frac{\xi_k}{E_k} \right)
\]

Bundling together the Gap equation with the constraint we arrive at what is usually referred to as the \textit{BCS Gap Equations}:

\[
\Delta_k = -\frac{1}{2} \sum_l V_{kl} \frac{\Delta_l}{E_l}
\]

\[\text{(2.11)}\]

\[
\langle N \rangle = \sum_k \left( 1 - \frac{\xi_k}{E_k} \right)
\]

\[\text{(2.12)}\]

The Eqs. (2.11) \& (2.12) are a set of coupled non linear equations. The unknowns are the Gap Distribution \(\Delta_k\) and the chemical potential \(\mu_{ch}\).

We can already see that the BCS ground state is not a state of a fixed particle number or in other words it is not an eigenstate of the number operator \(\hat{N} = \sum_{k\sigma} \hat{c}_{k\sigma}^\dagger \hat{c}_{k\sigma}\). Intuitively that can be understood from the fact that, in contrast with a free Fermi gas at \(T = 0 K\), the occupation of the states in the BCS ground state is fractional. That means that in the BCS ground state a \(k\) state is filled with a probability \(v_k^2\) or empty with a probability of \(u_k^2\) while in a free Fermi gas at \(T = 0 K\) any state with \(|k| < k_F\) is occupied with probability 1 and states with \(|k| > k_F\) have 0 probability to be found occupied. Since \(|\psi_{BCS}\rangle\) is not an eigenstate of the number operator it can be expressed on the basis of those eigenstates yielding a spectrum of eigenvalues \(\lambda_N\):

\[
|\psi_{BCS}\rangle = \sum_N \lambda_N |\psi_N\rangle
\]

\[\text{(2.13)}\]
This decomposition can be directly derived from the definition of the BCS ground state:

\[
|\psi_{BCS}\rangle = \prod_k \left( u_k + v_k \hat{c}_k^\dagger \hat{c}_{-k}^\dagger \right) |0\rangle
\]

by carrying out the product:

\[
|\psi_{BCS}\rangle = \prod_k \left( u_k + v_k \hat{p}_k^\dagger \right) |0\rangle
= \left( u_{k_1} + v_{k_1} \hat{p}_{k_1}^\dagger \right) \left( u_{k_2} + v_{k_2} \hat{p}_{k_2}^\dagger \right) \cdots \left( u_{k_{I/2}} + v_{k_{I/2}} \hat{p}_{k_{I/2}}^\dagger \right) |0\rangle = \\
= \prod_i u_{k_i} + \sum \prod_{i \neq j} v_{k_j} u_{k_i} \hat{p}_{k_j}^\dagger |0\rangle + \sum \prod_{m,n|m \neq n, i \neq n,m} v_{k_n} v_{k_m} u_{k_i} \hat{p}_{k_n}^\dagger \hat{p}_{k_m}^\dagger |0\rangle + \cdots = \\
= \lambda_0 |\psi_0\rangle + \lambda_2 |\psi_2\rangle + \lambda_4 |\psi_4\rangle \ldots
\]

which eventually leads to:

\[
\lambda_N |\psi_N\rangle = \sum_{\{l_1, \ldots, l_N\} k \notin \{l_1, \ldots, l_N/2\}} \prod_{i \in \{l_1, \ldots, l_N/2\}} u_{k_i} \prod_{l \in \{l_1, \ldots, l_N/2\}} v_{l} \hat{p}_{l}^\dagger |0\rangle \tag{2.14}
\]

where the sum \(\sum_{\{l_1, \ldots, l_N\}}\) runs over all possible sets of states \(l\) that contain \(N\) number of elements and \(\lambda_N\), as we show later, is related to the normalization of \(|\psi\rangle\). Finally, \(|\psi_{BCS}\rangle\) only contains components with an even number of particles. That can be seen in Eq. (2.1) where each term of the product in the right hand side creates a pair of particles on a specific \(k\) state. We can describe a system with an odd number of particles \(N + 1\) by considering the extra particle as a particle that will be residing on a \(k\)-state blocking it for any pairs to occupy the state. Mathematically that can be formulated as:
\[ |\psi_{BCS}^{b\gamma}\rangle = \hat{c}_{b\gamma}^\dagger \prod_{k \neq b} (u_k + v_k \hat{p}_k) |0\rangle \]  \hspace{1cm} (2.15)

We can expand the product the same way we did for the even case:

\[
\begin{align*}
|\psi_{BCS}^{b\gamma}\rangle &= \hat{c}_{b\gamma}^\dagger \prod_{k \neq b} (u_k + v_k \hat{p}_k) |0\rangle = \\
&= \hat{c}_{b\gamma}^\dagger (u_{k_1} + v_{k_1} \hat{p}_{k_1}^\dagger) (u_{k_2} + v_{k_2} \hat{p}_{k_2}^\dagger) \ldots (u_{k_i} + v_{k_i} \hat{p}_{k_i}^\dagger) \ldots |0\rangle = \\
&= \hat{c}_{b\gamma}^\dagger \prod_i u_{k_i} + \sum_j \prod_{i \neq j} v_{k_j} u_{k_i} \hat{p}_{k_j}^\dagger |0\rangle + \\
&\quad + \sum_{m,n|m \neq n,i \neq n,m} \prod v_{k_i} u_{k_m} v_{k_n} \hat{p}_{k_n}^\dagger \hat{p}_{k_m}^\dagger |0\rangle \ldots = \\
&= \hat{c}_{b\gamma}^\dagger (\lambda_0 |\psi_0\rangle + \lambda_2 |\psi_2\rangle + \lambda_4 |\psi_4\rangle \ldots )
\end{align*}
\]

and similarly:

\[
\lambda_{N+1} |\psi_{N+1}^{b\gamma}\rangle = \hat{c}_{b\gamma}^\dagger \sum_{\{l_1, \ldots, l_N\} \neq \{1, \ldots, l_{N/2}\}} \prod_{k \neq \{1, \ldots, l_{N/2}\}} u_{k_i} \prod_{l \in \{1, \ldots, l_{N/2}\}} v_{l_1} \hat{p}_{l_1}^\dagger |0\rangle \]  \hspace{1cm} (2.16)
Chapter 3

Restoring Particle Number

Conservation in BCS Theory

3.1 States that conserve Particle Number

The BCS ground state is not an eigenstate of the number operator and therefore it cannot describe a superfluid system with a fixed number of particles $N$. In order to describe such systems we need to restore the particle number conservation in the BCS ground state. A segue into the restoration of particle number conservation is to derive expression 2.14 making use of Projection operators. We begin by backtracking on the claim that $v_k$ and $u_k$ can be taken to be functions of $k$. For this section we will regard them as complex ones which can be written as:

\[
v_k = |v_k| e^{i\phi_v}
\]
\[
u_k = |u_k| e^{i\phi_u}
\]
It is worth noting that the BCS ground state is a coherent state of Cooper pairs and it should, therefore, have a well defined quantum phase. This case allows us to claim that the phases $\phi_v$ and $\phi_u$ are not dependent on $k$. Therefore $|\psi_{BCS}\rangle$ can be written as:

$$|\psi_{BCS}\rangle = \prod_k \left( |u_k|e^{i\phi_u} + |v_k|e^{i\phi_v} \hat{p}_k^\dagger \right) |0\rangle = e^{i\phi_u} \prod_k \left( |u_k| + |v_k|e^{i(\phi_v - \phi_u)} \hat{p}_k^\dagger \right) |0\rangle$$

For convenience, we can rename the magnitudes $|u_k|$ and $|v_k|$ as simply $u_k$ and $v_k$. The overall phase in front of the wave function does not have any physical significance since it is not an observable and therefore can be set to 0. Finally, renaming $\phi \equiv \phi_v - \phi_u$ we get:

$$|\psi_{BCS}\rangle = \prod_k \left( u_k + v_k e^{i\phi} \hat{p}_k^\dagger \right) |0\rangle$$

(3.1)

Now we can define the projection operator:

$$\hat{P}_N = \int \frac{d\phi}{2\pi} e^{-i\frac{N}{2}\phi}$$

which will project out the $N$-th term of the sum in Eq. (2.13). The motivation for that comes from observing that after giving a phase to $v_k$, if we were to carry out the derivation that led to Eq. 2.14, our decomposition of $|\psi_{BCS}\rangle$ into eigenstates of $\hat{N}$ would be:

$$|\psi_{BCS}\rangle = \prod_i u_{ki} + \sum_j \prod_{i\neq j} v_{kj} e^{i\phi} u_{ki} \hat{p}_{kj}^\dagger |0\rangle$$

(3.2)
$$+ \sum_{m,n|m \neq n} \prod_{i \neq n,m} v_{k_n} v_{k_m} e^{i2\phi} u_{k_i} \hat{p}_{k_n} \hat{p}_{k_m}^\dagger |0\rangle + \cdots =$$

$$= \lambda_0 |\psi_0\rangle + \lambda_2 e^{i\phi} |\psi_2\rangle + \lambda_4 e^{i2\phi} |\psi_4\rangle \ldots (3.3)$$

since every $v_k$ in those products carries a phase. We see that the $N$-th component of the above sum will have a product of $N/2$ phases making the decomposition eventually:

$$|\psi_{BCS}\rangle = \sum_{N} \lambda_N e^{i\frac{N}{2}\phi} |\psi_N\rangle$$

Multiplying with $e^{-i\frac{N}{2}\phi}$ and integrating over $[0, 2\pi]$ we get:

$$\int \frac{d\phi}{2\pi} e^{-i\frac{N}{2}\phi} |\psi_{BCS}\rangle = \int \frac{d\phi}{2\pi} e^{-i\frac{N}{2}\phi} \left[ \sum_{N'} \lambda_{N'} e^{i\frac{N'}{2}\phi} |\psi_{N'}\rangle \right] =$$

$$= \sum_{N'} \int \frac{d\phi}{2\pi} \lambda_{N'} e^{i\frac{N'-N}{2}\phi} |\psi_{N'}\rangle =$$

$$= \sum_{N'} \lambda_{N'} \int \frac{d\phi}{2\pi} e^{i\frac{N'-N}{2}\phi} |\psi_{N'}\rangle =$$

$$= \sum_{N'} \lambda_{N'} \delta_{NN'} |\psi_{N'}\rangle = \lambda_N |\psi_N\rangle$$

where we used one of the representations of the Kronecker Delta function:

where $n, n' \in \mathcal{Z}$. Finally:

$$|\psi_N\rangle = \frac{1}{\lambda_N} \int \frac{d\phi}{2\pi} e^{-i\frac{N}{2}\phi} |\psi_{BCS}\rangle (3.4)$$

As mentioned above, $\lambda_N$ will prove to be related to the normalization of $|\psi_N\rangle$. Indeed, taking the inner product of (3.4) with itself we get:
\[
\langle \psi_N | \psi_N \rangle = \frac{1}{\lambda_N^2} \int \frac{d\phi_1}{2\pi} e^{-i\frac{N}{2} \phi_1} \langle \psi_{BCS} | \int \frac{d\phi_2}{2\pi} e^{-i\frac{N}{2} \phi_2} | \psi_{BCS} \rangle = \\
\frac{1}{\lambda_N^2} \int \frac{d\phi_1}{2\pi} \int \frac{d\phi_2}{2\pi} e^{-i\frac{N}{2} (\phi_2 - \phi_1) \times} \\
\times \langle 0 | \prod \left( u_1 + v_1 e^{-i\phi_1} \hat{p}_1 \right) \prod \left( u_k + v_k e^{i\phi_2} \hat{p}_k \right) | 0 \rangle = \\
\frac{1}{\lambda_N^2} \int \frac{d\phi_1}{2\pi} \int \frac{d\phi_2}{2\pi} e^{-i\frac{N}{2} (\phi_2 - \phi_1) \times} \\
\times \langle 0 | \prod \left( u_k + v_k e^{-i\phi_1} \hat{p}_k \right) \left( u_k + v_k e^{i\phi_2} \hat{p}_k \right) | 0 \rangle = \\
\frac{1}{\lambda_N^2} \int \frac{d\phi_1}{2\pi} \int \frac{d\phi_2}{2\pi} e^{-i\frac{N}{2} (\phi_2 - \phi_1) \times} \\
\times \langle 0 | \prod \left( u_k^2 + u_k v_k e^{i\phi_2} \hat{p}_k + u_k v_k e^{i\phi_1} + v_k^2 e^{i(\phi_2 - \phi_1)} \hat{p}_k \hat{p}_k^\dagger \right) | 0 \rangle = \\
\frac{1}{\lambda_N^2} \int \frac{d\phi_1}{2\pi} \int \frac{d\phi_2}{2\pi} e^{-i\frac{N}{2} (\phi_2 - \phi_1) \times} \prod \left( u_k^2 + v_k^2 e^{i(\phi_2 - \phi_1)} \right)
\]

since (see Appendix A):

\[
\langle 0 | \hat{p}_k | 0 \rangle = \langle 0 | \hat{p}_k^\dagger | 0 \rangle = 0 \\
\langle 0 | \hat{p}_k \hat{p}_k^\dagger | 0 \rangle = 1
\]

We perform the change of variables:

with the Jacobian:

\[
|J| = \left| \frac{\partial (\phi_1, \phi_2)}{\partial (\varphi, \psi)} \right| = \left| \det \left( \begin{array}{cc} \frac{\partial \phi_1}{\partial \varphi} & \frac{\partial \phi_2}{\partial \varphi} \\ \frac{\partial \phi_1}{\partial \psi} & \frac{\partial \phi_2}{\partial \psi} \end{array} \right) \right| = \left| \det \left( \begin{array}{cc} -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{array} \right) \right| = \frac{1}{4} - \frac{1}{4} = \frac{1}{2}
\]

For the bounds:
\[ \phi_1 = 0 \iff \frac{1}{2} (\psi - \varphi) = 0 \Rightarrow \psi = \varphi \]
\[ \phi_1 = 2\pi \iff \frac{1}{2} (\psi - \varphi) = 2\pi \Rightarrow \psi = 4\pi + \varphi \]
\[ \phi_2 = 0 \iff \frac{1}{2} (\psi + \varphi) = 0 \Rightarrow \psi = -\varphi \]
\[ \phi_2 = 2\pi \iff \frac{1}{2} (\psi + \varphi) = 2\pi \Rightarrow \psi = 4\pi - \varphi \]

