Hartree-Fock theory for the electron gas in the mean-field regime

A Thesis

submitted to
Indian Institute of Science Education and Research Pune
in partial fulfillment of the requirements for the
BS-MS Dual Degree Programme

by

Ravish Mehta

Indian Institute of Science Education and Research Pune
Dr. Homi Bhabha Road,
Pashan, Pune 411008, INDIA.

April, 2024

Supervisor: Niels Benedikter

Certificate

This is to certify that this dissertation entitled Hartree-Fock theory for the electron gas in the mean-field regime towards the partial fulfilment of the BS-MS dual degree programme at the Indian Institute of Science Education and Research, Pune represents study/work carried out by Ravish Mehta at Indian Institute of Science Education and Research under the supervision of Niels Benedikter, Professor, Department of Mathematics, during the academic year 2023-2024.

Niels Benedikter

Committee:

Niels Benedikter

Phan Thanh Nam

Divyang Bhimani

This thesis is dedicated to my family.

Declaration

I hereby declare that the matter embodied in the report entitled "Hartree-Fock theory for the electron gas in the mean-field regime" are the results of the work carried out by me at the Department of Department of Mathematics, Indian Institute of Science Education and Research (IISER) Pune, under the supervision of Niels Benedikter, and the same has not been submitted elsewhere for any other degree. Wherever others contribute, every effort is made to indicate this clearly, with due reference to the literature and acknowledgement of collaborative research and discussions.

Ravish Mehta
20191132

Acknowledgments

My heartfelt thanks go to each member of my loving family for their unwavering love, encouragement, and support throughout my academic journey. Their constant support has been instrumental in my success.

I would like to express my deepest gratitude to my supervisors Prof Niels Benedikter and Prof Phan Thanh Nam for their guidance, patience, and unwavering support throughout the entire research process. Their expertise and invaluable feedback were crucial in shaping the direction of this thesis and the research conducted.

I would also like to extend my gratitude to my friends and colleagues in the institute for their support, encouragement, and their stimulating discussions, which provided me with new ideas and perspectives. Shoutout to Sascha, Nhi, Diwakar, Davide and Francois.

Special thanks to Sukrit Jaiswal, Kaustubh Gupta and Pranav Maheshwari who generously gave their time, listened to my woes and shared their experiences, while helping me stay positive, without which this research would not have been possible.

I would like to thank IISER Pune, University of Milan and LMU Munich for providing me with the opportunity to pursue my master's degree, and for their resources and facilities, which were essential in completing this thesis.

I acknowledge support of the ERC Starting Grant FermiMath, nr. 101040991, for part of my research activity in collaboration with Prof. Benedikter and Prof. Nam.

Abstract

The goal of this thesis is to explore the Hartree Fock ground state energy in the mean field approximation under Coulomb interaction. It was earlier believed that free Fermi gas energy is the true ground state energy in Hartree Fock approximation but Overhauser showed that there exists a state with energy lower than free Fermi gas energy. The question we explore in this thesis is whether we can multiply Coulomb potential by a small constant such that for any interaction with coupling parameter less than this constant, free Fermi gas energy is the true ground state energy and any interaction with coupling parameter greater than this constant, there exists some other state with energy lower than free fermi gas energy. We were able to derive a partial result in this direction proving that there exists some small constant such that free fermi gas energy is the true ground state energy in Hartree Fock approximation.

Contents

Chapter 1

Introduction

The concept of electron was suggested by JJ Thompson in 1897 [1] and since then systems of electrons have been widely studied. Diamagnetism and the low temperature specific heat were successfully explained by 1928 [2] considering electrons as independent particles obeying the Pauli exclusion principle which states that no two electrons can occupy the same state. It is very surprising that this non interacting model could explain these properties despite the fact that electrons are charged particles and under Coulomb repulsive forces. Since then a lot of work has been devoted to studying the effects resulting from interaction. The model that we use is the Jellium model which is a model in which electrons are particles in a positive charged background. This makes the model translation invariant with respect to the background and hence makes it easier to study interaction effects.

The exact Hamiltonian of the system is very difficult to handle because the degrees of freedom in a real world system are of the order of 10^{23}. To make our calculations easier, we make approximations. One such approximation is Hartree Fock approximation [3]. Under this, our effective Hamiltonian is quadratic in fermionic creation and annihilation operators. This makes it easier to diagonalise compared to the general case. It can be shown that a fermionic N particle state can be written as a complex linear combination of Slater determinants [4]. Under Hartree Fock approximation, we set the true ground state of the system as a single Slater determinant. We then determine the single particle states by requiring that the expectation value of Hamiltonian in this state is minimal. The problem with this approach is that even the true HF ground state is unknown till now.

As HF ground state is an approximation to the actual ground state, it becomes important to find the difference between the true ground state energy and the HF ground state energy. This difference is called the correlation energy. But this only makes sense if we know the true HF ground state energy, which we don't. Hence, it is common practice to define the correlation energy with respect to a particular HF state [4]. For jellium model, we commonly take it to be the free fermi gas state, i.e., the ground state of non interacting Hamiltonian.

The natural question that arises after this is to find the difference between the true HF ground state energy and the free fermi gas energy. It was shown by Gontier, Hainzl and Lewin that the difference between the two is exponentially small for Coulomb potentials in the thermodynamic (large volume) limit [5]. In my thesis, I worked on the mean field limit and tried to find this difference for Coulomb potentials multiplied by a constant.

Mean field limit is the case when we have the coupling constant in the interaction term of the order of N^{-1}. Because of this, we have both Kinetic term and interaction term to be of the same order [6].

The reason we are considering Coulomb potentials multiplied by a constant is that electromagnetic interactions between elementary charged particles have a constant multiplied which quantifies the interaction strength. This constant is called the fine structure constant and its value is roughly $\frac{1}{137}$. As a mathematical idealisation, we consider this constant to approach 0.

Chapter 2

Preliminaries

2.1 Operator theory

In this section, I follow the book by Gerald. (citation)
Suppose $\mathbf{h}$ is a vector space. A map $\langle .,. \rangle : \mathbf{h} \times \mathbf{h} \to C$ is called a sesquilinear form if it is conjugate linear in the first argument and linear in the second. A positive definite sesquilinear form is called an inner product. Associated with each inner product is a norm defined by

$$||\psi|| = \sqrt{\langle \psi, \psi \rangle}. \tag{2.1}$$

If $\mathbf{h}$ is complete with respect to the above norm, it is called a Hilbert space.
A linear map between two normed spaces is called a linear operator. A bijective linear operator $U \in \mathcal{L}(\mathbf{h}_1, \mathbf{h}_2)$ is called unitary if U preserves scalar products:

$$\langle U\phi, U\psi \rangle = \langle \phi, \psi \rangle, \quad \phi, \psi \in \mathbf{h}_1. \tag{2.2}$$

The adjoint of an operator is defined via

$$\langle \phi, A^* \psi \rangle = \langle A\phi, \psi \rangle. \tag{2.3}$$

A linear operator is called bounded if the operator norm

$$||A|| = \sup_{||\psi||=1} ||A\psi|| \tag{2.4}$$

is finite.
A densely defined linear operator is called symmetric if

$$\langle \phi, A\psi \rangle = \langle A\phi, \psi \rangle, \quad \psi, \phi \in \mathcal{D}(A). \tag{2.5}$$

It is clear that $A \subseteq A^*$ for symmetric operators. If we have, $A = A^*$, we call A to be a self adjoint operator.

Lemma 2.1. *Let A be symmetric. Then all eigenvalues are real and eigenvectors corresponding to different eigenvalues are orthogonal.*

Proof. If $A\psi_j = \lambda_j \psi_j, \qquad j = 1, 2$, we have

$$\lambda_1 ||\psi_1||^2 = \langle \psi_1, \lambda_1 \psi_1 \rangle = \langle \psi_1, A\psi_1 \rangle = \langle A\psi_1, \psi_1 \rangle = \langle \lambda_1 \psi_1, \psi_1 \rangle = \lambda_1^* ||\psi_1||^2$$

and

$$(\lambda_1 - \lambda_2)\langle \psi_1, \psi_2 \rangle = \langle A\psi_1, \psi_2 \rangle - \langle A\psi_1, \psi_2 \rangle = 0.$$

□

The closure of the set of all finite rank operators is called the set of compact operators. Among compact operators, two special cases are of particular importance. The first ones are integral operators

$$K\psi(x) = \int_M K(x, y)\psi(y) d\mu(y), \quad \psi \in L^2(M, d\mu), \tag{2.6}$$

where $K(x, y) \in L^2(M \times M, d\mu \otimes d\mu)$. Such an operator is called a Hilbert-Schmidt operator. It can be checked that K is a bounded operator.

Another class of operators is the trace class operator. An operator is called trace class if it can be written as the product of two Hilbert Schmidt operators, $K = K_1 K_2$, and in this case we have

$$||K||_1 \leq ||K_1||_2 ||K_2||_2 \tag{2.7}$$

If K is trace class, then for every orthonormal basis $\{\phi_n\}$ the trace

$$tr(K) = \sum_n \langle \phi_n, K\phi_n \rangle \tag{2.8}$$

is finite and independent of the orthonormal basis.

2.2 The principles of Quantum Mechanics

In this section, I used Prof. Phan Thanh Nam and Prof. Jan Philip Solovej's notes [7, 8]. In Quantum Mechanics, a pure state of the system is given by a unit vector ψ_0 in Hilbert space $\mathcal{H}$. The measurable quantities correspond to expectation values given by

$$\langle A\rangle_{\psi_0} = (\psi_0, A\psi_0), \tag{2.9}$$

of operators A on $\mathcal{H}$. This requires us to have $\psi_0 \in D(A)$. Since all measurable quantities are real, we must have that operators A are self-adjoint. The quantity $\langle A\rangle_{\psi_0}$ physically means taking average of many measurements of observable described by operator A in state ψ_0.

The general quantum mechanical state is not necessarily pure and given by a convex combination of pure states. The expectation values are given by

$$\langle A\rangle = \sum_{n=1}^{\infty} \lambda_n (\psi_n, A\psi_n), \tag{2.10}$$

where $0 \leq \lambda_n \leq 1$ and $\sum_n \lambda_n = 1$ and ψ_n is a family of orthonormal vectors. We will mainly work with ground states which are the lowest eigenvalue states of the energy operator called the Hamiltonian. Consider a physical system described by a Hamiltonian H acting on a Hilbert space $\mathcal{H}$. If

$$\inf_{\phi\in D(H), ||\phi||=1} (\phi, H\phi) > -\infty, \tag{2.11}$$

the system is called stable. If the system is stable, we define the ground state energy as

$$E = \inf_{\phi\in D(H), ||\phi||=1} (\phi, H\phi). \tag{2.12}$$

2.2.1 Many Body Quantum Mechanics

Consider N quantum particles on Hilbert spaces $\mathbf{h_1}, \mathbf{h_2}...\mathbf{h_N}$ and with Hamiltonian operators $h_1, ..., h_N$. The combined system of these particles is described on the tensor product

$$\mathcal{H}_N = \mathbf{h_1} \otimes \mathbf{h_2} \otimes ... \otimes \mathbf{h_N}. \tag{2.13}$$

We can identify operators $h_1, ..., h_N$ on this tensor product space i.e. operator h_i can be given by

$$I \otimes ... \otimes h_i \otimes ... \otimes I. \tag{2.14}$$

If particles are not interacting, the Hamiltonian for combined system is given by

$$H_N^{\text{nin}} = h_1 + ... + h_N. \tag{2.15}$$

The domain for this operator is given by

$$D(H_N^{\text{nin}}) = \text{span}\{\phi_1 \otimes ... \otimes \phi_N | \phi_1 \in D(h_1), ..., \phi_N \in D(h_N)\}. \tag{2.16}$$

Theorem 2.2. *If*

$$e_j = \inf_{\substack{\phi \in D(h_j), \\ ||\phi||=1}} (\phi, h_j \phi), \quad j = 1, ..., N$$

are ground state energies of the Hamiltonians $h_1, ..., h_N$, then the ground state energy of H_N^{nin} is $\sum_{j=1}^N e_j$. Also, if $\phi_1, ..., \phi_N$ are ground state eigenvectors of $h_1, ..., h_N$, then $\phi_1 \otimes ... \otimes \phi_N$ is a ground state eigenvector for H_N^{in}

Proof. If $\Psi \in D(H_N^{\text{nin}})$ is a unit vector, we may write

$$\Psi = \psi_1 \otimes \Psi_1 + ... + \psi_k \otimes \Psi_k, \tag{2.17}$$

where $\psi_1, ..., \psi_k \in D(h_1)$ and $\Psi_1, ..., \Psi_k \in \mathbf{h}_2 \otimes ... \otimes \mathbf{h}_N$ are orthonormal. Since Ψ is a unit vector, we have $||\Psi_1||^2 + ... + ||\Psi_k||^2 = 1$.
We have

$$(\Psi, h_1 \Psi) = \sum_{i=1}^K (\psi_i, h_1 \psi_i) \geq \sum_{i=1}^K ||\psi_i||^2 e_1 = e_1. \tag{2.18}$$

Hence, $(\Psi, H_N^{\text{nin}} \Psi) \geq \sum_{j=1}^N e_j$.