Graphically, this translates to a rotation of the initial integration domain and a scaling up of a factor of 2. With the new variables the integral becomes:

\[ \langle \psi_N | \psi_N \rangle = \frac{1}{\lambda_N^2} \left[ \int_{-2\pi}^{0} d\varphi \int_{-\varphi}^{4\pi + \varphi} d\psi \frac{1}{2\pi} e^{-i \frac{N}{2} \varphi} \prod_k (u_k^2 + v_k^2 e^{i\psi}) + \right. \\
\left. + \int_0^{2\pi} d\varphi \int_{\varphi}^{4\pi - \varphi} d\psi \frac{1}{2\pi} e^{-i \frac{N}{2} \varphi} \prod_k (u_k^2 + v_k^2 e^{i\psi}) \right] = \\
= \frac{1}{8\pi^2 \lambda_N^2} \left[ \int_{-2\pi}^{0} d\varphi 2(2\pi + \varphi) e^{-i \frac{N}{2} \varphi} \prod_k (u_k^2 + v_k^2 e^{i\varphi}) + \right. \\
\left. + \int_0^{2\pi} d\varphi 2(2\pi - \varphi) e^{-i \frac{N}{2} \varphi} \prod_k (u_k^2 + v_k^2 e^{i\varphi}) \right] = \\
= \frac{1}{4\pi^2 \lambda_N^2} \left[ \int_{0}^{2\pi} d\omega \omega e^{-i \frac{N}{2} (\omega - 2\pi)} \prod_k (u_k^2 + v_k^2 e^{i(\omega - 2\pi)}) + \right. \\
\left. + \int_0^{2\pi} d\varphi (2\pi - \varphi) e^{-i \frac{N}{2} \varphi} \prod_k (u_k^2 + v_k^2 e^{i\varphi}) \right] \\
\]

where we performed the following additional change of variables in the first integral:

\[ \omega \equiv 2\pi + \varphi \iff \varphi = \omega - 2\pi \quad \text{and} \quad d\omega = d\varphi, \]

\[ (\varphi_1 = -2\pi, \varphi_2 = 0) \rightarrow (\omega_1 = 0, \omega_2 = 2\pi) \]

At this point we observe that only terms even in \( N \) will show up in the expansion
(2.13). That means that $\frac{N}{2}$ in the exponents above is an integer. That is an artifact of the fact that the product in the state (3.1) essentially adds pairs on $k$ states with a probability amplitude of $v_k$ and because of that this state can only describe systems with an even number of particles. We see later how that gives rise to the theory of blocked states as an attempt to describe a ground state for systems with an odd particle number. For now we will only use the fact that $\frac{N}{2} \in \mathbb{Z}$ to simplify the first integral since:

$$e^{-i \frac{N}{2} (\omega - 2 \pi)} = e^{i \frac{N}{2} \omega} e^{i \frac{N}{2} 2 \pi}$$

Using that and renaming the dummy variable of the first integral from $\omega$ back to $\varphi$ we get:

$$\langle \psi_N | \psi_N \rangle = \frac{1}{4 \pi^2 \lambda_N^2} \left[ \int_{-2\pi}^{0} d\varphi e^{i \frac{N}{2} \varphi} \prod_k (u_k^2 + v_k^2 e^{i \varphi}) + \right.$$

$$\left. + \int_{0}^{2\pi} d\varphi (2\pi - \varphi) e^{-i \frac{N}{2} \varphi} \prod_k (u_k^2 + v_k^2 e^{i \varphi}) \right] =$$

$$= \frac{1}{4 \pi^2 \lambda_N^2} \int_{0}^{2\pi} d\varphi 2\pi e^{-i \frac{N}{2} \varphi} \prod_k (u_k^2 + v_k^2 e^{i \varphi}) =$$

$$= \frac{1}{\lambda_N^2} \int_{0}^{2\pi} \frac{d\varphi}{2\pi} e^{-i \frac{N}{2} \varphi} \prod_k (u_k^2 + v_k^2 e^{i \varphi})$$

Finally, demanding from $|\psi_N\rangle$ to be normalized we get $\lambda$:

$$1 = \frac{1}{\lambda_N^2} \int_{0}^{2\pi} \frac{d\varphi}{2\pi} e^{-i \frac{N}{2} \varphi} \prod_k (u_k^2 + v_k^2 e^{i \varphi}) \Leftrightarrow$$

$$\lambda_N^2 = \int_{0}^{2\pi} \frac{d\varphi}{2\pi} e^{-i \frac{N}{2} \varphi} \prod_k (u_k^2 + v_k^2 e^{i \varphi})$$  (3.5)
We define the quantities:

\[
R^N_n (k_1, k_2, \ldots, k_N) = \frac{1}{2\pi i} \oint d\zeta z^{-(M-n)-1} \prod_{k \neq k_1, k_2, \ldots, k_N} (u_k^2 + z v_k^2) = \\
= \int_0^{2\pi} \frac{d\phi}{2\pi} e^{-i(M-n)\phi} \prod_{k \neq k_1, k_2, \ldots, k_N} (u_k^2 + e^{i\phi} v_k^2)
\]

Using that notation we can write:

\[
R_0^0 = \lambda_N^2 = \int_0^{2\pi} \frac{d\phi}{2\pi} e^{-i\frac{M-1}{2} \phi} \prod_k (u_k^2 + v_k^2 e^{i\phi}) = \oint d\zeta z^{-M-1} \prod_k (u_k^2 + z v_k^2)
\]

As it has been hinted above, BCS theory is defined in a Grand Canonical Ensemble meaning that the BCS Ground State does not describe a system with a fixed number of particles but rather a system with a fixed average number of particles. In other words, the ground state of BCS is not an eigenstate of the number operator \( \hat{N} \) but rather a linear combination of the eigenstates of \( \hat{N} \). The spectrum of \( \lambda_N \) is sharply picked around \( N = \langle N \rangle \) since the major contribution to \( |\psi_{BCS}⟩ \) comes from wavefunctions that describe a system with \( N = \langle N \rangle \) particles. We aim to simulate finite systems and as such we will need to describe the ground state of systems with fixed particle numbers.

The process of restoring the particle conservation in BCS is called a Projection and it can be done in different ways. The two most used are:

- **Projection After Variation (PAV)**
- **Variation After Projection (VAP)**

It is expected that VAP gives a better description of the finite system than PAV since the former performs a variation on the projected state while the latter projects
the desired component of an already optimized state. BCS theory can be seen as a Saddle Point approximation of VAP (see Appendix D). This approximation becomes more reliable as we move to more strongly paired systems [18] such as neutron matter. Therefore one expects the VAP description of a finite superfluid system of neutrons to not differ much from that of BCS. Since PAV already provides a better description of finite superfluid systems than BCS, one can also expect that both PAV and VAP will provide a good description of a finite superfluid system of neutrons. In the section below we present the theory of PAV. In Appendix D we will present the theory of VAP.

**Projection After Variation (PAV): PBCS Theory**

In Section 3.1 we saw how the BCS ground state comes from a variational approach. That means that $v_k$ and $u_k$ in the state (3.1) are determined so that the $|\psi_{BCS}\rangle$ minimizes the Free Energy $F = E - \mu N$. Once we have $|\psi_{BCS}\rangle$ we can choose to project out the component that describes a system with a fixed number of particles $N$ the same way that it was described above:

$$
|\psi_N\rangle = \hat{P}_N |\psi_{BCS}\rangle = \oint \frac{dz}{2\pi i} z^{-M-1} \prod_k \left( u_k + z v_k \hat{p}_k^\dagger \right) |0\rangle = \\
= \int_0^{2\pi} \frac{d\phi}{2\pi} e^{-iM\phi} \prod_k \left( u_k + e^{i\phi} v_k \hat{p}_k^\dagger \right) |0\rangle
$$

(3.8)

where we define:

$$
M = \frac{N}{2}, \quad \text{the number of pairs}
$$
PBCS is the theory where this $|\psi_N\rangle$ is used to describe the eigenstate of a finite system with $N$ particles. Using this ground state we can calculate the energy of a system with $N$ particles where $N$ is an even number (see Appendix E):

$$E_{\text{even}}(N) = \frac{\langle \psi_N | \mathcal{H} | \psi_N \rangle}{\langle \psi_N | \psi_N \rangle} = \sum_k \epsilon_k 2v_k^2 \frac{R^2_1(k)}{R_0^2} + \sum_k V_{kk} v_k^2 \frac{R^2_1(k)}{R_0^2} + \sum_{k,l|k\neq l} V_{kl} u_k u_l v_k v_l \frac{R^2_1(kl)}{R_0^2} \quad (3.9)$$

In order to find the energy of a system with an odd number of particles we have to employ the theory of blocked states that was described above where the ground state of the system in BCS is (2.15). From that ground state we can again project the state with $N+1$ particles:

$$|\psi^{b\gamma}_{N+1}\rangle = \hat{\mathcal{P}}_N |\psi^{b\gamma}_{BCS}\rangle = \epsilon_{b\gamma}^+ \int \frac{dz}{2\pi i} z^{-\frac{N}{2}} \prod_{k\neq b} (u_k + z v_k \hat{p}_k^\dagger) |0\rangle =$$

$$= \epsilon_{b\gamma}^+ \int_0^{2\pi} \frac{d\phi}{2\pi} e^{-iM\phi} \prod_{k\neq b} (u_k + e^{i\phi} v_k \hat{p}_k^\dagger) |0\rangle \quad (3.10)$$

Using this ground state the expression of the energy can be found in an identical way as the expression for the even systems:

$$E_{\text{odd}}(N + 1) = \sum_k \epsilon_k 2v_k^2 \frac{R^2_1(k)}{R_0^2(b)} + \epsilon_b + \sum_k V_{kk} v_k^2 \frac{R^2_1(bk)}{R_0^2(b)} + \sum_{k,l|k\neq l} V_{kl} u_k u_l v_k v_l \frac{R^2_1(bkl)}{R_0^2(b)} \quad (3.11)$$
3.2 Analytical and Numerical Solution of the Residuum Integrals

The analytical solution

The Residuum integrals as defined in Eq. (3.7) can be evaluated analytically. If we expand the product on the left hand side of Eq. (3.7) we get:

\[
R_n^N (k_1, \ldots, k_N) = \int_0^{2\pi} \frac{d\phi}{2\pi} e^{-i(M-n)\phi} \prod_{k\neq k_1, k_2, \ldots, k_N} (u_k^2 + e^{i\phi} v_k^2) = \\
= \int_0^{2\pi} \frac{d\phi}{2\pi} e^{-i(M-n)\phi} (u_{k_1}^2 + e^{i\phi} v_{k_1}^2) (u_{k_2}^2 + e^{i\phi} v_{k_2}^2) (u_{k_3}^2 + e^{i\phi} v_{k_3}^2) \cdots = \\
= \prod_{k\neq k_1, k_2, \ldots, k_N} u_k^2 + \\
+ \sum_{l_1 \neq k_1, k_2, \ldots, k_N} u_{l_1}^2 \prod_{k\neq l_1, l_2, k_1, k_2, \ldots, k_N} u_k^2 \int_0^{2\pi} \frac{d\phi}{2\pi} e^{-i(M-n)\phi} e^{i\phi} + \\
+ \sum_{l_1, l_2 \neq k_1, k_2, \ldots, k_N} u_{l_1}^2 u_{l_2}^2 \prod_{k\neq l_1, l_2, l_3, k_1, k_2, \ldots, k_N} u_k^2 \int_0^{2\pi} \frac{d\phi}{2\pi} e^{-i(M-n)\phi} e^{i2\phi} + \\
+ \sum_{l_1, l_2, l_3 \neq k_1, k_2, \ldots, k_N} u_{l_1}^2 u_{l_2}^2 u_{l_3}^2 \prod_{k\neq l_1, l_2, l_3, k_1, k_2, \ldots, k_N} u_k^2 \int_0^{2\pi} \frac{d\phi}{2\pi} e^{-i(M-n)\phi} e^{i3\phi} + \\
+ \cdots + \\
+ \sum_{\{l\}_H} \prod_{l \in \{l\}_H} v_l^2 \prod_{k \notin \{l\}_H} u_k^2 \int_0^{2\pi} \frac{d\phi}{2\pi} e^{-i(M-n)\phi} e^{iH\phi} + \cdots
\]

where the sum \( \sum_{\{l\}_H} \) runs over all sets \( \{l\}_H \) with \( H \) elements and the integrals serve as Kronecker delta functions which will pick the terms with \( M - n \) terms of \( v_k \)'s since:

Finally:

\[
R_n^N (k_1, \ldots, k_N) = \sum_H \left[ \sum_{\{l\}_H} \prod_{l \in \{l\}_H} v_l^2 \prod_{k \notin \{l\}_H} u_k^2 \delta_{H, M-n} \right] = 
\]

25
\[ A \{l\}_1 \times \cdots \times \{l\}_N = \sum_{\{l\}_1 \times \cdots \times \{l\}_N} A_{\{l\}_1} \cdots A_{\{l\}_N} \quad \text{where} \quad A_L = \prod_{l \in L} v_l^2 \prod_{k \notin L} u_k^2 \]

we also observe that:

\[ \prod_k (u_k^2 + v_k^2 e^{i\phi}) \bigg|_{\phi = 0} = \prod_k (u_k^2 + v_k^2) = 1 \]

and so:

\[ \prod_k (u_k^2 + v_k^2 e^{i\phi}) \bigg|_{\phi = 0} = \sum_{\{l\}_1 \times \cdots \times \{l\}_N} \prod_{l \in \{l\}_1} v_l^2 \prod_{k \notin \{l\}_1} u_k^2 = 1 \]

where the sum runs over all possible sets \{l\} with no constraint on the cardinalities.

Finally if we also define:

\[ \eta_{\mu} = \sum_{\{l\}_\mu \times \{l\}_\mu} \prod_{l \in \{l\}_\mu} v_l^2 \prod_{k \notin \{l\}_\mu} u_k^2 \]

then:

\[ \langle \psi_{BCS} | \psi_{BCS} \rangle = \prod_k (u_k^2 + v_k^2 e^{i\phi}) = \sum_{\mu = 0}^{\infty} \eta_{\mu} e^{i\mu\phi} \]

where \( \sum_{\mu = 0}^{\infty} \eta_{\mu} = 1 \). The projection operator introduced before will pick one term
from the sum in the right hand side of Eq. (3.13). This points to a simple interpretation for $A_{\{l\}_\mu}$ and for the Residuum Integrals:

- $A_{\{l\}_\mu}$ : “the probability of finding the set $\{l\}_\mu$ of $k$-states occupied”
- $R_n^N(k_1, \ldots, k_N)$: “the probability of finding any set of $k$-states with cardinality $M - n$ occupied, excluding $k_1, \ldots, k_N”$

Equation (3.12) provides an analytical form of the Residuum Integrals but it is not fit for an actual evaluation. The sum $\sum_{\{l\}}^{M-n}$ contains $\binom{\Omega}{M-n}$ terms where $\Omega$ is the number of $k$-states available to the particles (the implicit upper bound of the product in Eq. (3.1)). Each one of those terms corresponds to a different choice of $M - n$ $k$-states out of the $\Omega$ $k$-states available. Even though one could exploit the degeneracies in the $k$-states to reduce that number of terms, that reduction is still not enough to allow for an evaluation using Eq. (3.12). Alternatively, the Residuum Integrals can be evaluated numerically using their definition (3.7) and a numerical integration method, such as the Gauss-Legendre quadrature. Figures of the 1-state Residuum Integrals evaluated numerically can be found in Fig. 3.1. Similar plots of the 2-state Residuum integrals can be found in Figs. 3.2, 3.3 & 3.4.
Figure 3.1: The 1D Residuum Integrals $R_0^1(k)$ & $R_1^1(k)$ as a function of the dimensionless momentum $n = \frac{2\pi}{L}k$. 