If we, given $\epsilon > 0$, choose unit vectors $\phi_j \in D(h_j), j = 1, ..., N$ such that $(\phi_j, h_j\phi_j) < e_j + \epsilon$ for $j = 1, ..., N$ and define $\Psi = \phi_1 \otimes ... \otimes \phi_N$. We find that Ψ is a unit vector and

$$(\Psi, H_N^{\text{nin}}\Psi) = \sum_{j=1}^{N}(\phi_j, h_j\phi_j) \leq \sum_{j=1}^{N} e_j + N\epsilon. \tag{2.19}$$

It is clear that if $\phi_1, ..., \phi_N$ are ground state eigenvectors for $h_1, ..., h_N$, then Ψ is a ground state eigenvector for H_N^{in} □

It is more interesting to look at interacting systems. The interaction of particle i and particle j is described by an operator W_{ij} acting in the Hilbert space $\mathbf{h}_i \otimes \mathbf{h}_j$. This can also be identified as an operator on $\mathbf{h}_1 \otimes ... \otimes \mathbf{h}_N$. The interacting Hamiltonian is formally

$$H_N = H_N^{\text{nin}} + \sum_{1\leq i<j\leq N} W_{ij} = \sum_{j=1}^{N} h_j + \sum_{1\leq i<j\leq N} W_{ij} \tag{2.20}$$

Determining the ground state energy and possible ground state eigenfunctions of an interacting many particle quantum Hamiltonian is a very difficult problem. For this, approximate methods have been developed.

Let us now discuss statistics of identical particles. Assume that the N particles discussed above are identical, i.e.,

$$\mathbf{h}_1 = ... = \mathbf{h}_N = \mathbf{h}, \ h_1 = ... = h_N = h. \tag{2.21}$$

For interacting particles, we have that the two-body potential W_{ij} is the same operator W for all i and j and ExWEx $= W$, where Ex is the unitary exchange operator.

The non-interacting operator H_N^{in} maps vectors in the subspaces $\otimes_{sym}^N \mathbf{h}$ and $\wedge^N \mathbf{h}$ into the same subspaces. The operator can therefore be restricted to domains

$$P_+ D(H_N^{in}) \text{ or } P^- D(H_N^{in}). \tag{2.22}$$

If we restrict to the symmetric subspace $\otimes_{sym}^N \mathbf{h}$, we refer to the particles as bosons and antisymmetric subspace for fermions. The physics is very different for these two types of systems.

The interaction Hamiltonian will also map the symmetric and antisymmetric subspaces to themselves.

2.3 Hartree Fock Variational Problem

We will look at a simpler problem first. We will try to get the Schrodinger Equation $H\Psi = E\Psi$. Lets say we have to find $\inf_{||\Psi||=1}\langle\Psi, H\Psi\rangle$. For this we use the method of Lagrange multipliers and do a variation of Ψ in the above equation and set it to 0.

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}\varepsilon}(\langle\Psi+\varepsilon\chi, H(\Psi+\varepsilon\chi)\rangle - E(||\Psi+\varepsilon\chi||^2-1))|_{\varepsilon=0} = 0,\\
&\frac{d}{d\varepsilon}(\varepsilon(\langle\chi, H\Psi\rangle + \langle\Psi, H\chi\rangle) - 2E\varepsilon\langle\Psi,\chi\rangle) = 0,\\
&\langle(H-E)\Psi,\chi\rangle = 0,\\
&H\Psi = E\Psi. \qquad (2.23)
\end{aligned}$$

In this, we have expanded the inner product and kept only the terms with order 1 in ϵ because we are differentiating with respect to ϵ. We have also used that H is a self-adjoint operator. Now we will consider the Hartree Fock case. We have to find $\inf_{\substack{\{\phi_j\}_{j=1}^n,\\ ||\phi_j||=1}}\langle\bigwedge_j\phi_j, H\bigwedge_j\phi_j\rangle$. For this, we again use the method of Lagrange multipliers and do a variation in ϕ_k. We get

$$\begin{aligned}
&\frac{d}{d\varepsilon}(\langle\phi_1\wedge...\wedge(\phi_k+\varepsilon\chi)\wedge..\wedge\phi_n, H(\phi_1\wedge...\wedge(\phi_k+\varepsilon\chi)\wedge..\wedge\phi_n)\rangle\\
&-\sum_{j=1,j\neq k}^{n}\lambda_j(||\phi_j||^2-1) - \lambda_k(||\phi_k+\varepsilon\chi||^2-1) = 0, \qquad (2.24)\\
H = &-\sum_{i=1}^{n}(\frac{1}{2}\nabla_i^2 - G_i) + \sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\frac{1}{r_{ij}} = \sum_{i=1}^{n}H_i^{\text{core}} + \sum{}'\frac{1}{r_{ij}}. \qquad (2.25)
\end{aligned}$$

Here we have specified the exact form of our interaction Hamiltonian. Let us first focus on H_k^{core}.

$$\frac{d}{d\varepsilon}(\langle\phi_1\wedge...\wedge(\phi_k+\varepsilon\chi)\wedge..\wedge\phi_n, H_k^{\text{core}}(\phi_1\wedge...\wedge(\phi_k+\varepsilon\chi)\wedge..\wedge\phi_n)\rangle. \qquad (2.26)$$

The antisymmetric product is just the Slater determinant of

$$\frac{1}{\sqrt{N!}}\begin{vmatrix}\phi_1(x_1) & . & . & \phi_n(x_1)\\ \phi_1(x_2) & . & . & .\\ . & . & . & .\\ \phi_1(x_n) & . & . & \phi_n(x_n)\end{vmatrix}. \qquad (2.27)$$

It can be checked that all terms of the Slater determinant give 0 when we take derivative with respect to ε, other than terms of the form

$$\langle \phi_1(x_a)..(\phi_k + \varepsilon\chi)(x_k)..\phi_n(x_b), H_k^{\text{core}}(\phi_1(x_a)..(\phi_k + \varepsilon\chi)(x_k)..\phi_n(x_b))\rangle. \tag{2.28}$$

After taking derivative with respect to ε, we finally get

$$\frac{d}{d\varepsilon}(\langle \phi_1 \wedge ... \wedge (\phi_k + \varepsilon\chi) \wedge .. \wedge \phi_n, H_k^{\text{core}}(\phi_1 \wedge ... \wedge (\phi_k + \varepsilon\chi) \wedge .. \wedge \phi_n)\rangle = 2\langle H_k^{\text{core}}(\phi_k(x_k)), \chi\rangle. \tag{2.29}$$

Now we will look at the other term $\frac{1}{r_{ij}}$.

Like the case with H_i^{core}, it can be checked that all terms will be 0 except those where product on both sides differ by at most 1 permutation. The 2 types of terms we get are

$$\langle \phi_k'(x_i)\phi_l(x_j), \frac{1}{r_{ij}}\phi_k'(x_i)\phi_l(x_j)\rangle, \tag{2.30}$$

$$-\langle \phi_k'(x_i)\phi_l(x_j), \frac{1}{r_{ij}}\phi_k'(x_j)\phi_l(x_i)\rangle. \tag{2.31}$$

The expressions that we get from (2.30) and (2.31) are

$$2\sum_{j=1}^{n}\langle \phi_j^*(x_j)\frac{1}{r_{kj}}\phi_k(x_k)\phi_j(x_j), \chi\rangle, \tag{2.32}$$

$$-2\sum_{j=1}^{n}\langle \phi_j^*(x_j)\frac{1}{r_{kj}}\phi_k(x_j)\phi_j(x_k), \chi\rangle. \tag{2.33}$$