1-D Residuum Integrals in BCS

$R_0^1$ & $R_1^1$ vs k for $\langle N \rangle = 66$
Figure 3.2: The 2D Residuum Integral $R_0^2(k_1, k_2)$ as a function of $k_2$ for $k_1 = 0, 1, 2$ and $k_1 = k_2$. The momenta have once again been made dimensionless.
2-states Residuum Integrals in BCS

$R_1^2$ vs $k$ for $\langle N \rangle = 66$

Figure 3.3: The 2D Residuum Integral $R_1^2(k_1, k_2)$ as a function of the $k_2$ for $k_1 = 0, 1, 2$ and $k_1 = k_2$. The momenta have once again been made dimensionless.
Figure 3.4: The 2D Residuum Integral $R_2^2(k_1, k_2)$ as a function of the $k_2$ for $k_1 = 0, 1, 2$ and $k_1 = k_2$. The momenta have once again been made dimensionless.
Chapter 4

Simulating Finite Systems of Neutron Matter

We wish to describe a system of superfluid neutron matter. Superfluid neutrons can be found in the inner crust of cold neutron stars at densities less than about the density of nuclear matter \( n_n \approx 1.6 \times 10^{-2} \text{fm}^{-3} \). The sheer magnitude of the dimensions of the inner crust, compared to the scale of the neutron-neutron interaction, renders the crust essentially an infinite system. As has been mentioned above, extracting properties of the ground state of infinite systems is no simple task. Some of the most exact methods fall under the category of Quantum Monte Carlo (QMC) methods where one solves the problem of minimizing the energy of the system stochastically. The input that those methods require is the Hamiltonian of the system and a trial wave function which is a guess for the actual ground state of the system. The efficiency of a QMC simulation relies heavily on the ability of the trial wave function to capture the physics of the simulated system. However, QMC techniques are still simulating finite systems and they scale unfavourably with the number of particles. Eventually one faces the problem of finding a trial wave function that can capture the
physics of a system at the Thermodynamic Limit (an infinite system) while keeping
the number of particles to be simulated at a minimum. That form of optimization
requires one to know the way that a finite system of neutron matter approaches the
Thermodynamic Limit as the number of particles is increased while it is kept to a
fixed density.

4.1 BCS in A Box - Computation for Finite Systems

We carried out calculations for finite systems of neutron matter at $k_F a = -10$ and
at $k_F a = -5$. These belong to a range of densities low enough so that the details and
the shape of the interaction are irrelevant (see subsection 4.1.2). Our finite systems
were constrained in a box under PBC. That means that our results correspond to
a twist of $\theta = 0$ (see section 1.2). As mentioned in Chapter 2, pairing requires
an attractive interaction. In those densities the attractive interaction is provided
mostly by the $^1S_0$ channel of the neutron-neutron interaction which turns repulsive
at $k \approx 1.7 \text{ fm}^{-1}$. For higher momenta the main attractive contribution comes from the
$^3P_2$ channel of the interaction [19]. It has been shown that the change in the pairing
Gap due to $p$-wave contributions in the interaction is small (approximately 7% in the
density discussed here [20] [21]). We model the neutron-neutron interaction using the
Modified Pöschl-Teller potential (see section 4.1.2). Equations (2.11) & (2.12) have
to be expanded in partial waves to isolate the $^1S_0$ component. Following expression
(S1.1), equation (2.11) becomes:
\[
[\Delta_k]_{00} = -\frac{4\pi}{L^3} \sum_{k'} \langle k| V |k' \rangle \left[ \frac{\Delta_{k'}}{2E_{k'}} \right]_{00}
\]

where \([\Delta_k]_{00}\) is the \(l = 0, m = 0\) component of the expansion \(\Delta_k = \sum_{lm} \sqrt{\frac{4\pi}{2l+1}} Y_{lm}[\Delta_k]_{lm}\). The angle dependence in the denominator prevents the kernel of the sum to separate into different partial-wave components. We get rid of that angle dependence by performing an angle averaging on \(\Delta_k\). That is, we define

\[
|\tilde{\Delta}(k)|^2 = \int \frac{d\Omega_k}{4\pi} \Delta^*_k \Delta_k = \int \frac{d\Omega_k}{4\pi} |\Delta_k|^2 = \sum_{lm} \frac{1}{2l+1} |\Delta_{lm}(k)| \text{ (see Appendix C)}
\]

and we approximate \(\Delta_k\) with \(\tilde{\Delta}(k)\). This angle-average approximation is valid as long as the quantity of interest is the average value of the Gap on the Fermi surface, namely \(\tilde{\Delta}(k_F)\) and not the angle dependence of the Gap functions \([\Delta_k]_l\) [22]. Thus, we remove the angle dependence in the denominator of Eq. (2.11) and the S-wave expansion can be written as:

\[
[\Delta_k]_{00}(k) = -\frac{4\pi}{L^3} \sum_{k'} V_0(k, k') \frac{[\Delta_{k'}]_{00}(k')}{2E_{k'}}
\]

We define the population function \(M(x)\) which takes the value of the number of \(k\) states with \(|k| = x\) so that the sum \(\sum_{k'}\) can be replaced by \(\sum_{k'} M(k')\). We also introduce the notation \(\Delta(k) = [\Delta_k]_{00}(k)\). Using those and the fact that the second Gap equation (2.12) has a trivial S-wave expansion, we arrive at the Gap equations in the S-wave:

\[
\Delta(k) = -\frac{4\pi}{L^3} \sum_{k'} M(k') V_0(k, k') \frac{\Delta(k')}{2E(k')}
\]

(4.1)
\[ \langle N \rangle = \sum_k M(k) \left( 1 - \frac{\xi(k)}{E(k)} \right) \]  \hspace{1cm} (4.2)

where

- \( V_0(k, k') = \int_0^\infty dr r^2 j_0(kr)V(r)j_0(k'r) \) and \( j_0(x) = \frac{\sin x}{x} \) the 0th Spherical Bessel function of the first kind

- \( \xi(k) = \frac{\hbar^2}{2m} k^2 - \mu_{ch} \), the single particle energies measured from the chemical potential

- \( E(k) = \sqrt{\xi^2(k) + \Delta^2(k)} \), the quasi-particle excitation energy

- \( L = \left( \frac{\langle N \rangle}{n} \right)^{1/3} \) the length of the box which is taken such that the particles in the box yield the desired density \( n_0 = 5.3341 \times 10^{-3} \text{ fm}^{-3} \)

In the weak coupling regime, where \( \Delta/\mu_{ch} \ll 1 \) Eqs. (4.1) & (4.2) can be decoupled giving what is sometimes referred to as the BCS approximation [23] since it was employed in the initial introduction of the theory [24]. However this approximation is invalid for the values of density considered here. For a specific particle number \( \langle N \rangle \), Eqs. (4.1) & (4.2) are solved self-consistently in an iterative scheme. That is, for a given \( \mu_{ch} \) we can solve Eq. (4.1) iteratively starting with a flat Gap distribution \( \Delta^{(0)}(k) = 1 \) which we plug in the right hand side. From the left hand side we extract an updated Gap function \( \Delta^{(1)}(k) \) which we then plug in the right hand side to get the new \( \Delta^{(2)}(k) \) from the left hand side again and so on. This iterative procedure stops when the updated Gap distribution on the left is equal to the input on the right (up to some accuracy). Mathematically that criterion can be written as:
\[ \Delta(k) \text{ vs } n \]

\( \Delta(k) \) as the solution of the BCS Gap equations

Figure 4.1: The gap function \( \Delta(k) \) as a function of the dimensionless momentum \( n = \frac{2\pi}{L} k \) for different average particle numbers.

\[ \sqrt{\sum_k \left[ \frac{\Delta^{(i+1)}(k) - \Delta^{(i)}(k)}{\Delta^{(i)}(k)} \right]^2} \approx 0 \quad (4.3) \]

Once Eq. (4.1) has been solved giving us the correct \( \Delta(k) \) that corresponds to the given \( \mu_{ch} \), we calculate \( \langle N \rangle \) using Eq. (4.2) and our solution from Eq. (4.1). Essentially this is a function \( f(\mu_{ch}) = \langle N \rangle \) and we wish to find the root of \( f(\mu_{ch}) - \langle N \rangle_0 = 0 \) where \( \langle N \rangle_0 \) is the particle number of the system we wish to describe.

Typically, the Gap \( \Delta \) is defined as the value of \( \Delta(k) \) on the Fermi Surface. However, in systems with strong pairing the Fermi surface is not well defined since the
occupation distribution is highly smeared (see section 4.1.3). Therefore, we define as Gap the minimum of the excitation energy $E(k)$. From the definition of $E(k)$ we can see that $\min_k E(k)$ occurs at the value of $k$ which makes the single particle energy $\epsilon_k = \frac{\hbar^2}{2m} k^2$ be the closest to the chemical potential $\mu_{ch}$ (since $\Delta(k)$ is a decreasing function of $k$ as can be seen in Fig. 4.1). Therefore $\min_k E(k)$ will be the energy gain of the system when a new particle is added. A figure of the Excitation energy (at $\langle N \rangle = 66$) and the Gap as it is extracted from its minimum can be seen in Fig. 4.2.

In sections 4.1.3 & 4.1.4 we analyse the results of the above treatment. That is, in
section 4.1.3 we discuss the dependence of the Gap $\Delta$ to the average particle number $\langle N \rangle$ as a result of the procedure described above. In section 4.1.4 we present a similar discussion on the chemical potential $\mu$.

4.1.1 BCS in the continuum - The Thermodynamic Limit

Solutions

As has been mentioned in the beginning of the chapter our goal is to study the approach of a finite superfluid system to its Thermodynamic Limit (TL). In order to quantify convergence and various errors we need to know the thermodynamic limit values of the calculated intensive quantities. Typically an extrapolation to the TL is no trivial task. However, in BCS Theory the calculation in the TL can be carried out in a fairly straightforward way.

We can begin by observing that a system in the TL corresponds to a system in a box of an infinite length $L$. Taking this limit in Eqs. (2.11) & (2.12) the sums turn into integrals since the separation between the lattice points in $k$ space is $\frac{2\pi}{L}$ (Periodic Boundary Conditions) which tends to 0 as $L \to \infty$:

$$\sum_{k} = \sum_{k_x} \sum_{k_y} \sum_{k_z} = \sum_{k_x} \sum_{k_y} \sum_{k_z} \frac{\delta k_x \delta k_y \delta k_z}{\delta k_x \delta k_y \delta k_z} = \frac{1}{\delta k_x \delta k_y \delta k_z} \left[ \sum_{k_x k_y k_z} \delta k_x \delta k_y \delta k_z \right] =$$

$$= \left( \frac{L}{2\pi} \right)^3 \left[ \sum_{k_x k_y k_z} \delta k_x \delta k_y \delta k_z \right]$$

Substituting that into Eq. (4.1), the factor of $L^3$ cancels and we can take the limit $L \to \infty$. Working in an identical way on Eq. (4.2) we arrive at the TL version of the Gap equations in the $^1S_0$ channel [22]:

38
Figure 4.3: The Gap as a fraction of the Fermi energy in the TL. In the figure we can also see the Gap at $\langle N \rangle = 66$ of a finite system for $k_F a = -5$ and $k_F a = -10$.

\[
\Delta(k) = -\frac{1}{\pi} \int_0^\infty dk'(k')^2 V_0(k, k') \frac{\Delta(k')}{E(k')}
\]  

(4.4)

\[
\frac{\langle N \rangle}{L^3} = n = \frac{1}{2\pi^2} \int_0^\infty dk k^2 \left( 1 - \frac{\xi(k)}{E(k)} \right)
\]  

(4.5)

Equations (4.4) & (4.2) are solved using the same iterative scheme described for finite systems. That is, we created a function $f_{TL}(\mu_{ch})$ which, given a chemical potential $\mu_{ch}$, solves equation (4.1) iteratively and uses the solution to calculate the corresponding
density. Ultimately we solved for the root of the equation \( f_{TL}(\mu_{ch}) - n_0 = 0 \). The solution of the Gap Eqs in the continuum can provide us with the dependence of the Gap of an infinite system for different densities (and therefore different \( k_F \)). A figure of the Gap as a fraction of the Fermi energy can be seen in Fig. 4.3.

Once those equations were solved, we employed the same procedure to extract the Gap \( \Delta \) as the minimum of the excitation energy \( E(k) \) which is the TL value that appears in Fig. 4.1. The root of the equation \( f_{TL}(\mu_{ch}) - n_0 = 0 \) is the one that corresponds to the TL value of the chemical potential \( \mu_{ch} \).

### 4.1.2 The Modified Pöschl - Teller Potential

At the densities that we consider here the neutron-neutron interaction is dominated by the \( ^1S_0 \) channel (spin 0 isospin 1). This interaction is attractive enough to almost create a bound system (dineutron). The neutron-neutron scattering length and effective range are \( a = -18.5 \text{ fm} \) and \( r_e = 2.7 \text{ fm} \), respectively [25]. Those are quantities that arise from solving Schrödinger’s equation and they capture the physics of the interaction at low energies. That is, the low-energy cross section does not depend on the details of the interaction but only on \( a \) and \( r_e \). That tells us that any potential, regardless of the details of its shape, that can be tuned to reproduce the scattering length and effective range of neutron matter will describe the correct physics at low energies. We choose the Modified Pöschl - Teller potential since it can be treated analytically [20].

Therefore, we model the neutron-neutron interaction using the Modified Pöschl - Teller potential:
\[
V(r) = -\frac{\hbar}{m_n} \frac{\lambda(\lambda - 1)\mu^2}{\cosh^2(\mu r)} \tag{4.6}
\]

where:

\[
\lambda = 1.93672
\]

\[
\mu = 0.79959 \text{ fm}^{-1}
\]

These parameters are tuned to reproduce the \(^1\!S_0\) scattering length and effective range of neutron matter. As mentioned above, in the \(^1\!S_0\) channel the potential is:

\[
V_0(k, k') = \int_0^\infty dr r^2 j_0(kr)V(r)j_0(k'r) =
\]

\[
= \frac{A\pi}{4\mu k k'} \left( \frac{k - k'}{\sinh \left( \frac{(k-k')\pi}{2\mu} \right)} - \frac{k + k'}{\sinh \left( \frac{(k+k')\pi}{2\mu} \right)} \right) \quad \text{for} \quad k \neq k', \ k, k' \neq 0
\]

\[
= \frac{A}{2\mu^2 k^2} \left( \mu - k' \frac{\pi}{\sinh \left( \frac{k\pi}{\mu} \right)} \right) \quad \text{for} \quad k = k' \neq 0
\]

\[
= \frac{A}{2\mu^2 k^2} \left[ \frac{1}{\sinh \left( \frac{\pi k}{2\mu} \right)} \left( \frac{\pi k}{2\mu} \coth \left( \frac{\pi k}{2\mu} \right) - 1 \right) \right] \quad \text{for} \quad k \neq k', \ k' = 0
\]

\[
= \frac{A\pi^2}{12\mu^3} \quad \text{for} \quad k = k' = 0
\]

where \(j_0(x)\) are the spherical Bessel functions of the first kind.

The derivation of the above expressions can be found in Appendix E. A plot of \(V_0(k, k')\) can be seen in Fig. 4.4.
4.1.3 The Gap in finite superfluid systems

The Gap of a superfluid system is defined as the value of the Gap function $\Delta(k)$ on the Fermi surface. However, one key feature of the BCS theory is that it yields no well defined Fermi surface. That is, as can be seen in Fig. 4.5, the occupation probabilities experience no sharp drop but they are rather smeared over a region. This smearing effect becomes larger as the system becomes more and more strongly interacting. Neutron matter is an inherently strongly interacting system and that can be seen by the substantial smearing of $v^2(k)$ in Fig. 4.5.

This absence of a well defined Fermi surface introduces an ambiguity in how one would calculate the Gap of a finite system. One approach is the one described above where the Gap is taken to be the minimum of the excitation energy $\min_k E(k)$. Calculations of the Gap using this prescription for different densities can be seen in Figs. 4.6 & 4.7.
Figure 4.5: The occupation probabilities in BCS as a function of the dimensionless momentum $n = \frac{2\pi}{L} k$. The smearing of the Fermi surface can easily be seen getting larger as the particle number increases. The circled points correspond to the k-states where $E(k)$ is minimum and can therefore be understood as the points where $\epsilon_k \approx \mu_{ch}$.

4.1.4 The Chemical Potential

The treatment of the chemical potential requires some additional care. By definition the chemical potential is a Lagrange multiplier, as can be seen in Eq. (2.9) where it was introduced to keep $\langle N \rangle$ fixed during the variation. This definition makes it, while still an intensive quantity, different to the energy (per particle) or the Gap. A second difference that makes it somewhat special is that there is no projected version of it. The projection takes us from a grand canonical ensemble, where the chemical potential is defined to a canonical ensemble where there is no analogous quantity.
Figures of the chemical potential with respect to the average particle number as a solution of the BCS Gap equations (4.1) & (4.2) for different density values can be seen in Figs. 4.8 & 4.9.

We can see that, compared to the Gap and the energy (per particle), the chemical potential is affected more by the finite size effects and it is affected less by the shell closure, see for example the inset of Fig. 4.8 which focuses on the region of $\langle N \rangle = 66$ where we expect a shell closure.

4.1.5 The energy per particle in Finite Systems

Once the solution to Eqs. (4.1) & (4.2) is identified we can use expressions (2.7) & (3.9) to calculate the energy in BCS and PBCS, respectively. In Figs (4.10) & (4.11) we present the energy per particle in BCS and PBCS divided by the energy per particle of a free Fermi gas $E_{N_{Free}} = \frac{3}{5} \epsilon_F$ for $k_F a = -10$ and $k_F a = -5$, respectively. As an intensive quantity, the energy per particle converges to the corresponding quantity in the TL which is calculated by taking $L \to \infty$ in the expression (2.7). That yields:

$$\frac{E_{TL}}{V} = \frac{1}{2\pi^2} \int_0^\infty dk k^2 2\epsilon(k)v(k) + \frac{1}{\pi^3} \int_0^\infty dk dk' k^2 k'^2 V_0(k, k') u(k) v(k) u(k') v(k')$$

(4.7)

and:

$$\frac{E_{TL}}{V} = \frac{E_{TL}}{N} \Rightarrow \frac{E_{TL}}{N} = \frac{1}{n} \frac{E_{TL}}{V}$$

where:
\[ n = \frac{1}{2\pi^2} \int_0^{\infty} dk k^2 2v^2(k) \]

Again we can see in the inset of Figs. (4.10) & (4.11) that in the region of \( N = 66 \) the FS Effects reach a minimum as expected by the shell closure.

Finally, an expression that holds for zero range interactions in the thermodynamic limit is:

\[ \frac{E/N}{\frac{3}{5} \epsilon_F} = \frac{\mu_{ch}}{\epsilon_F} \]  

(4.8)

In our case, we find that this expression is true up to 2% which is attributed to the fact that the neutron-neutron interaction is a finite range interaction.
Figure 4.6: The Gap for finite systems for $k_Fa = -10$. The inset focuses on the region of $\langle N \rangle = 66$ where we anticipate a shell closure. That is, following the comments in chapter 1.2, we expect the Gap at $\langle N \rangle = 66$ to roughly match the Gap at the TL.

Figure 4.7: The Gap for finite systems for $k_Fa = -5$. The inset focuses on the region of $\langle N \rangle = 66$ where we anticipate a shell closure. That is, following the comments in chapter 1.2, we expect the Gap at $\langle N \rangle = 66$ to roughly match the Gap at the TL.
Figure 4.8: The chemical potential in BCS as a solution of the Gap equations Eqs. (4.1) & (4.2) for $k_Fa = -10$. The inset focuses on the region of $\langle N \rangle = 66$ where anticipate a shell closure. Even though for the rest of the intensive quantities the shell closure is characterized by minimum FS Effects, as was mentioned above, for the chemical potential the difference of the value at $\langle N \rangle = 66$ from the TL value is substantial.

Figure 4.9: The chemical potential in BCS as a solution of the Gap equations Eqs. (4.1) & (4.2) for $k_Fa = -5$. The inset focuses on the region of $\langle N \rangle = 66$ where anticipate a shell closure. Even though for the rest of the intensive quantities the shell closure is characterized by minimum FS Effects, as was mentioned above, for the chemical potential the difference of the value at $\langle N \rangle = 66$ from the TL value is substantial.
Figure 4.10: The energy per particle as a function of the average particle number in BCS & PBCS for $k_F a = -10$. The inset focuses on the region of $\langle N \rangle = 66$ where we anticipate a shell closure. That is, following the comments in chapter 1.2, we expect the energy per particle at $\langle N \rangle = 66$ to, roughly, match the energy at the TL.

Figure 4.11: The energy per particle as a function of the average particle number in BCS & PBCS for $k_F a = -5$. The inset focuses on the region of $\langle N \rangle = 66$ where we anticipate a shell closure. That is, following the comments in chapter 1.2, we expect the energy per particle at $\langle N \rangle = 66$ to, roughly, match the energy at the TL.
Chapter 5

Summary & Conclusions

To summarize, in this thesis we investigate the problem of simulating infinite superfluid neutron matter with finite systems under PBC. Exact calculations for those systems are typically carried out by QMC methods that scale unfavourably with the number of particles simulated. This constraint imposed by QMC methods motivates a study of the way one can minimize Finite Size effects while keeping the number of particles to a minimum. We started by describing ways that have been used in QMC methods to manipulate variables introduced by the PBC to alleviate FS effects. Then we presented a review of the BCS Theory of superconductivity and a thorough analysis of how one can extend the theory to include systems with fixed particle numbers was made. That is, we described the procedure of restoring the particle number conservation in the BCS ground state by projecting eigenstates of the number operator out of it. That provided us with the Projected BCS (PBCS) theory that can describe finite systems with a fixed particle number.

We then reported on our BCS calculations of the Gap and energy of finite superfluid systems in densities relevant to that of the inner crust of cold neutron stars. Those
results allowed us to study the approach of the Gap, the energy and the chemical potential to the Thermodynamic Limit. This study was able to confirm the assumption that finite superfluid systems exhibit minimum Finite Size effects on the shell closure of the free Fermi gas. Finally we presented calculations of the energy in the context of PBCS and compared it with the analogous calculation in the BCS case.

Even though the work presented in this thesis has allowed us to study the Finite Size effects in systems of superfluid neutrons, there is still much to be explored. All calculations presented were carried out without any manipulation of the Twists introduced by the PBC. It is expected that a Twist averaging on those results will minimize the effects of the finite volume and will make the quantities calculated here reach their Thermodynamic Limit faster. That will provide one with a way to capture the physics of an infinite system in a wavefunction of a finite system of several particles allowing for QMC simulations with fewer particles. Once those results are obtained for the density considered here, a study of their dependency on different densities that are relevant to the inner crust of cold neutron stars will also be made.
Appendix A

Commutation Relations of $\hat{\rho}_k$

The pair creation and annihilation operators $\hat{\rho}_k^\dagger$ and $\hat{\rho}_k$ are defined as:

$$\hat{\rho}_k^\dagger = \hat{c}_{-k\uparrow}\hat{c}_{k\uparrow}$$

$$\hat{\rho}_k = \hat{c}_{k\uparrow}\hat{c}_{-k\uparrow}^\dagger$$

Using the anticommutation relations of $\hat{c}_{k\sigma}$ one can show that:

$$[\hat{\rho}_k^\dagger, \hat{c}_{l\sigma}] = \hat{c}_{k\uparrow}^\dagger \hat{c}_{l\downarrow} - \hat{c}_{k\downarrow} \hat{c}_{l\uparrow}$$

$$[\hat{\rho}_k, \hat{c}_{l\sigma}^\dagger] = \hat{c}_{-k\uparrow}^\dagger \hat{c}_{l\downarrow} - \hat{c}_{-k\downarrow} \hat{c}_{l\uparrow}$$

$$[\hat{\rho}_k^\dagger, \hat{c}_{l\sigma}^\dagger] = [\hat{\rho}_k, \hat{c}_{l\sigma}] = 0$$

Using those one can show that:

$$[\hat{\rho}_k^\dagger, \hat{n}] = \left(\hat{c}_{k\uparrow}^\dagger \hat{c}_{k\uparrow} + \hat{c}_{-k\downarrow}^\dagger \hat{c}_{-k\downarrow} - 1\right) \delta_{l,k} = (\hat{n}_{k\uparrow} + \hat{n}_{k\downarrow} - 1) \delta_{l,k} = \hat{M}_{k}\delta_{l,k}$$

$$[\hat{\rho}_k, \hat{n}] = [\hat{\rho}_k^\dagger, \hat{n}^\dagger] = 0$$

where we have defined $\hat{n}_k = \hat{c}_{k\sigma}^\dagger \hat{c}_{k\sigma}$ the density operator and $\hat{M}_k = (\hat{n}_{k\uparrow} + \hat{n}_{k\downarrow} - 1)$
Also:

\[
\begin{align*}
[\hat{n}_{k\sigma}, \hat{p}_l^\dagger] &= \hat{p}_l^\dagger [\delta_{-k,l}\delta_{\sigma\downarrow} + \delta_{kl}\delta_{\sigma\uparrow}] \\
[\hat{n}_{k\sigma}, \hat{p}_l] &= -\hat{p}_l [\delta_{-k,l}\delta_{\sigma\downarrow} + \delta_{kl}\delta_{\sigma\uparrow}]
\end{align*}
\]

Using those:

\[
\begin{align*}
[\hat{M}_k, \hat{p}_l^\dagger] &= 2\hat{p}_l^\dagger \delta_{kl} \\
[\hat{M}_k, \hat{p}_l] &= -2\hat{p}_l \delta_{kl}
\end{align*}
\]

Some useful relations also are:

\[
[\hat{M}_k, \hat{M}_l] = 0 \quad \forall k, l
\]

\[
\hat{p}_l^\dagger |0\rangle = 0
\]

\[
\hat{p}_l^\dagger \hat{M}_k |0\rangle = 0 \quad \forall k, l
\]

\[
\hat{p}_l^\dagger \hat{M}_k \hat{M}_n |0\rangle = 0 \quad \forall k, l, n
\]

\[
\vdots
\]

\[
\hat{p}_l^\dagger \prod_k \hat{M}_k |0\rangle = 0
\]

As an extension of the \(\hat{n}_{k\sigma}\) and \(\hat{p}_k\) commutation rules, one can show:

\[
\begin{align*}
[\hat{n}_{k\sigma}^{m+1}, \hat{p}_l^\dagger] &= (\delta_{-k,l}\delta_{\sigma\downarrow} + \delta_{kl}\delta_{\sigma\uparrow}) \sum_{r=0}^{m} \binom{m}{r} \hat{n}_{k\sigma}^{m-r} \hat{p}_l^\dagger \hat{n}_{k\sigma}^r \\
[\hat{n}_{k\sigma}^{m+1}, \hat{p}_l] &= - (\delta_{-k,l}\delta_{\sigma\downarrow} + \delta_{kl}\delta_{\sigma\uparrow}) \sum_{r=0}^{m} \binom{m}{r} \hat{n}_{k\sigma}^{m-r} \hat{p}_l \hat{n}_{k\sigma}^r
\end{align*}
\]
Similar relations can be derived for $\hat{M}_k$ as well:

\[
[\hat{M}_k^{m+1}, \hat{p}_l] = (\delta_{kl} + \delta_{-k,l}) \sum_{r=0}^{m} \binom{m}{r} \hat{M}_k^{m-r} \hat{p}_l \hat{M}_k^r
\]

\[
[\hat{M}_k^{m+1}, \hat{p}_l] = - (\delta_{kl} + \delta_{-k,l}) \sum_{r=0}^{m} \binom{m}{r} \hat{M}_k^{m-r} \hat{p}_l \hat{M}_k^r
\]
Appendix B

The derivation of $V_0(k, k')$

For $k \neq k'$:

$$ V_0(k, k') = \int dr r^2 j_0(kr) V(r) j_0(k'r) = \int dr r^2 \frac{\sin(kr)}{kr} V(r) \frac{\sin(k'r)}{k'r} = $$

$$ = \frac{1}{kk'} \int dr \sin kr \sin k'r V(r) = $$

$$ = \frac{1}{kk'} \int dr [\cos (k - k')r - \cos (k + k')r] V(r) = $$

$$ = \frac{A}{2kk'} \left[ \int dr \frac{\cos \alpha(-) r}{\cosh^2 \mu r} - \int dr \frac{\cos \alpha(+) r}{\cosh^2 \mu r} \right] $$

where we defined, for convenience:

$$ A = -\frac{\hbar}{m_n} \lambda(\lambda - 1)\mu^2 $$

$$ \alpha(-) = k - k' $$

$$ \alpha(+) = k + k' $$

From [26] we find:

$$ I_1(\alpha, \mu) \int dr \frac{\cos \alpha r}{\cosh^2 \mu r} = \frac{\alpha\pi}{2\mu^2 \sinh \frac{\alpha\pi}{2\mu}} \text{ for } \alpha > 0, \mu > 0 $$
Both of those constraints are satisfied in our case since \( \mu > 0 \) and \( k, k' > 0 \Rightarrow \alpha^{(+)} > 0 \) and for the cases where \( \alpha^{(-)} < 0 \) we can always use the fact the \( \cos(-\alpha^{(-)} r) = \cos(\alpha^{(-)} r) \). Substituting:

\[
V_0(k, k') = \frac{A \mu}{2 k k' 2} \left[ \frac{\alpha^{(-)} \pi}{2 \mu} \sinh \frac{\alpha^{(-)} \pi}{2 \mu} - \frac{\alpha^{(+)} \pi}{2 \mu} \sinh \frac{\alpha^{(+)} \pi}{2 \mu} \right]
\]

\[
= \frac{A \mu}{4 \mu^2 k k' 2} \left[ \frac{k - k'}{2 \mu^2} \sinh \frac{k - k'}{2 \mu} - \frac{k + k'}{2 \mu^2} \sinh \frac{k + k'}{2 \mu} \right] \quad \text{for} \quad k \neq k', \; k, k' \neq 0
\]