We also get $-2\lambda_k\langle \phi_k, \chi\rangle$ by taking derivative of the term $-\lambda_k(||\phi_k + \varepsilon\chi||^2 - 1)$.
The resulting equation we get is

$$H_k^{\text{core}}(\phi_k(x_k)) + \sum_{j=1}^{n}\langle \phi_j^*(x_j)\frac{1}{r_{kj}}\phi_k(x_k)\phi_j(x_j) - \sum_{j=1}^{n}\langle \phi_j^*(x_j)\frac{1}{r_{kj}}\phi_k(x_j)\phi_j(x_k) = \lambda_k\phi_k. \tag{2.34}$$

2.4 Fock space

We return to the study of the N-body operator

$$H_N = H_N^{\text{nin}} + \sum_{1\leq i<j\leq N} W_{ij} = \sum_{j=1}^{N} h_j + \sum_{1\leq i<j\leq N} W_{ij} \tag{2.35}$$

defined on the Hilbert space $\mathcal{H}_N = \mathbf{h}_1 \otimes ... \otimes \mathbf{h}_N$. This situation where we study a fixed number of particles is called canonical picture. But we can also define a new space to study all particle numbers at the same time. This would make it easier to study the creation and annihilation of particles in our system. We define this space as the Fock Hilbert space and it is given by

$$\mathcal{F} = \bigoplus_{N=0}^{\infty} \mathbf{h}_1 \otimes ... \otimes \mathbf{h}_N \tag{2.36}$$

(where $N = 0$, we interpret $\mathbf{h}_1 \otimes ... \otimes \mathbf{h}_N$ as simply $\mathbf{C}$ and refer to it as the 0-particle space, the vector $1 \in \mathbf{C}$ is often called the vacuum vector and denoted by Ω or $|\Omega\rangle$ and the operator

$$H = \bigoplus_{N=0}^{\infty} H_N, \quad H \bigoplus_{N=0}^{\infty} \Psi_N = \bigoplus_{N=0}^{\infty} H_N \Psi_N \tag{2.37}$$

This situation when all particles are considered at the same time is called the grand canonical picture.

Of special interest are the cases when we have identical particles. In this case, we can introduce the bosonic Fock space

$$\mathcal{F}^B(\mathbf{h}) = \bigoplus_{N=0}^{\infty} \bigotimes_{\text{sym}}^{N} \mathbf{h} \tag{2.38}$$

and the fermionic Fock space

$$\mathcal{F}^B(\mathbf{h}) = \bigoplus_{N=0}^{\infty} \bigwedge^{N} \mathbf{h} \tag{2.39}$$

In this case, we refer to $\mathbf{h}$ as the one particle space.

2.5 Fermion density matrices

This section is based on the method suggested in Prof. Phan Thanh Nam and Prof. Jan Philip Solovej's notes [7, 8]. We take our Hilbert space $\mathcal{H} := L^2(\mathbf{R}^3) \otimes \mathbf{C}^{\mathbf{q}}$. We can define Fock space corresponding to this Hilbert space as $\mathcal{H} = \bigoplus_{N=0}^{\infty} \mathcal{H}^{(N)}$ where $\mathcal{H}^{(0)} = \mathbf{C}$, and $\mathcal{H}^{(N)} = \bigwedge_{i=1}^{N} \mathcal{H}$. The fermionic creation and annihilation operators obey the anti-commutation relations given by

$$a(f)a^{\dagger}(g) + a^{\dagger}(g)a(f) := \{a(f), a^{\dagger}(g)\} = \langle f, g\rangle, \tag{2.40}$$

$$\{a(f), a(g)\} = \{a^{\dagger}(f), a^{\dagger}(g)\} = 0. \tag{2.41}$$

Given N orthonormal elements $\chi_1, ..., \chi_N \in \mathcal{H}$, we compute

$$a^{\dagger}(\chi_1)....a^{\dagger}(\chi_N)|0\rangle = (N!)^{-1/2} \sum_{\pi} (-1)^{\pi} \chi_{\pi(1)} \otimes .... \otimes \chi_{\pi(N)} \in \mathcal{H}^{(N)}, \tag{2.42}$$

where the sum runs over all permutations π of (1,2,...,N). These wavefunctions are called slater dterminants and the set of all slater determinants is represented by $\mathrm{SD}_N \subseteq \mathcal{H}^{(N)}$.
Let ρ_N be an N-particle density matrix i.e. $\rho_N = \sum_i |\Psi_{N,i}\rangle \lambda_i \langle \Psi_{N,i}|$ for orthonormal set $\{\Psi_{N,i}\}_{i \in \mathbf{N}} \subseteq \mathcal{H}^{(N)}\}$ and nonnegative numbers $0 \leq \lambda_i \leq 1$, $\sum_i \lambda_i = 1$. The expectation value of an operator A with respect to state ρ_N is given by

$$\begin{aligned} \langle A \rangle &= tr_N\{A\rho_N\} = \frac{1}{p!} tr_p\{A^{(p)}\rho_N^{(p)}\} \\ &= \frac{1}{p!} \sum_{i_1,...,i_p} \sum_{j_1,...,j_p} A^{(p)}_{i_1,...,i_p;j_1,...,j_p} \langle a^{\dagger}_{i_p}...a^{\dagger}_{i_1} a_{j_1}..a_{j_p}\rangle. \end{aligned} \tag{2.43}$$

The reduced density matrices are given by

$$\rho_{N\ j_1,...,j_p;i_1,...,i_p}^{(p)} = \langle a^{\dagger}_{i_p}...a^{\dagger}_{i_1} a_{j_1}..a_{j_p}\rangle. \tag{2.44}$$

Now call γ_ρ and Γ_ρ to be the 1-particle density matrix and 2-particle density matrix respectively.

$$\gamma_\rho = \sum_{i=1}^{N} |\xi_i\rangle\langle\xi_i|, \tag{2.45}$$

$$\Gamma_\rho = \sum_{i,j=1}^{N} |\xi_i \wedge \xi_j\rangle\langle\xi_i \wedge \xi_j| \tag{2.46}$$

$$= (\gamma_\rho \otimes \gamma_\rho) - \mathrm{Ex}(\gamma_\rho \otimes \gamma_\rho), \tag{2.47}$$

where Ex is the exchange operator given by

$$\mathrm{Ex} = \sum_{i,j} |\phi_i \otimes \phi_j\rangle\langle\phi_j \otimes \phi_i|. \tag{2.48}$$

2.6 Lieb's Variational principle

The HF energy is given by

$$E_{\mathrm{HF}}(N, Z, R) = inf\{\langle\Psi_N|H_N(Z, R)|\Psi_N\rangle|\Psi_N \in \mathrm{SD}_N \cap \mathrm{D}_N\}. \tag{2.49}$$

We know $E_Q(N, Z, R) \leq E_{\mathrm{HF}}(N, Z, R)$. We can write E_{HF} as

$$E_{\mathrm{HF}}(N, Z, R) = inf\{\varepsilon_{\mathrm{HF}}(\gamma)|\gamma = \gamma^2, tr_1\{\gamma\} = N, tr_1\{h\gamma\} < \infty\}, \tag{2.50}$$

where

$$\varepsilon_{HF}(\gamma) = tr_1\{h\gamma\} + \frac{1}{2}tr_2\{V(1 - \mathrm{Ex})(\gamma \otimes \gamma)\}. \tag{2.51}$$

We will show that we don't lose anything if we don't assume γ to be a projection.