For \( k = k' \neq 0 \):

\[
V_0(k, k)(\neq) = \frac{A \mu}{2 k^2} \int dr \frac{\sin^2 kr}{\cosh^2 \mu r} = \frac{A \mu}{2 k^2} \int dr \frac{1 - \cos 2kr}{\cosh^2 \mu r} =
\]

\[
= \frac{A \mu}{2 k^2} \int dr \left[ \frac{1}{\cosh^2 \mu r} - \frac{\cos 2kr}{\cosh^2 \mu r} \right]
\]

Recognizing the first term as the integral of tanh and using the integral cited above we get:

\[
V_0(k, k)(\neq) = \frac{A \mu}{2 k^2} \left[ \left\{ \tanh \frac{\mu r}{\mu} \right\}_0^\infty - \frac{k \pi}{\mu^2 \sinh \frac{k \pi}{\mu}} \right] =
\]

\[
= \frac{A \mu}{2 \mu^2 k^2} \left[ \mu - \frac{k \pi}{\sinh \frac{k \pi}{\mu}} \right] \quad \text{for} \quad k = k' \neq 0
\]

For \( k \neq k', \; k' = 0 \):

\[
V_0(k, 0) = V_0(0, k) = \int dr r^2 j_0(kr) V(r) j_0(0) = \frac{1}{k} \int drr^2 \frac{\sin kr}{kr} \frac{A}{\cosh^2 \mu r} =
\]

\[
= \frac{A}{k} \int dr \frac{r \sin kr}{\cosh^2 \mu r} = \frac{A}{k} \int dx x r \sin \frac{k x}{\mu} \frac{\mu}{\mu \mu \cosh^2 x}
\]

55
where we performed the change of variables $\mu r = x$. From [26] we find:

$$I_2(\beta) = \int dx \frac{r \sin \beta x}{\cosh^2 x} = \frac{\pi}{2} \frac{1}{\sinh \frac{\pi \beta}{2}} \left( \frac{\pi \beta}{2} \coth \frac{\pi \beta}{2} - 1 \right)$$

Substituting:

$$V_0(k, 0) = \frac{A\pi}{2\mu^2 k} \left[ \frac{1}{\sinh \frac{\pi k}{2\mu}} \left( \frac{\pi k}{2\mu} \coth \frac{\pi k}{2\mu} - 1 \right) \right] \quad \text{for} \quad k \neq k', \; k' = 0$$

For $k = k' = 0$:

$$V_0(0, 0) = \int dr \frac{r^2 j_0(\theta)}{\cosh^2 \mu r} = A \int dr \frac{r^2}{\cosh^2 x} = A \int dr \frac{(\frac{r}{\mu})^2}{\cosh^2 x} = \frac{A\pi^2}{12\mu^3} \quad \text{for} \quad k = k' = 0$$

where we employed the same change of variable $\mu r = x$
Appendix C

The Partial Wave Expansion

In this section we will present the $S$-wave expansion of functions of vectors that are in the form of sums of the potential multiplied with other functions of vectors. We will use the final expressions in our $S$-wave expansion of the Gap Equations where the vectors are momenta on a 3D $k$-lattice (see Eqs. (4.1) & (4.2)) or in a continuum 3D $k$-space see Eqs. ((4.4) & 94.5)). The momenta in the following derivation are denoted by general vectors $\tilde{\nu}$ in an attempt to hint that those expressions are applicable outside BCS theory as well.

Single-Sum quantities Let $S(\tilde{\nu})$ be a quantity that depends on $\tilde{\nu}$ in the following way:

$$S(\tilde{\nu}) = \sum_{\tilde{\nu}_1} \langle \tilde{\nu} | V | \tilde{\nu}_1 \rangle B(\tilde{\nu}_1)$$

where $B(\tilde{\nu})$ an arbitrary function of $\tilde{\nu}$. We can separate the dependencies of the quantity $S$ from different channels of the potential and eventually express it as:

$$S(\tilde{\nu}) = \sum_l S_l$$
To that end we separate the potential’s radial and angular dependence on the momenta:

$$\langle \vec{\nu} | V | \vec{\nu}_1 \rangle = \frac{4\pi}{L^3} \sum_{l=0}^{\infty} (2l + 1)V_l(\nu, \nu_1)P_l(\hat{\nu} \cdot \hat{\nu}_1)$$

where:

$$V_l(\nu, \nu_1) = \int drr^2 j_l(k_\nu r) V(r) j_l(k_{\nu_1} r)$$

$$P_l: \text{ the Legendre Polynomials}$$

Using that, the quantity $S$ becomes:

$$S(\vec{\nu}) = \sum_{\vec{\nu}_1} \frac{4\pi}{L^3} \sum_{l=0}^{\infty} (2l + 1)V_l(\nu, \nu_1)P_l(\hat{\nu} \cdot \hat{\nu}_1)B(\vec{\nu}_1) =$$

$$= \sum_{l=0}^{\infty} \frac{4\pi}{L^3} \sum_{\vec{\nu}_1} [(2l + 1)V_l(\nu, \nu_1)P_l(\hat{\nu} \cdot \hat{\nu}_1)]B(\vec{\nu}_1) =$$

$$= \sum_l S_l(\vec{\nu})$$

where:

$$S_l(\vec{\nu}) = \frac{4\pi}{L^3} \sum_{\vec{\nu}_1} [(2l + 1)V_l(\nu, \nu_1)P_l(\hat{\nu} \cdot \hat{\nu}_1)]B(\vec{\nu}_1) \quad \text{(S1)}$$

and therefore:

$$S_0(\vec{\nu}) = \frac{4\pi}{L^3} \sum_{\vec{\nu}_1} [V_0(\nu, \nu_1)P_0(\hat{\nu} \cdot \hat{\nu}_1)]B(\vec{\nu}_1) = \frac{4\pi}{L^3} \sum_{\vec{\nu}_1} V_0(\nu, \nu_1)B(\vec{\nu}_1) \quad \text{(S1.1)}$$
Having separated $S$ into different channels we can also separate the radial and angular dependencies of $S$. To do so we can use the expansion of the Legendre polynomials in Spherical Harmonics:

$$P_l(\hat{\nu} \cdot \hat{\nu}_1) = \frac{4\pi}{2l + 1} \sum_{m=-l}^{l} Y_{lm}(\hat{\nu})Y_{lm}^*(\hat{\nu}_1)$$  \(1\)

With that, $S$ becomes:

$$S(\vec{\nu}) = \sum_{lm} \frac{4\pi}{l^3} \sum_{\vec{\nu}_1} [4\pi V_l(\nu, \nu_1)Y_{lm}(\hat{\nu})Y_{lm}^*(\hat{\nu}_1)]B(\vec{\nu}_1) = $$

$$= \sum_{lm} \sqrt{\frac{4\pi}{2l + 1}} Y_{lm}(\hat{\nu}) \left[ \frac{4\pi}{l^3} \sum_{\vec{\nu}_1} (2l + 1) \sqrt{\frac{4\pi}{2l + 1}} Y_{lm}^*(\hat{\nu}_1)V_l(\nu, \nu_1)B(\vec{\nu}_1) \right]$$

Expanding $S$ in a Laplace series:

$$S(\vec{\nu}) = \sum_{lm} \sqrt{\frac{4\pi}{2l + 1}} Y_{lm}(\hat{\nu})S_{lm}(\nu)$$

and using the orthogonality of the Spherical Harmonics we can identify $S_{lm}$ as:

$$S_{lm}(\nu) = \frac{4\pi}{l^3} \sum_{\vec{\nu}_1} (2l + 1) \sqrt{\frac{4\pi}{2l + 1}} Y_{lm}^*(\hat{\nu}_1)V_l(\nu, \nu_1)B(\vec{\nu}_1) \quad (S1^*)$$

and therefore:

$$S_{00}(\nu) = \frac{4\pi}{l^3} \sum_{\vec{\nu}_1} \sqrt{4\pi} Y_{00}^*(\hat{\nu}_1)V_0(\nu, \nu_1)B(\vec{\nu}_1) = \frac{4\pi}{l^3} \sum_{\vec{\nu}_1} V_0(\nu, \nu_1)B(\vec{\nu}_1) \quad (S1.1^*)$$

At this point we can also identify the ways that $S$ depends on different moments of $B$. To do so we have to expand $B$ in its own Laplace series:
\[ B(\hat{\nu}_1) = \sum_{l' m'} \sqrt{\frac{4\pi}{2l' + 1}} Y_{l'm'}(\hat{\nu}_1) B_{l'm'}(\nu_1) \]

If we substitute that in the expression for \( S \) we get:

\[
S(\hat{\nu}) = \sum_{\hat{\nu}_1} \frac{4\pi}{L^3} \sum_{l=0}^{\infty} (2l + 1)V_l(\nu, \nu_1) \frac{4\pi}{2l + 1} \times \\
\times \sum_{m=-l}^{l} Y_{lm}(\hat{\nu}) Y_{lm}^*(\hat{\nu}_1) \sum_{l'm'} \sqrt{\frac{4\pi}{2l' + 1}} B_{l'm'}(\nu_1) Y_{l'm'}(\hat{\nu}_1) = \\
= \sum_{lm} \sqrt{\frac{4\pi}{2l + 1}} Y_{lm}(\hat{\nu}) \times \\
\times \left[ \frac{4\pi}{L^3} \sum_{\hat{\nu}_1} \sum_{l'm'} 4\pi \sum_{l=0}^{\infty} \frac{2l + 1}{2l' + 1} Y_{lm}^*(\hat{\nu}) Y_{l'm'}(\hat{\nu}_1) V_l(\nu, \nu_1) B_{l'm'}(\nu_1) \right]
\]

Again, using the orthogonality of the Spherical Harmonics we can identify \( S_{lm} \) as:

\[
S_{lm}(\nu) = \frac{4\pi}{L^3} \sum_{\hat{\nu}_1} \sum_{l'm'} 4\pi \sqrt{\frac{2l + 1}{2l' + 1}} Y_{lm}^*(\hat{\nu}_1) Y_{l'm'}(\hat{\nu}_1) V_l(\nu, \nu_1) B_{l'm'}(\nu_1) \quad (S2)
\]

Therefore:

\[
S_{00} = \frac{4\pi}{L^3} \sum_{\hat{\nu}_1} \sum_{l'm'} 4\pi \sqrt{\frac{1}{2l' + 1}} Y_{00}^*(\hat{\nu}_1) Y_{l'm'}(\hat{\nu}_1) V_0(\nu, \nu_1) B_{l'm'}(\nu_1) = \\
= \frac{4\pi}{L^3} \left\{ \sum_{\hat{\nu}_1} V_0(\nu, \nu_1) B_{00}(\nu_1) + \sum_{\hat{\nu}_1} \sum_{l'm'} \sqrt{\frac{4\pi}{2l' + 1}} Y_{l'm'}(\hat{\nu}_1) V_0(\nu, \nu_1) B_{l'm'}(\nu_1) \right\}
\]

where:

\[
\sum_{l'm'} = \sum_{l'=1}^{\infty} \sum_{m'=-l'}^{l'}
\]
Finally keeping only the $B_{00}$ term:

$$S_{00} = \frac{4\pi}{L^3} \sum_{\nu_1} V_0(\nu, \nu_1) B_{00}(\nu_1)$$  \hspace{1cm} (2.1)

**Double-Sum quantities**  Let $Q(\vec{\nu})$ be a quantity that depends on $\vec{\nu}$ in the following way:

$$Q(\vec{\nu}) = \sum_{\vec{\nu}_1, \vec{\nu}_2} \langle \vec{\nu}_1 | V | \vec{\nu}_2 \rangle B(\vec{\nu}_1, \vec{\nu}_2, \vec{\nu})$$

where $B(\vec{\nu}_1, \vec{\nu}_2, \vec{\nu})$ is an arbitrary function of $\vec{\nu}_1, \vec{\nu}_2, \vec{\nu}$. Carrying out a similar derivation as the one presented for the Single-Sum quantities we have to separate the radial and angular dependencies of the potential:

$$\langle \vec{\nu}_1 | V | \vec{\nu}_2 \rangle = \frac{4\pi}{L^3} \sum_{l=0}^{\infty} (2l + 1) V_l(\nu_1, \nu_2) P_l(\hat{\nu}_1 \cdot \hat{\nu}_2)$$

Substituting that in:

$$Q(\vec{\nu}) = \sum_{l=0}^{\infty} \frac{4\pi}{L^3} \sum_{\vec{\nu}_1, \vec{\nu}_2} [(2l + 1)V_l(\nu_1, \nu_2)P_l(\hat{\nu}_1 \cdot \hat{\nu}_2)] B(\vec{\nu}_1, \vec{\nu}_2, \vec{\nu}) = \sum_l Q_l(\vec{\nu})$$

where:

$$Q_l(\vec{\nu}) = \frac{4\pi}{L^3} \sum_{\vec{\nu}_1, \vec{\nu}_2} [(2l + 1)V_l(\nu_1, \nu_2)P_l(\hat{\nu}_1 \cdot \hat{\nu}_2)] B(\vec{\nu}_1, \vec{\nu}_2, \vec{\nu})$$  \hspace{1cm} (D1)

and therefore:
Following similar steps as before, we can separate the radial and angular $\vec{\nu}$-dependencies of $B$ by expanding it in a Laplace Series:

\[ B(\vec{\nu}_1, \vec{\nu}_2, \nu) = \sum_{lm} \sqrt{\frac{4\pi}{2l+1}} Y_{lm}(\hat{\nu}) B_{lm}(\vec{\nu}_1, \vec{\nu}_2, \nu) \]

using that in the expression for $Q$ and using the expansion of the Legendre Polynomials (1), we get:

\[ Q(\vec{\nu}) = \sum_{lm} \sqrt{\frac{4\pi}{2l+1}} Y_{lm}(\hat{\nu}) \left\{ \frac{4\pi}{L^3} \sum_{\vec{\nu}_1, \vec{\nu}_2, \nu_0} V_0(\nu_1, \nu_2) Y^*_l(\hat{\nu}_1) Y^*_m(\hat{\nu}_2) B_{lm}(\vec{\nu}_1, \vec{\nu}_2, \nu) \right\} \]