Lemma 2.3. *Define $\mathcal{H}$,h, V, and ε_{HF} as above. Let $0 \leq \gamma \leq 1$, $tr_1\{\gamma\} = N$ be a 1-particle density matrix of finite rank. Then there exists a projection $\hat{\gamma} = \hat{\gamma}^2$, $tr_1\{\hat{\gamma}\} = N$, such that*

$$\varepsilon_{HF}(\gamma) \geq \varepsilon_{HF}(\hat{\gamma}). \tag{2.52}$$

Furthermore, $V > 0$ implies the strictness of this inequality unless γ is a projection itself.

Proof. We may assume $\varepsilon_{HF} < \infty$. We can take the eigenbasis of γ because it is a 1-particle density matrix. Working in an eigenvector basis of γ, we may write

$$\gamma = \sum_{k=1}^{M} |\phi_k\rangle \lambda_k \langle \phi_k|, \ \sum_{k=1}^{M} \lambda_k = N, \ 0 < \lambda_k \leq 1, \ \langle \phi_k | \phi_l \rangle = \delta_{kl}, \tag{2.53}$$

for some $M < \infty$. Let us abbreviate $\bar{h_k} = h_{kk}$ and $\bar{V_k} l = V_{kl;kl} - V_{kl;lk}$. We get

$$\varepsilon_{HF}(\gamma) = \sum_{k=1}^{M} \lambda_k \bar{h_k} + \frac{1}{2} \sum_{k,l=1}^{M} \lambda_k \lambda_l \bar{V_{kl}}. \tag{2.54}$$

We assume that $M > N$. Then there are at least 2 eigenvalues $0 < \lambda_p, \lambda_q < 1$ and we may assume

$$\bar{h_q} + \sum_{k=1}^{M} \lambda_k \bar{V_{kq}} \leq \bar{h_p} + \sum_{k=1}^{M} \lambda_k \bar{V_{kp}}. \tag{2.55}$$

Let $\delta = \min\{\lambda_p, 1 - \lambda_q\} > 0$ and define

$$\overline{\gamma} = \left(\sum_{p,q \neq k=1}^{M} |\phi_k\rangle \lambda_k \langle \phi_k| \right) + |\phi_p\rangle(\lambda_p - \delta)\langle \phi_p| + |\phi_p\rangle(\lambda_p + \delta)\langle \phi_q| \tag{2.56}$$

We get $\varepsilon_{\mathrm{HF}}(\overline{\gamma}) - \varepsilon_{\mathrm{HF}}(\gamma) < 0$. Define

$$n(\gamma) = |\{\lambda_k | 0 < \lambda_k < 1\}| \tag{2.57}$$

We can see that $n(\overline{\gamma}) \leq n(\gamma) - 1$. After at most $M - N$ iterations of this, we get a 1-particle density matrix $\hat{\gamma}$ which obeys $\varepsilon_{\mathrm{HF}}(\hat{\gamma}) < \varepsilon_{\mathrm{HF}}(\gamma)$ and $n(\hat{\gamma}) = 0$. But the latter means that $\hat{\gamma} = \hat{\gamma}^2$. □

Using this lemma, we get Lieb's variational principle as a Corollary.

Corollary 2.4. *(Lieb's Variational Principle)*

$$E_{HF}(N, Z, R) = inf\{\varepsilon_{HF}(\gamma) | 0 \leq \gamma \leq 1, \mathrm{Tr}_1\{\gamma\} = N, \mathrm{Tr}_1\{h\gamma\} < \infty\} \tag{2.58}$$

Chapter 3

Direct Method

3.1 1 fermion outside fermi sphere

As an exercise, I try to calculate the energy difference between the plane wave state and the state with 1 electron outside the fermi sphere. For this, we will introduce a map $\mathtt{R} : F \to F$ with the properties:

$$\mathtt{R}\Omega = \bigwedge_{k \in B_f} f_k \text{ where } f_k = (2\pi)^{-\frac{3}{2}} e^{ikx}, \tag{3.1}$$

$$Ra_k^* R^* = \begin{cases} a_k^* \text{ if } k \in B_f^c \\ a_k \text{ if } k \in B_f. \end{cases} \tag{3.2}$$

Ground state energy is given by $\inf_{||\Psi||=1} \langle \Psi, H\Psi \rangle$. We can rewrite this using the above map as

$$\langle \Psi, H\Psi \rangle = \langle R^* R\Psi, HR^* R\Psi \rangle = \langle R\Psi, RHR^* R\Psi \rangle = \langle \xi, H'\xi \rangle, \tag{3.3}$$

$$\inf_{\substack{||\Psi||=1, \\ \mathcal{N}\Psi = N\Psi}} \langle \Psi, H\Psi \rangle = \inf_{\substack{||\xi||=1, \\ (\mathcal{N}_\mathrm{p} - \mathcal{N}_\mathrm{h})\xi = 0}} \langle \xi, H'\xi \rangle. \tag{3.4}$$

We return to our N-body Hamiltonian and we will now try to write it in the second quantised form.

$$H = \bigoplus_{N=1}^{\infty} \sum_{j=1}^{N} h_j + \bigoplus_{N=2}^{\infty} \sum_{1 \le i < j \le N} W_{ij} \tag{3.5}$$

Lemma 3.1. *The 1-body operator $\bigoplus_{N=1}^{\infty} \sum_{j=1}^{N} h_j$ can be written in second quantised form*

as

$$\sum_{n=1}^{\infty}\sum_{m=1}^{\infty}(u_m, Hu_n)a_m^* a_n \tag{3.6}$$

where we have used the notation $a_m^* = a^*(u_m)$ *and* $\{u_i\}_{i=1}^{\infty}$ *is an orthonormal basis in* $\mathbf{h}$.

Proof. It suffices to prove that

$$\sum_{i=1}^{N} h_i \Psi_N = \sum_{m,n\geq 1}(u_m, hu_n)a_m^* a_n \Psi_N \tag{3.7}$$

for all $\Psi_N \in \mathcal{H}$ and for all N. We have

$$(a_m^* a_n \Psi_N)(x_1, .., x_N) = \sum_{i=1}^{N}(-1)^{N-i}u_m(x_i)\int \overline{u_n(y)}\Psi_N(x_1, .., x_{i-1}, x_{i+1}, .., x_N, y)dy \tag{3.8}$$

So,

$$\begin{aligned}
&\sum_{m,n}(u_m, hu_n)(a_m^* a_n \Psi_N)(x_1, .., x_N) \\
&\quad = \sum_{m,n}(u_m, hu_n)\sum_{i=1}^{N}(-1)^{N-i}u_m(x_i)\int \overline{u_n(y)}\Psi_N(x_1, .., x_{i-1}, x_{i+1}, .., x_N, y)dy \\
&\quad = \sum_{i=1}^{N}(-1)^{N-i}\sum_{n}\left(\sum_{m}(u_m, hu_n)u_m(x_i)\right)\int \overline{u_n(y)}\Psi_N(x_1, .., x_{i-1}, x_{i+1}, .., x_N, y)dy \\
&\quad = \sum_{i=1}^{N}(-1)^{N-i}\sum_{n}(hu_n)(x_i)\int \overline{u_n(y)}\Psi_N(x_1, .., x_{i-1}, x_{i+1}, .., x_N, y)dy \\
&\quad = \sum_{i=1}^{N}(-1)^{N-i}\sum_{n}[(|hu_n\rangle\langle u_n|)_N \Psi_N](x_1, .., x_{i-1}, x_{i+1}, .., x_N, x_i) \\
&\quad = \sum_{i=1}^{N}(-1)^{N-i}[\left((h\sum_{n}|u_n\rangle\langle u_n|\right)_N \Psi_N](x_1, .., x_{i-1}, x_{i+1}, .., x_N, x_i) \\
&\quad = \sum_{i=1}^{N}(-1)^{N-i}[h_N \Psi_N](x_1, .., x_{i-1}, x_{i+1}, .., x_N, x_i) \\
&\quad = \sum_{i=1}^{N}[h_i \Psi_N](x_1, .., x_{i-1}, x_i, x_{i+1}, .., x_N)
\end{aligned}$$

Here we have use the Parseval's identity

$$\sum_m (u_m, hu_n)u_m = hu_n, \tag{3.9}$$

the resolution of identity operator

$$\sum_n |u_n\rangle\langle u_n| = \mathbf{1}, \tag{3.10}$$

and the antisymmetry of fermionic wave function. □

Similarly the two-body operator can be written in second quantised form as

$$\bigoplus_{n=0}^{\infty}\Big(\sum_{1\le i<j\le N} W_{ij}\Big) = \frac{1}{2}\sum_{m,n,p,q\ge 1}(u_m\otimes u_n, Wu_p\otimes u_q)a_m^* a_n^* a_q a_p \tag{3.11}$$

The Hamiltonian H can be written as an operator on fermionic Fock space $\mathcal{F}$ as

$$H = \sum_{m,n} h_{mn}a_m^* a_n + \frac{1}{2}\sum_{m,n,p,q} W_{mnpq}a_m^* a_n^* a_q a_p \tag{3.12}$$

The interaction Hamiltonian H can be written in the second quantised form as

$$H = \hbar^2\sum_{k\in Z^3} k^2 a_k^* a_k + \lambda\sum_{k,l,q\in Z^3}\hat{V}(k)a_{l+k}^* a_{q-k}^* a_q a_l, \tag{3.13}$$

$$H' = RHR^* = \hbar^2\sum_{k\in B_f^c} k^2 a_k^* a_k + \hbar^2\sum_{k\in B_f} k^2 a_k a_k^* + \text{ (16 interaction terms)}. \tag{3.14}$$

The 16 interaction terms correspond to $(q-k), (l+k), q, l \in B_f$ or $\in B_f^c$ and are given by (3.18).

Now we can use commutation rules for creation and annihilation operators to get

$$H' = \hbar^2\sum_{k\in B_f^c} k^2 a_k^* a_k - \hbar^2\sum_{k\in B_f} k^2 a_k^* a_k + \hbar^2\sum_{k\in B_f} k^2 + \text{ (16 interaction terms)}, \tag{3.15}$$

$$\langle\Psi, H'\Psi\rangle = E_{\text{pw}} + E_{\text{kin}} + E_{\text{int}}. \tag{3.16}$$

This makes it easy to find the difference between plane wave energy and the energy of our system in which we have 1 electron outside the fermi sphere with momentum p and 1 hole

inside it with momentum h. We will have to evaluate $E_{\text{kin}} + E_{\text{int}}$.

$$E_{\text{kin}} = \langle \Psi, (\hbar^2 \sum_{k \in B_f^c} k^2 a_k^* a_k - \hbar^2 \sum_{k \in B_f} k^2 a_k^* a_k)\Psi \rangle = \hbar^2(p^2 - h^2), \tag{3.17}$$

where $\Psi = a_p^* a_h^* \Omega$.

$$\begin{aligned}
H_{\text{int}} = \lambda \Bigg(& \sum_{\substack{l+k \in B_f^c, \\ q-k \in B_f^c, \\ q \in B_f^c, \\ l \in B_f}} \hat{V(k)} a_{l+k}^* a_{q-k}^* a_q a_l^* + \sum_{\substack{l+k \in B_f^c, \\ q-k \in B_f^c, \\ q \in B_f, \\ l \in B_f}} \hat{V(k)} a_{l+k}^* a_{q-k}^* a_q^* a_l^* + \sum_{\substack{l+k \in B_f^c, \\ q-k \in B_f^c, \\ q \in B_f, \\ l \in B_f^c}} \hat{V(k)} a_{l+k}^* a_{q-k}^* a_q^* a_l \\
& + \sum_{\substack{l+k \in B_f^c, \\ q-k \in B_f, \\ q \in B_f^c, \\ l \in B_f^c}} \hat{V(k)} a_{l+k}^* a_{q-k} a_q a_l + \sum_{\substack{l+k \in B_f^c, \\ q-k \in B_f, \\ q \in B_f^c, \\ l \in B_f}} \hat{V(k)} a_{l+k}^* a_{q-k} a_q a_l^* + \sum_{\substack{l+k \in B_f^c, \\ q-k \in B_f, \\ q \in B_f, \\ l \in B_f^c}} \hat{V(k)} a_{l+k}^* a_{q-k} a_q^* a_l \\
& + \sum_{\substack{l+k \in B_f^c, \\ q-k \in B_f, \\ q \in B_f, \\ l \in B_f}} \hat{V(k)} a_{l+k}^* a_{q-k} a_q^* a_l^* + \sum_{\substack{l+k \in B_f, \\ q-k \in B_f^c, \\ q \in B_f^c, \\ l \in B_f^c}} \hat{V(k)} a_{l+k} a_{q-k}^* a_q a_l + \sum_{\substack{l+k \in B_f, \\ q-k \in B_f^c, \\ q \in B_f^c, \\ l \in B_f}} \hat{V(k)} a_{l+k} a_{q-k}^* a_q a_l^* + \\
& + \sum_{\substack{l+k \in B_f, \\ q-k \in B_f^c, \\ q \in B_f, \\ l \in B_f^c}} \hat{V(k)} a_{l+k} a_{q-k}^* a_q^* a_l + \sum_{\substack{l+k \in B_f, \\ q-k \in B_f^c, \\ q \in B_f^c, \\ l \in B_f^c}} \hat{V(k)} a_{l+k} a_{q-k} a_q a_l + \sum_{\substack{l+k \in B_f, \\ q-k \in B_f^c, \\ q \in B_f, \\ l \in B_f}} \hat{V(k)} a_{l+k} a_{q-k}^* a_q^* a_l^* \\
& + \sum_{\substack{l+k \in B_f, \\ q-k \in B_f, \\ q \in B_f, \\ l \in B_f^c}} \hat{V(k)} a_{l+k} a_{q-k} a_q^* a_l + \sum_{\substack{l+k \in B_f, \\ q-k \in B_f, \\ q \in B_f^c, \\ l \in B_f}} \hat{V(k)} a_{l+k} a_{q-k} a_q a_l^* \\
& + \sum_{\substack{l+k \in B_f, \\ q-k \in B_f, \\ q \in B_f, \\ l \in B_f}} \hat{V(k)} a_{l+k} a_{q-k} a_q^* a_l^* + \sum_{\substack{l+k \in B_f^c, \\ q-k \in B_f^c, \\ q \in B_f^c, \\ l \in B_f^c}} \hat{V(k)} a_{l+k}^* a_{q-k}^* a_q a_l \Bigg)
\end{aligned} \tag{3.18}$$