Expanding $Q$ in its own Laplace Series and using the orthogonality of the Spherical Harmonics we identify $Q_{lm}$ as:

\[ Q_{lm}(\nu) = \frac{4\pi}{L^3} \sum_{\vec{\nu}_1, \vec{\nu}_2, \nu_0} V_l'(\nu_1, \nu_2) Y^*_l'(\hat{\nu}_1) Y^*_m'(\hat{\nu}_2) B_{lm}(\vec{\nu}_1, \vec{\nu}_2, \nu) = \]

\[ = \frac{4\pi}{L^3} \sum_{\vec{\nu}_1, \vec{\nu}_2} \left[ V_0(\nu_1, \nu_2) + \sum_{\nu_0} V_l'(\nu_1, \nu_2) Y^*_l'(\hat{\nu}_1) Y^*_m'(\hat{\nu}_2) \right] B_{lm}(\vec{\nu}_1, \vec{\nu}_2, \nu) \]  

\[ \text{(D2)} \]

therefore:

\[ Q_{00}(\nu) = \frac{4\pi}{L^3} \sum_{\vec{\nu}_1, \vec{\nu}_2} V_0(\nu_1, \nu_2) B_{00}(\vec{\nu}_1, \vec{\nu}_2, \nu) \]  

\[ \text{(D2.1)} \]
Appendix D

Variation After Projection (VAP): FBCS Theory

In PBCS Theory that was presented in chapter 3 $v_k$ and $u_k$ are determined such that $|\psi_{BCS}\rangle$ minimizes the Free Energy. However, in PBCS, $|\psi_{BCS}\rangle$ is no longer our ground state. Our new ground state $|\psi_N\rangle$ is only one component of the full $|\psi_{BCS}\rangle$ which means that it does not minimize the Free Energy:

$$\langle \psi_N | (\hat{H} - \mu \hat{N}) | \psi_N \rangle > F_0 = \langle \psi_{BCS} | (\hat{H} - \mu \hat{N}) | \psi_{BCS} \rangle$$

The fact that the PBCS ground state is not a minimum of the Free Energy means that it is not a good enough description of the ground state of a system with $N$ particles. In order to achieve better accuracy, the variation that provides us with $v_k$ and $u_k$ has to be done directly to $|\psi_N\rangle$. However, now $|\psi_N\rangle$ is a state with a definite particle number and therefore belongs to a canonical ensemble. As such the relevant quantity that has to be made stationary is the Energy (as opposed to the Free Energy in the grand canonical ensemble). That can be done by projecting $|\psi_N\rangle$ out of $|\psi_{BCS}\rangle$ before doing the variation and then using $|\psi_N\rangle$ as the ground state on which we will employ the variation. Mathematically that translates to:
\[ \delta \langle \psi_N | \hat{H} | \psi_N \rangle = 0 \iff \frac{\delta}{\delta v_k} \left[ 2 \sum_k v_k^2 \frac{R_1^1(k)}{R_0^0} + \sum_k v_{kk} v_k^2 \frac{R_1^1(k)}{R_0^0} + \sum_{k,l \mid k \neq l} V_{kl} u_k v_k v_l \frac{R_1^2(kl)}{R_0^0} \right] = 0 \]

where we consider \( v_k \) and \( u_k \) related through the relation \( v_k^2 + u_k^2 = 1 \) and therefore we can vary \( v_k \) taking \( u_k \) to be just a function of \( v_k \). Thus we defined:

\[
\frac{\delta}{\delta v_k} \equiv \frac{\partial}{\partial v_k} + \frac{\partial u_k}{\partial v_k} \frac{\partial}{\partial u_k} = \frac{\partial}{\partial v_k} - \frac{v_k}{u_k} \frac{\partial}{\partial u_k}
\]

It is evident that this variation is not equivalent to the variation (2.9) and therefore it will result in different Gap Equations. Indeed, performing the variation, which is outlined below, we arrive at:

\[
(\tilde{\epsilon}_k + \Lambda_k) u_k v_k + \Delta_k (u_k^2 - v_k^2) = 0 \forall k
\]

where:

\[
\tilde{\epsilon}_k = (\epsilon_k + \frac{1}{2} V_{kk}) \frac{R_1^1(k)}{R_0^0}
\]

\[
\Delta_k = \frac{1}{2} \sum_{k_1} V_{kk_1} u_{k_1} v_{k_1} \frac{R_1^2(k_1 k)}{R_0^0}
\]

\[
\Lambda_k = \sum_{k_1} (\epsilon_{k_1} + \frac{1}{2} V_{k_1 k_1}) v_{k_1}^2 \frac{R_1^1(k) R_2^2(k_1 k) - R_1^1(k) R_2^2(k_1 k_1)}{(R_0^0)^2} + \]

\[
+ \frac{1}{2} \sum_{k_1 k_2} V_{k_1 k_2} u_{k_1} v_{k_1} u_{k_2} v_{k_2} \frac{R_1^1(k) R_2^2(k_1 k_2) - R_1^1(k) R_2^2(k_1 k_2 k)}{(R_0^0)^2} + \]

\[
+ [\tilde{\epsilon}_k v_k^2 + 2 \Delta_k v_k u_k] \frac{R_1^1(k) - R_1^1(k)}{R_0^0}
\]
and the energy of the system:

\[ E_{\text{even}}(N) = \frac{\langle \psi_N | \mathcal{H} | \psi_N \rangle}{\langle \psi_N | \psi_N \rangle} = 2 \sum_k \epsilon_k v_k^2 \frac{R_1^1(k)}{R_0^0} + \sum_k V_{kk} v_k^2 \frac{R_1^1(k)}{R_0^0} + \sum_{k,l|k \neq l} V_{kl} u_k v_k v_l \frac{R_1^2(kl)}{R_0^2} \] (6)

Expression (5) is identical to the expression for the energy in PBCS (3.9). The difference in the two approaches is in the \( v_k \) and \( u_k \) that go into each expression. For PBCS \( v_k \) and \( u_k \) come form the BCS Gap equations (2.11) & (2.12) while in FBCS they come from the FBCS Gap equation (2).

In PBCS we saw that systems with an Odd number of particles need different treatment. This is true in FBCS as well. To describe a system with \( N + 1 \) particles where \( N \) is an even number we have to start from a different ground state. That ground state is the state provided by the theory of blocking (3.10). The energy corresponding to that state is:

\[ E_{\text{odd}}(N + 1) = \sum_k \epsilon_k 2v_k^2 \frac{R_1^1(k)}{R_0^0} + \epsilon_b + \sum_k V_{kk} v_k^2 \frac{R_1^1(bk)}{R_0^0(b)} + \sum_{k,l|k \neq l} V_{kl} u_k v_k v_l \frac{R_1^2(bkl)}{R_0^2(b)} \] (7)

Following a logic identical to that for the even \( N \) case, while the energy expression for FBCS carries over from PBCS the difference in the two theories comes from the fact that \( v_k \) and \( u_k \) in FBCS are determined such that they minimize (7). Performing that variation we arrive at (2) where now the coefficients are:
The variation in FBCS

FBCS is the theory that arises by the variation of the energy that occurs in PBCS, namely Eq. (3.9). Determining \( v_k \) and \( u_k \) so that they minimize that energy instead of using the \( v_k \) and \( u_k \) that minimize the BCS Free Energy (2.3), provides a more accurate description of a system with particle number conservation. In this section we will show how this variation is performed. We first name the different terms in Eq. (3.9) as:

\[
E_1 = \sum_k \epsilon_k^2 v_k^2 \frac{R_1^1(k)}{R_0^0(k)}
\]

\[
E_2 = \sum_k V_{kk} v_k^2 \frac{R_1^1(k)}{R_0^0(k)}
\]

\[
E_3 = \sum_{k,l|k \neq l} V_{kl} u_k u_l v_k v_l \frac{R_1^2(kl)}{R_0^0(kl)}
\]

As mentioned above, the variation has to be done taking into consideration the fact that \( v_k \) and \( u_k \) are related through the constraint (2.2). That is, the variation has to be done as:
Thus the variation of the Residuum Integrals is:

$$\frac{\delta}{\delta v_k} R_N^N(k_1, \ldots, k_N) = 2v_k \left[ R_{n+1}^N(k_1, \ldots, k_N, k) - R_n^N(k_1, \ldots, k_N, k) \right]$$

Applying the variation to $E_1, E_2, E_3$ we get: For $E_1$

$$\frac{\delta}{\delta v_l} E_1 = \frac{\delta}{\delta v_l} \left[ \sum_k \epsilon_k v_k^2 R_1^1(k) \right] = \epsilon_k 4v_l R_0^0 + 2\epsilon v_l^2 \left[ \frac{\delta}{\delta v_l} R_0^0 \right]$$

For $E_2$, we observe that it has the same form as $E_1$ and therefore it will be:

$$\frac{\delta}{\delta v_l} E_2 = \frac{\delta}{\delta v_l} \left[ \sum_k V_k v_k R_1^1(k) \right] = 2V_l v_l R_0^0 + V_l v_l^2 \left[ \frac{\delta}{\delta v_l} R_0^0 \right]$$

For $E_3$:

$$\frac{\delta}{\delta v_a} E_3 = \frac{\delta}{\delta v_a} \left[ \sum_{k,l|k \neq l} V_{kl} u_k u_l v_k v_l \frac{R_2^2(kl)}{R_0^0} \right] =$$

$$= \sum_{k,l|k \neq l} V_{kl} \left[ \frac{\delta}{\delta v_a} u_k u_l v_k v_l + \frac{\delta}{\delta v_a} u_k u_l v_k v_l + \frac{\delta}{\delta v_a} u_k u_l v_k v_l \right] \frac{R_2^2(kl)}{R_0^0} +$$

$$+ \sum_{k,l|k \neq l} V_{kl} u_k u_l v_k v_l \left[ \frac{\delta}{\delta v_a} R_0^0 \right] =$$

$$= \sum_{l} V_{al} \left[ \frac{v_a^2}{u_a^2} u_l v_l + u_a u_l v_l - \frac{R_1^1(al)}{R_0^0} \right] + \sum_k V_{ka} \left[ \frac{v_a^2}{u_a^2} u_k v_k + u_a u_k v_k - \frac{R_1^1(ka)}{R_0^0} \right] +$$

$$+ \sum_{k,l|k \neq l} V_{kl} u_k u_l v_k v_l \left[ \frac{\delta}{\delta v_a} R_0^0 \right] =$$
where we used that $V_{k \ell}$ is symmetric. Finally, the variation of the Energy is the sum of all three:

$$\frac{\delta}{\delta v_a} E = \frac{\delta}{\delta v_a} E_1 + \frac{\delta}{\delta v_a} E_2 + \frac{\delta}{\delta v_a} E_3 =$$

$$= (4\epsilon_a + 2V_{aa}) v_a \frac{R_1^1(a)}{R_0^0} + 2\frac{u_a^2 - v_a^2}{u_a} \sum_k V_{ka}u_k v_k \frac{R_1^0(ka)}{R_0^0} +$$

$$+ \sum_k (2\epsilon_a + V_{aa}) v_k^2 \left[ \frac{\delta}{\delta v_a} \frac{R_1^1(k)}{R_0^0} \right] + \sum_{k,l | k \neq l} V_{k\ell}u_k v_k \left[ \frac{\delta}{\delta v_a} \frac{R_1^0(\ell)}{R_0^0} \right] =$$

$$= \left( \epsilon_a + \frac{1}{2} V_{aa} \right) v_a u_a \frac{R_1^1(a)}{R_0^0} + \left( u_a^2 - v_a^2 \right) \sum_k \frac{1}{2} V_{ka}u_k v_k \frac{R_1^0(ka)}{R_0^0} +$$

$$+ \frac{u_a}{4} \left( \sum_k (2\epsilon_k + V_{kk}) v_k^2 \left[ \frac{\delta}{\delta v_a} \frac{R_1^1(k)}{R_0^0} \right] + \sum_{k,l | k \neq l} V_{k\ell}u_k v_k \left[ \frac{\delta}{\delta v_a} \frac{R_1^0(\ell)}{R_0^0} \right] \right)$$

Setting $\frac{\delta}{\delta v_a} E = 0$ we can see right away how the different coefficients from Eq. (2) start to form. The first two terms in the above equation will be $\bar{\epsilon}_a v_a u_a + (u_a^2 - v_a^2) \Delta_a$. The last term, which is related to the variation of the Residuum Integrals, will, after the use of Eq. (11), give rise to $\Lambda_a$.