All terms other than 5,6,9,10,15 give 0 in the state $a_p^* a_h^* \Omega$ because we need to have equal number of creation and annihilation operators to get back the same state. The 16th term gives 0 because we can't apply two successive annihilation operators in B_f^c. The contribution

of the non-zero terms are

$$\langle\Psi, \sum_{\substack{l+k\in B_f^c,\\ q-k\in B_f,\\ q\in B_f^c,\\ l\in B_f}} \hat{V(k)} a_{l+k}^* a_{q-k} a_q a_l^* \Psi\rangle = -\sum_{l\in B_f\setminus\{h\}} \hat{V}(p-l), \tag{3.19}$$

$$\langle\Psi, \sum_{\substack{l+k\in B_f^c,\\ q-k\in B_f,\\ q\in B_f,\\ l\in B_f^c}} \hat{V(k)} a_{l+k}^* a_{q-k} a_q^* a_l \Psi\rangle = \sum_{q\in B_f\setminus\{h\}} \hat{V}(0), \tag{3.20}$$

$$\langle\Psi, \sum_{\substack{l+k\in B_f,\\ q-k\in B_f^c,\\ q\in B_f^c,\\ l\in B_f}} \hat{V(k)} a_{l+k} a_{q-k}^* a_q a_l^* \Psi\rangle = \sum_{l\in B_f\setminus\{h\}} \hat{V}(0), \tag{3.21}$$

$$\langle\Psi, \sum_{\substack{l+k\in B_f,\\ q-k\in B_f^c,\\ q\in B_f,\\ l\in B_f^c}} \hat{V(k)} a_{l+k} a_{q-k}^* a_q^* a_l \Psi\rangle = -\sum_{q\in B_f\setminus\{h\}} \hat{V}(q-p), \tag{3.22}$$

$$\langle\Psi, \sum_{\substack{l+k\in B_f,\\ q-k\in B_f,\\ q\in B_f,\\ l\in B_f}} \hat{V(k)} a_{l+k} a_{q-k} a_q^* a_l^* \Psi\rangle = -\sum_{q,l\in B_f\setminus\{h\}, q\neq l} \hat{V}(q-l) + \hat{V}(0). \tag{3.23}$$

Now we have to evaluate the difference between this and the energy for paramagnetic state in which only 1 term contributes. For the paramagnetic state,

$$\langle\Omega, \sum_{\substack{l+k\in B_f,\\ q-k\in B_f,\\ q\in B_f,\\ l\in B_f}} \hat{V(k)} a_{l+k} a_{q-k} a_q^* a_l^* \Omega\rangle = -\sum_{q,l\in B_f, q\neq l} \hat{V}(q-l) + \hat{V}(0). \tag{3.24}$$

The energy difference becomes

$$\langle a_p^* a_h^* \Omega, H' a_p^* a_h^* \Omega\rangle - \langle\Omega, H'\Omega\rangle = E_{\rm int} - E_{\rm int}^{\rm pw} + \hbar^2(p^2 - h^2), \tag{3.25}$$

$$\begin{aligned} E_{\rm int} - E_{\rm int}^{\rm pw} &= -2\sum_{q\in B_f\setminus\{h\}} \hat{V}(q-p) + 2\sum_{q\in B_f\setminus\{h\}} \hat{V}(q-h) \\ &= 2\sum_{q\in B_f\setminus\{h\}} \left(\frac{1}{|q-h|^2} - \frac{1}{|q-p|^2}\right). \end{aligned} \tag{3.26}$$

Theorem 3.2. *The energy difference* $E_{int} - E_{int}^{pw} \geq 0$.

Proof. Suppose there exists a bijective map $M : B_f \to B_f$ such that $d(q,h) \leq d(M(q),p), \forall q \in B_f \setminus \{h\}$. We have

$$\sum_{q \in B_f \setminus \{h\}} \left(\frac{1}{|q-h|^2} - \frac{1}{|q-p|^2} \right) = \sum_{q \in B_f \setminus \{h\}} \left(\frac{1}{|q-h|^2} - \frac{1}{|M(q)-p|^2} \right) \geq 0. \tag{3.27}$$

Now we construct the map M.
Without loss of generality, we can assume the points h and p lie on the XY plane and assume that the line connecting these points is the x axis. Consider the plane of points equidistant from both p and h. The equation of this plane would be given by $\frac{p+h}{2}$. Consider the reflection of the fermi ball B_f under this plane and call it B_f^r. Define the map as

$$M(q) = \begin{cases} q \text{ if } q \notin B_f^r \cap B_f \\ r(q) \text{ if } q \in B_f^r \cap B_f \end{cases} \tag{3.28}$$

where r(q) is the reflection of q under that plane.
Clearly this map satisfies the requirements. □

3.2 n fermions outside fermi ball

Now we generalise the calculation in previous section to n particles n holes system. The state is given by $\Psi = a_{p_n}^* a_{h_n}^* .... a_{p_1}^* a_{h_1}^* \Omega$
We have to evaluate

$$\langle \Psi, H' \Psi \rangle = E_{\text{pw}} + E_{\text{kin}} + E_{\text{int}}. \tag{3.29}$$

$$E_{\text{kin}} = \sum_{i=1}^{n} \hbar^2 (p_i^2 - h_i^2) \tag{3.30}$$

$E_{\rm int}$ will have contribution from the terms 5,6,9,10,15,16 of $H_{\rm int}$. Their contribution is given by

$$\langle\Psi, \sum_{\substack{l+k\in B_f^c,\\ q-k\in B_f,\\ q\in B_f^c,\\ l\in B_f}} \hat{V(k)} a^*_{l+k}a_{q-k}a_q a^*_l\Psi\rangle = -\sum_{l\in B_f\setminus\{h_1,h_2,..,h_n\}}\sum_{i=1}^{n}\hat{V}(p_i-l), \tag{3.31}$$

$$\langle\Psi, \sum_{\substack{l+k\in B_f^c,\\ q-k\in B_f,\\ q\in B_f,\\ l\in B_f^c}} \hat{V(k)} a^*_{l+k}a_{q-k}a^*_q a_l\Psi\rangle = \sum_{q\in B_f\setminus\{h_1,h_2,..,h_n\}}\sum_{i=1}^{n}\hat{V}(0) = n(N-n)\hat{V}(0), \tag{3.32}$$