The $^1S_0$ channel of FBCS

The coefficients that come into Eq. (2) are:

$$\bar{\epsilon}_k = (\epsilon_k + \frac{1}{2} V_{kk}) \frac{R_1^1(k)}{R_0^0}$$

$$\Delta_k = \frac{1}{2} \sum_{k_1} V_{kk_1}u_{k_1} v_{k_1} \frac{R_1^0(k_1, k)}{R_0^0}$$
\[ \Lambda_k = \sum_{k_1} (\epsilon_{k_1} + \frac{1}{2} V_{k_1, k_1}) v_{k_1}^2 \frac{R_{0}^1(k) R_{2}^1(k_1, k)}{(R_{0}^0)^2} + \]
\[ + \frac{1}{2} \sum_{k_1, k_2} V_{k_1, k_2} u_{k_1} u_{k_2} v_{k_1} v_{k_2} \frac{R_{0}^1(k) R_{2}^3(k_1, k_2, k) - R_{1}^1(k) R_{3}^3(k_1, k_2, k)}{(R_{0}^0)^2} + \]
\[ + [\tilde{\epsilon}_k v_k^2 + 2\Delta_k v_k u_k] \frac{R_{0}^1(k) - R_{1}^1(k)}{R_{0}^0} \]

where:

\[ V_{k_1, k_2} = \langle k_1 - k_1| V | k_2 - k_2 \rangle \]

is the matrix element of the pure pairing interaction. Using the above results the FBCS equations in the \(^1S_0\) channel become: (Using expansions (S2) and (D2))

\[ \tilde{\epsilon}(k)_{00} = \left[ \epsilon_k + \frac{2\pi}{L^3} V_0(k, k) \right] \left[ R_{0}^1(k) \right]_{00} \]
\[ \Delta(\nu)_{00} = \frac{2\pi}{L^3} \sum_{k_1} V_0(k, k_1) \left[ u_{k_1} v_{k_1} \frac{R_{1}^2(k_1, k)}{R_{0}^0} \right]_{00} \]
\[ \Lambda(k)_{00} = \sum_{k_1} \left[ \epsilon_{k_1} + \frac{2\pi}{L^3} V_0(k_1, k_1) \right] \left[ u_{k_1} v_{k_1} \frac{R_{0}^1(k) R_{2}^3(k_1, k_2, k) - R_{1}^1(k) R_{3}^3(k_1, k_2, k)}{(R_{0}^0)^2} \right]_{00} + \]
\[ + \frac{2\pi}{L^3} \sum_{k_1, k_2} V_0(k_1, k_2) \left[ u_{k_1} v_{k_1} u_{k_2} v_{k_2} \frac{R_{0}^1(k) R_{2}^3(k_1, k_2, k) - R_{1}^1(k) R_{3}^3(k_1, k_2, k)}{(R_{0}^0)^2} \right]_{00} + \]
\[ + \left[ \tilde{\epsilon}_k v_k^2 + 2\Delta_k v_k u_k \right] \frac{R_{0}^1(k) - R_{1}^1(k)}{R_{0}^0} \]_00

The Angle-Averaged Products

In chapter 4 we approximated the Gap function \(\Delta_k\) with an angle-averaged Gap function \(\tilde{\Delta}_k\). Here we justify this angle-averaging and present a method that can be used for any form of product of the form \(z_1^* z_2\). We write:
\[ \tilde{\Delta}_k^2 = \int \frac{d\Omega_k}{4\pi} \Delta_k^* \Delta_k = \int \frac{d\Omega_k}{4\pi} \sum_{lm,l'm'} \frac{4\pi}{2l + 1} \Delta_{lm}(k)^* \Delta_{l'm'}(k) Y_{lm}^*(\hat{k}) Y_{l'm'}(\hat{k}) = \]

\[ = \sum_{lm,l'm'} \frac{4\pi}{2l + 1} \Delta_{lm}(k)^* \Delta_{l'm'}(k) \int \frac{d\Omega_k}{4\pi} Y_{lm}^*(\hat{k}) Y_{l'm'}(\hat{k}) = \]

\[ = \sum_{lm,l'm'} \frac{4\pi}{2l + 1} \Delta_{lm}(k)^* \Delta_{l'm'}(k) \frac{1}{4\pi} \delta_{l''l'} \delta_{m'm'} = \sum_{lm} \frac{1}{2l + 1} \Delta_{lm}(k)^* \Delta_{lm}(k) = \]

\[ = \sum_{lm} \frac{1}{2l + 1} |\Delta_{lm}(k)|^2 \]

As mentioned in chapter 4, \( \tilde{\Delta}_k \) is a very good approximation of \( \Delta_k \) as long as one is interested only in the value of \( \tilde{\Delta}_k \) on the Fermi surface and not the angle dependence of \( \Delta_k \).

**The Angle-Averaged Residuum Integrals**

An angle-averaged version of the residuum integrals can be derived as follows:

Starting from the original Residuum Integrals:

\[ R^N_n(k_1, \ldots, k_N) = \frac{1}{2\pi i} \oint dz \frac{f(z)}{\chi^N_n(k_1, \ldots, k_N)} \]

where:

\[ \chi^N_n(k_1, \ldots, k_N) = \frac{z^{n-1}}{\prod_{k=k_1, \ldots, k_N} (u_k^2 + zv_k^2)} \]

we can perform an angle-averaging on \( \chi \) as follows by defining the quantities:

\[ \tilde{u}^2(k) = \sum_{lm} \frac{1}{2l + 1} |u_{lm}(k)|^2 \]

\[ \tilde{v}^2(k) = \sum_{lm} \frac{1}{2l + 1} |v_{lm}(k)|^2 \]
and:

\[ \tilde{\chi}_N^n(k_1, \ldots, k_N) = \frac{z^{n-1}}{\prod_{k=k_1 \ldots k_N} [\tilde{u}^2(k) + z\tilde{v}^2(k)]} \]

where the connection with the original \( \chi \) is just an angle averaging of the denominator:

\[
\int \frac{d\Omega_{k_1} \ldots d\Omega_{k_N}}{(4\pi)^N} \prod_{k=k_1 \ldots k_N} (u_k^2 + zv_k^2) = \prod_{k=k_1 \ldots k_N} \int \frac{d\Omega_k}{4\pi} (u_k^2 + zv_k^2) = \prod_{k=k_1 \ldots k_N} [\tilde{u}^2(k) + z\tilde{v}^2(k)]
\]

where:

\[
\int \frac{d\Omega_k}{4\pi} u_k^2 = \int \frac{d\Omega_k}{4\pi} u_k^* u_k = \int \frac{d\Omega_k}{4\pi} \sum_{lm,l'm'} u_{lm}(k)^* u_{l'm'}(k) Y_{lm}^*(\hat{k}) Y_{l'm'}(\hat{k}) = \sum_{lm,l'm'} \frac{4\pi}{2l+1} u_{lm}(k)^* u_{l'm'}(k) \int \frac{d\Omega_k}{4\pi} Y_{lm}^*(\hat{k}) Y_{l'm'}(\hat{k}) = \sum_{lm,l'm'} \frac{4\pi}{2l+1} u_{lm}(k)^* u_{l'm'}(k) \frac{1}{4\pi} \delta_{ll'} \delta_{mm'} = \sum_{lm} \frac{1}{2l+1} |u_{lm}|^2 = \tilde{u}^2(k)
\]

Finally the angle-averaged Residuum Integrals are:

\[ \tilde{R}_N^n(k_1, \ldots, k_N) = \frac{1}{2\pi i} \oint dz e^{f(z)} \tilde{\chi}_N^n(k_1, \ldots, k_N) \]

where:

\[ \tilde{\chi}_N^n(k_1, \ldots, k_N) = \frac{z^{n-1}}{\prod_{k=k_1 \ldots k_N} (u_k^2 + zv_k^2)} = \frac{z^{n-1}}{\prod_{k=k_1 \ldots k_N} [\tilde{u}^2(k) + z\tilde{v}^2(k)]} \]
We can use those to approximate the fractions of the form $\left[ \frac{R}{R_0} \right]_{00}$ in the $^1S_0$ expansion of the FBCS Gap equation.

**Computing the residuum Integrals using the Saddle Point Approximation**

It has been shown by Bayman [27] that BCS Theory can be viewed as a saddle point approximation of FBCS Theory. That is, if we approximate the Residuum Integrals (3.7) by a saddle point approximation then the FBCS Gap equation (2) will turn into the first BCS Gap equation (2.11) while the equation guaranteeing that the integrand in Eq. (3.7) has a saddle point will become the second BCS Gap Equation (2.12).

In order to see that we can recast Eq. (3.7) into:

$$R_n^N(k_1, \ldots, k_N) = \frac{1}{2\pi i} \oint dz e^{f(z)} \chi_n^N(k_1, \ldots k_N; z)$$

(12)

where:

$$f(z) \equiv -M \log z + \sum_k \log(u_k^2 + zv_k^2)$$

$$\chi_n^N(k_1, \ldots k_N; z) \equiv \frac{z^{n-1}}{\prod_{k=k_1 \ldots k_N} (u_k^2 + zv_k^2)}$$

The path of integration is a closed path around $z = 0$. Both $f(z)$ and $\chi_n^N(k_1, \ldots k_N; z)$ are analytic functions of $z$ along this path. The path of integration can be taken to pass through the Saddle Point of $f(z)$ which is defined by:

$$f'(z_0) = -\frac{M}{z_0} + \sum_k \frac{v_k^2}{u_k^2 + z_0v_k^2} = 0$$

(13)

Rearranging:
\[ M = \sum_k \frac{z_0 v_k^2}{u_k^2 + z_0 v_k^2} = \sum_k \frac{z_0 r_k^2}{1 + z_0 r_k^2} \] where \( r_k^2 \equiv \frac{r_k^2}{u_k^2} \)

Setting \( z_0 = a + ib \) the above equation becomes:

\[
\sum_k \frac{ar_k^2 (1 + ar_k^2) + (br_k^2)^2}{(1 + ar_k^2)^2 + (br_k^2)^2} = M \\
\sum_k \frac{br_k^2}{(1 + ar_k^2)^2 + (br_k^2)^2} = 0
\]

(14)  
(15)

For \( b \neq 0 \) Eq. (15) becomes:

\[
\sum_k \frac{r_k^2}{(1 + ar_k^2)^2 + (br_k^2)^2} = 0
\]

But \( \frac{r_k^2}{(1 + ar_k^2)^2 + (br_k^2)^2} > 0, \quad \forall k \) and finite \( a, b \). Therefore:

\[
\sum_k \frac{r_k^2}{(1 + ar_k^2)^2 + (br_k^2)^2} > 0, \quad \forall a, b < \infty
\]

and hence Eq. (15) can only be satisfied for \( b = 0 \). In that case, Eq. (14) becomes:

\[
\sum_k \frac{ar_k^2 (1 + ar_k^2) + (br_k^2)^2}{(1 + ar_k^2)^2 + (br_k^2)^2} = M \iff \sum_k \frac{ar_k^2}{1 + ar_k^2} = M \iff h(a) = M
\]

where we defined:

\[
h(a) \equiv \sum_k \frac{ar_k^2}{1 + ar_k^2}
\]

Now, \( f(a) \) is a monotonically increasing function since:
\[ dh(a) = \sum_k \left( \frac{r_k^2}{1 + ar_k^2} - \frac{a(r_k^2)^2}{(1 + ar_k^2)^2} \right) = \sum_k \frac{r_k^2(1 + ar_k^2) - a(r_k^2)^2}{(1 + ar_k^2)^2} = \sum_k \frac{r_k^2}{(1 + ar_k^2)^2} > 0 \quad \forall a \in \mathcal{R} \]

Therefore, \( h(a) = M \) has one or no solutions. However for \( a = 1 \) we find:

\[ h(1) = \sum_k \frac{r_k^2}{1 + r_k^2} = \sum_k \frac{v_k^2}{u_k^2 + v_k^2} = \sum_k v_k^2 = M \]

since by the definition of \( M \) and \( v_k^2, u_k^2 \):

\[ M = \frac{\langle N \rangle}{2} = \frac{\sum_k 2v_k^2}{2} = \sum_k v_k^2 \quad (16) \]

Finally the only solution to the equations is \( (a, b) = (1, 0) \):

Applying the Saddle Point approximation to the Residuum Integrals we get:

\[ R_n^N(k_1, \ldots, k_N) \approx \frac{1}{(2\pi)^{1/2}} \frac{e^{f(z_0)} \chi_n^N(k_1, \ldots, k_N; z_0)}{|f''(z_0)|^{1/2}} \quad (17) \]

where:

\[ f''(z) = \frac{M}{z^2} - \sum_k \frac{(u_k^2)^2}{(u_k^2 + vz_k^2)^2} \]

It is:

\[ \chi_n^N(k_1, \ldots, k_N; z_0) = 1 \]
\[ f(z_0) = 0 \iff e^{f(z_0)} = 1 \]
\[ f''(z_0) = M - \sum_k v_k^4 = \sum_k v_k^2 - \sum_k v_k^4 = \sum_k v_k^2 u_k^2 \]

Substituting in 17 we get:

\[ R_n^N(k_1, \ldots, k_N) \approx \frac{1}{(2\pi \sum_k v_k^2 u_k^2)^{1/2}} \]

It becomes apparent that \( R_n^N(k_1, \ldots, k_N) \) is a constant in the Saddle Point approximation. Thus all quantities in Eq. (5) containing differences of Residuum Integrals will become zero. Additionally both in Eq. (5) and in Eq. (3.9) the Residuum Integrals appear in fractions leading to them cancelling with each other once the Saddle Point approximation is employed. With the Residuum Integrals out of the equations we recover the BCS theory: The energy Eq. (3.9) turns into Eq. (2.7) while Eq. (2) will turn into the definition for \( \Delta_k \). Finally Eq. 16, which guarantees that Eqs. 14 & 15 have a solution, will turn into the second BCS Gap equation 2.12. It is important to know that throughout our review of the FBCS theory we have remained consistent with the original sign convention that was introduced by [18]. That is, \( \Delta_k \) is defined as a negative quantity in FBCS as opposed to \( \Delta_k \) in BCS. That can be seen clearly by the absence of the minus sign in the FBCS definition of \( \Delta_k \) in (5) in contrast with \( \Delta_k \) from Eq. (2.11). This convention has to be taken into account if one wishes to carry out the Saddle Point approximation and recover the BCS theory.
The derivation of the Energy expressions

The derivations of the Energy expressions for BCS and PBCS are relatively similar. In this Appendix we will begin with the derivation of the PBCS Energy and show how the corresponding BCS expression can be derived in an identical way.

In PBCS, the ground state is the state (3.4). Bracketing the Hamiltonian (2.7) with that state we get:

\[ K = \langle \psi_N | \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} | \psi_N \rangle = \]

\[ = \frac{1}{R_0^0} \sum_{k\sigma} \epsilon_k \int_{0}^{2\pi} \frac{d\phi_1}{2\pi} \frac{d\phi_2}{2\pi} e^{iM\phi_1} e^{-iM\phi_2} \times \]

\[ \times \langle 0 | \prod_{l \neq k} (u_l + v_l e^{-i\phi_2} p_l^\dagger) \hat{n}_{k\sigma} \prod_{m} (u_m + v_m e^{i\phi_2} p_m^\dagger) | 0 \rangle = \]

\[ = \frac{1}{R_0^0} \sum_{k\sigma} \epsilon_k \int_{0}^{2\pi} \frac{d\phi_1}{2\pi} \frac{d\phi_2}{2\pi} e^{iM\phi_1} e^{-iM\phi_2} \langle 0 | (u_k + v_k e^{-i\phi_1} p_k) \hat{n}_{k\sigma} (u_k + v_k e^{i\phi_2} p_k^\dagger) \times \]

\[ \times \prod_{1 \neq k} (u_1 + v_1 e^{-i\phi_1} p_1)(u_1 + v_1 e^{i\phi_2} p_1^\dagger) | 0 \rangle = \]

\[ \]

\[ = \frac{1}{R_0^0} \sum_{k} \epsilon_k \int_{0}^{2\pi} \frac{d\phi_1}{2\pi} \frac{d\phi_2}{2\pi} e^{iM\phi_1} e^{-iM\phi_2} \times \]

\[ \times \langle 0 | (u_k + v_k e^{-i\phi_1} p_k)(\hat{n}_{k\uparrow} + \hat{n}_{k\downarrow})(u_k + v_k e^{i\phi_2} p_k^\dagger) \times \]

\[ \times \prod_{1 \neq k} (u_1 + v_1 e^{-i\phi_1} p_1)(u_1 + v_1 e^{i\phi_2} p_1^\dagger) | 0 \rangle = \]
\[
= \frac{1}{R_0^0} \sum_k \epsilon_k \int_0^{2\pi} \frac{d\phi_1}{2\pi} \frac{d\phi_2}{2\pi} e^{iM\phi_1} e^{-iM\phi_2} \times \\
\times \langle 0 \rvert (u_k + v_k e^{-i\phi_1} p_k)(\hat{n}_{k\uparrow} + \hat{n}_{k\downarrow})(u_k + v_k e^{i\phi_2} p_k^\dagger) \rvert 0 \rangle \\
\times \prod_{l \neq k} (u_l + v_l e^{-i\phi_1} p_l)(u_l + v_l e^{i\phi_2} p_l^\dagger) \rvert 0 \rangle
\]

Where in the last line we have re-summed the the sum containing \(\hat{n}_{-k} \), to run the \(k\) indices in the opposite "direction". In other words we matched the terms with \(\hat{n}_{k\uparrow}\) from the first sum with the terms with \(\hat{n}_{k\downarrow}\) from the second sum. The motivation for that is that from the commutation relations we can see that \([\hat{n}_{-k\downarrow}, p_l] = -p_l(\delta_{kl}\delta_{\sigma\downarrow} + \delta_{-kl}\delta_{\sigma\uparrow}) \Rightarrow [\hat{n}_{-k\downarrow}, p_l] = p_l\delta_{kl} = -p_k\delta_{kl}\). We also have: \([\hat{n}_{-k\downarrow}, p_l] = -p_l\delta_{kl} = -p_k\delta_{kl}\). Therefore, the only term from the products that the number operators actually see is the \(k\) term. The terms outside the product are:

\[
\langle 0 \rvert (u_k + v_k e^{-i\phi_1} p_k)(n_{k\uparrow} + n_{k\downarrow})(u_k + v_k e^{i\phi_2} p_k^\dagger) \rvert 0 \rangle = \\
= \langle 0 \rvert u_k^2 (n_{k\uparrow} + n_{k\downarrow}) + u_k v_k e^{i\phi_2} (n_{k\uparrow} + n_{k\downarrow}) p_k^\dagger + \\
+ u_k v_k e^{-i\phi_1} p_k (n_{k\uparrow} + n_{k\downarrow}) + v_k^2 e^{i(\phi_2 - \phi_1)} p_k (n_{k\uparrow} + n_{k\downarrow}) p_k^\dagger \rvert 0 \rangle = \\
= v_k^2 e^{i(\phi_2 - \phi_1)} \langle 0 \rvert p_k (n_{k\uparrow} + n_{k\downarrow})^\dagger p_k^\dagger \rvert 0 \rangle = v_k^2 e^{i(\phi_2 - \phi_1)} \langle 0 \rvert p_k n_{k\uparrow} p_k^\dagger + p_k n_{-k\downarrow} p_k^\dagger \rvert 0 \rangle = \\
= v_k^2 e^{i(\phi_2 - \phi_1)} \langle 0 \rvert (n_{k\uparrow} p_k + p_k p_k^\dagger + (n_{-k\downarrow} p_k + p_k^\dagger) p_k^\dagger \rvert 0 \rangle = \\
= v_k^2 e^{i(\phi_2 - \phi_1)} \langle 0 \rvert p_k n_{k\uparrow} p_k^\dagger + p_k n_{-k\downarrow} p_k^\dagger + p_k p_k^\dagger \rvert 0 \rangle = \\
= v_k^2 e^{i(\phi_2 - \phi_1)} \left( \langle 0 \rvert p_k p_k^\dagger \rvert 0 \rangle + \langle 0 \rvert p_k^\dagger p_k^\dagger \rvert 0 \rangle \right) = 2v_k^2 e^{i(\phi_2 - \phi_1)}
\]

And:

\[
\langle 0 \rvert \prod_{l \neq k} (u_l + v_l e^{-i\phi_1} p_l)(u_l + v_l e^{i\phi_2} p_l^\dagger) \rvert 0 \rangle =
\]
\[
= \langle 0 | \prod_{l \neq k} (u_l^2 + u_1 v_1 e^{i \phi_2} p_l^0 + u_1 v_1 e^{-i \phi_1} p_l^0 + v_1^2 e^{i(\phi_2 - \phi_1)} p_l p_l^\dagger) | 0 \rangle = \\
= \prod_{l \neq k} (u_l^2 + v_1^2 e^{i(\phi_2 - \phi_1)}) \langle 0 | p_l p_l^\dagger | 0 \rangle = \prod_{l \neq k} (u_l^2 + v_1^2 e^{i(\phi_2 - \phi_1)}) 
\]

Finally:

\[
K = \frac{1}{R_0^2} \sum_k \epsilon_k \int_0^{2\pi} \frac{d \phi_1}{2\pi} \int_0^{2\pi} \frac{d \phi_2}{2\pi} e^{iM \phi_1} e^{-iM \phi_2} 2v_k^2 e^{i(\phi_2 - \phi_1)} \prod_{l \neq k} (u_l^2 + v_1^2 e^{i(\phi_2 - \phi_1)}) = \\
= \frac{1}{R_0^2} \sum_k \epsilon_k v_k^2 \int_0^{2\pi} \frac{d \phi_1}{2\pi} \int_0^{2\pi} \frac{d \phi_2}{2\pi} e^{iM (\phi_2 - \phi_1)} e^{i(\phi_2 - \phi_1)} \prod_{l \neq k} (u_l^2 + v_1^2 e^{i(\phi_2 - \phi_1)}) 
\]

Using definition (3.7) we get:

\[
K = 2 \sum_k \epsilon_k v_k^2 \frac{R_1^l(k)}{R_0^l} \tag{18}
\]

At this point there are two ways to derive the BCS expression for the Kinetic energy.

The first way relies on the fact that the BCS ground state (2.1) is the integrand of the PBCS ground state (3.4) and that we did not carry out the integration until the last step. That means that if we were to do the BCS derivation the steps would look the same without the integrals and setting both phases \(\phi_1\) and \(\phi_2\) to zero. The second way comes from the fact that, as was noted in chapter 3, BCS is the saddle point approximation of FBCS and since FBCS and PBCS share the same energy expression, the saddle point approximation of PBCS should provide us with the BCS Energy expression. Indeed, performing a saddle point approximation as it was described in chapter 3, \(\frac{R_1^l(k)}{R_0^l}\) goes to 1 leaving us with the BCS Energy expression.

Working in a similar way the potential energy is:
\[ V = \langle \psi_N | \sum_{kl} V_{kl} \hat{p}_k \hat{p}_l | \psi_N \rangle = \langle \psi_N | \sum_{k} V_{kk} \hat{p}_k \hat{p}_k + \sum_{k \neq 1} V_{kl} \hat{p}_k \hat{p}_l | \psi_N \rangle = \]
\[ = \frac{1}{P_0} \int_0^{2\pi} \frac{d\phi_1}{2\pi} \frac{d\phi_2}{2\pi} e^{iM\phi_1} e^{-iM\phi_2} \times \]
\[ \times \left[ \sum_k V_{kk} \langle 0 | (u_k + v_k e^{-i\phi_1} \hat{p}_k) \hat{p}_k (u_k + v_k e^{i\phi_2} \hat{p}_k) \times \]
\[ \times \prod_{n \neq k} (u_n + v_n e^{-i\phi_1} \hat{p}_n) (u_n + v_n e^{i\phi_2} \hat{p}_n) |0\rangle + \]
\[ + \sum_{k,l \neq 1} V_{kl} \langle 0 | (u_k + v_k e^{-i\phi_1} \hat{p}_k) (u_l + v_l e^{-i\phi_1} \hat{p}_l) \hat{p}_k \hat{p}_l (u_k + v_k e^{i\phi_2} \hat{p}_k) (u_l + v_l e^{i\phi_2} \hat{p}_l) \times \]
\[ \times \prod_{m \neq k,l} (u_m + v_m e^{-i\phi_1} \hat{p}_m) (u_m + v_m e^{i\phi_2} \hat{p}_m) |0\rangle \right] \]

For the first sum:

\[ \langle 0 | (u_k + v_k e^{-i\phi_1} \hat{p}_k) \hat{p}_k (u_k + v_k e^{i\phi_2} \hat{p}_k) |0\rangle = \]
\[ = \langle 0 | u_k^2 \hat{p}_k^\dagger \hat{p}_k + u_kv_k e^{i\phi_2} \hat{p}_k^\dagger \hat{p}_k + u_kv_k e^{-i\phi_1} \hat{p}_k \hat{p}_k + v_k^2 e^{i(\phi_2-\phi_1)} \hat{p}_k^\dagger \hat{p}_k |0\rangle = \]
\[ = v_k^2 e^{i(\phi_2-\phi_1)} \langle 0 | (\hat{p}_k^\dagger \hat{p}_k - M_k) (\hat{p}_k^\dagger \hat{p}_k - M_k) |0\rangle = \]
\[ = v_k^2 e^{i(\phi_2-\phi_1)} \langle 0 | (\hat{p}_k^\dagger \hat{p}_k - M_k) (\hat{p}_k^\dagger \hat{p}_k - M_k - M_k + M_k) |0\rangle = \]
\[ = v_k^2 e^{i(\phi_2-\phi_1)} \langle 0 | M_k M_k |0\rangle = v_k^2 e^{i(\phi_2-\phi_1)} \]

For the second sum:

\[ \langle 0 | (u_k + v_k e^{-i\phi_1} \hat{p}_k) (u_l + v_l e^{-i\phi_1} \hat{p}_l) \hat{p}_k \hat{p}_l (u_k + v_k e^{i\phi_2} \hat{p}_k) (u_l + v_l e^{i\phi_2} \hat{p}_l) |0\rangle = \]
\[ = \langle 0 | (u_k u_l + u_k v_l e^{-i\phi_1} \hat{p}_l + u_l v_k e^{-i\phi_1} \hat{p}_k + v_k v_l e^{-i\phi_1} \hat{p}_k \hat{p}_l) \hat{p}_k \hat{p}_l \times \]
\[ \times (u_k u_l + u_k v_l e^{i\phi_2} \hat{p}_l^\dagger + u_l v_k e^{i\phi_2} \hat{p}_k^\dagger + v_k v_l e^{i\phi_2} \hat{p}_k \hat{p}_l) |0\rangle = \]
\[ 0^\dagger \begin{pmatrix} p_k \dagger \end{pmatrix} \begin{pmatrix} p_1 \dagger \end{pmatrix} \begin{pmatrix} 0 \end{pmatrix} = \langle 0 | p_k \dagger p_1 \dagger | 0 \rangle = 0 \]

Since:

- \[ \langle 0 | p_k \dagger p_1 \dagger | 0 \rangle = \langle 0 | p_k \dagger p_1 | 0 \rangle = 0 \]
- \[ \langle 0 | p_k \dagger p_1 | 0 \rangle = \langle 0 | p_k \dagger p_1 \dagger | 0 \rangle = 0 \]
- \[ \langle 0 | p_k \dagger p_1 \dagger | 0 \rangle = \langle 0 | p_k \dagger p_1 | 0 \rangle = 0 \]
- \[ \langle 0 | p_k \dagger p_1 | 0 \rangle = \langle 0 | p_k \dagger p_1 \dagger | 0 \rangle = 0 \]

All of the above are direct consequences of the commutation relation \[ [p_k \dagger, p_1] = M_k \delta_{kl} \]
(see Appendix A) which for \( k \neq 1 \) becomes \[ [p_k \dagger, p_1] = 0. \] The terms that require a little more care are:

- \[ \langle 0 | p_k \dagger p_1 | 0 \rangle = \langle 0 | p_k \dagger p_k - M_k (p_1 \dagger p_1 - M_1) | 0 \rangle = \langle 0 | p_k \dagger p_k (p_1 \dagger p_1 + M_k M_1) | 0 \rangle = 0 \]
- \[ \langle 0 | p_k \dagger p_1 | 0 \rangle = \langle 0 | p_k \dagger p_k - M_k (p_1 \dagger p_1 - M_1) | 0 \rangle = \langle 0 | p_k \dagger p_k (p_1 \dagger p_1 + M_k M_1) | 0 \rangle = 0 \]

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\[ \langle 0 | p_k p_k^\dagger p_k p_k^\dagger | 0 \rangle = \langle 0 | p_k p_k^\dagger p_k p_k^\dagger | 0 \rangle = \langle 0 | (p_k p_k^\dagger p_k p_k^\dagger)^\dagger | 0 \rangle \] which is just the conjugate of the \( k \leftrightarrow 1 \) case of the second step of the previous point and therefore it is 0

\[ \langle 0 | p_k p_k^\dagger p_k p_k^\dagger | 0 \rangle = \langle 0 | p_k p_k^\dagger p_k p_k^\dagger | 0 \rangle \\
= \langle 0 | (p_k p_k^\dagger - M_k)p_k^\dagger p_k (p_1^\dagger p_1 - M_1) | 0 \rangle = \langle 0 | (p_k p_k^\dagger - M_k)p_k^\dagger p_k | 0 \rangle = \langle 0 | (p_k^\dagger M_k + p_k^\dagger) p_1 M_1 | 0 \rangle = \langle 0 | (p_k^\dagger M_k + p_k^\dagger) p_1 | 0 \rangle = \langle 0 | (p_k^\dagger M_k + p_k^\dagger) p_1 M_1 | 0 \rangle = \langle 0 | (p_k^\dagger M_k + p_k^\dagger) p_1 | 0 \rangle = 0 \]

Finally:

\[ V = \frac{1}{R_0^2} \int_0^{2\pi} \frac{d\phi_1}{2\pi} \frac{d\phi_2}{2\pi} e^{iM(\phi_2-\phi_1)} \times \left[ \sum_k v_k^2 e^{i(\phi_2-\phi_1)} \prod_{n \neq k} \left( u_n^2 + v_n^2 e^{i(\phi_2-\phi_1)} \right) + \sum_{k,l|k \neq l} v_k v_l e^{i(\phi_2-\phi_1)} \prod_{m \neq k,l} \left( u_m^2 + v_m^2 e^{i(\phi_2-\phi_1)} \right) \right] = \frac{1}{R_0^2} \sum_k v_k^2 \left( \int_0^{2\pi} \frac{d\phi_1}{2\pi} \frac{d\phi_2}{2\pi} e^{iM(\phi_2-\phi_1)} \prod_{n \neq k} \left( u_n^2 + v_n^2 e^{i(\phi_2-\phi_1)} \right) + \sum_{k,l|k \neq l} v_k v_l e^{i(\phi_2-\phi_1)} \prod_{m \neq k,l} \left( u_m^2 + v_m^2 e^{i(\phi_2-\phi_1)} \right) \right) = \sum_k v_k^2 \frac{R_1^1(k)}{R_0^2} + \sum_{k,l|k \neq l} v_k v_l \frac{R_1^1(kl)}{R_0^2} \]

As was noted in the Kinetic Energy, the corresponding BCS expression can be recovered by ignoring the integration and the phases. Alternatively, one can perform a saddle point approximation to the Residuum Integrals in the above expression. Doing so the fractions \( \frac{R_1^1(k)}{R_0^2} \) and \( \frac{R_1^1(kl)}{R_0^2} \) go to 1 and we arrive at the BCS expression for the Energy.
Bibliography