$$\langle\Psi, \sum_{\substack{l+k\in B_f,\\ q-k\in B_f^c,\\ q\in B_f^c,\\ l\in B_f}} \hat{V(k)} a_{l+k}a^*_{q-k}a_q a^*_l\Psi\rangle = \sum_{l\in B_f\setminus\{h_1,h_2,..,h_n\}}\sum_{i=1}^{n}\hat{V}(0) = n(N-n)\hat{V}(0), \tag{3.33}$$

$$\langle\Psi, \sum_{\substack{l+k\in B_f,\\ q-k\in B_f^c,\\ q\in B_f,\\ l\in B_f^c}} \hat{V(k)} a_{l+k}a^*_{q-k}a^*_q a_l\Psi\rangle = -\sum_{q\in B_f\setminus\{h_1,h_2,..,h_n\}}\sum_{i=1}^{n}\hat{V}(q-p_i), \tag{3.34}$$

$$\begin{aligned}\langle\Psi, \sum_{\substack{l+k\in B_f,\\ q-k\in B_f,\\ q\in B_f,\\ l\in B_f}} \hat{V(k)} a_{l+k}a_{q-k}a^*_q a^*_l\Psi\rangle &= -\sum_{q,l\in B_f\setminus\{h_1,h_2,..,h_n\},q\neq l}\hat{V}(q-l)-\hat{V}(0)\\ &= -\sum_{q,l\in B_f,q\neq l}\hat{V}(q-l)\\ &\quad + 2\sum_{i=1}^{n}\sum_{l\in B_f\setminus\{h_1,h_2,..,h_n\}}\hat{V}(h_i-l)\\ &\quad + \sum_{\substack{i,j=1,\\ i\neq j}}^{n}\hat{V}(h_i-h_j) + (N-n)(N-n-1)\hat{V}(0),\end{aligned} \tag{3.35}$$

$$\langle\Psi, \sum_{\substack{l+k\in B_f^c,\\ q-k\in B_f^c,\\ q\in B_f^c,\\ l\in B_f^c}} \hat{V(k)} a^*_{l+k}a^*_{q-k}a_q a_l\Psi\rangle = -\sum_{q,l\in\{p_1,p_2,..,p_n\},q\neq l}\hat{V}(q-l)-\hat{V}(0). \tag{3.36}$$

The energy difference becomes

$$E_{\text{int}} - E_{\text{int}}^{\text{pw}} = \sum_{\substack{i,j=1,\\ i\neq j}}^{n} \hat{V}(h_i - h_j) - \sum_{\substack{i,j=1,\\ i\neq j}}^{n} \hat{V}(p_i - p_j) + 2\sum_{i=1}^{n} \sum_{l\in B_f\setminus\{h_1,h_2,..,h_n\}} \hat{V}(h_i - l)$$
$$- \sum_{q\in B_f\setminus\{h_1,h_2,..,h_n\}} \sum_{i=1}^{n} \hat{V}(q - p_i). \tag{3.37}$$

From this, we can't conclusively tell if the energy difference is positive or negative. It appears that it would depend on the relative positions of particles and holes.

Chapter 4

Improving the lower bound

In the previous chapter, we have tried using the direct approach to find the difference between the Hartree Fock ground state energy and the energy of the state of completely filled fermi ball but as we have seen, it is difficult to comment on this as we don't know the true Hartree Fock ground state. In this chapter, we intend to prove the following 3 theorems.

Theorem 4.1. *Consider the Hamiltonian*

$$H_N = \hbar^2 \sum_{i=1}^{N} (-\Delta_{x_i}) + \lambda \sum_{1 \leq i \leq j \leq N} V(x_i - x_j),$$

where V is the L-periodic Coulomb potential multiplied with a constant κ and $N = |B_F|$. Then for κ sufficiently small, the free fermi gas state or the state with completely filled fermi ball denoted by Ψ_{pw} is the unique minimiser for E_N^{HF}.

Theorem 4.2. *Consider the Hamiltonian H_N given as above.*
Then for κ sufficiently large, Ψ_{pw} is not a global minimizer for E_N^{HF}.

Conjecture 4.3. *There exists a critical value κ_c such that $\forall \kappa > \kappa_c$, the slater determinant of plane waves is not a unique minimizer for E_N^{HF} and for $\kappa < \kappa_c$, slater determinant of plane waves is the unique minimizer for E_N^{HF}.*

4.1 Theorem 1

Proof. Following the calculations of [9], we get

$$\begin{aligned}\langle \Psi, H_N \Psi \rangle - \langle \Psi_{\text{pw}}, H_N \Psi_{\text{pw}} \rangle = tr(-\hbar^2 \Delta(\gamma - \gamma_{\text{pw}})) \\ - \frac{\lambda}{2} \int \int [|\gamma(x,y)|^2 - |\gamma_{\text{pw}}(x,y)|^2] V(x-y) dxdy \\ + \frac{\lambda}{2} \int \int [\rho_\gamma(x)\rho_\gamma(y) - \rho_{\gamma_{\text{pw}}}(x)\rho_{\gamma_{\text{pw}}}(y)] V(x-y) dxdy. \quad (4.1)\end{aligned}$$

We have to find a lower bound to the above expression. There are 3 terms in the above expression that is Kinetic term, Exchange term and Direct term. It was shown in [9] that direct term is strictly positive. So we get

$$\langle \Psi, H_N \Psi \rangle - \langle \Psi_{\text{pw}}, H_N \Psi_{\text{pw}} \rangle \geq tr(-\hbar^2 \Delta(\gamma - \gamma_{\text{pw}})) - \frac{\lambda}{2} \int \int [|\gamma(x,y)|^2 - |\gamma_{\text{pw}}(x,y)|^2] V(x-y) dxdy. \quad (4.2)$$

Let us look at the exchange term first.
We can decompose this term as

$$|\gamma(x,y)|^2 - |\gamma_{\text{pw}}(x,y)|^2 = |\gamma(x,y) - \gamma_{\text{pw}}(x,y)|^2 + 2Re[(\gamma(x,y) - \gamma_{\text{pw}}(x,y))\gamma_{\text{pw}}(y-x)]. \quad (4.3)$$

We get the first term as

$$\int \int |\gamma(x,y) - \gamma_{\text{pw}}(x-y)|^2 V(x-y) dxdy. \quad (4.4)$$

For the second part of the exchange term, we write

$$\int \int (\gamma(x,y) - \gamma_{\text{pw}}(x-y))\gamma_{\text{pw}}(x-y) V(y-x) dxdy = tr(G(\gamma - \gamma_{\text{pw}})), \quad (4.5)$$

where G is an operator on $L^2(\mathbf{T^3})$ with kernel $\gamma_{\text{pw}}(y-x)V(y-x)$. Equivalently, G is the multiplication operator in Fourier space with

$$G(k) = \sum_{p \in B_f} \hat{V}(k-p). \quad (4.6)$$

In particular, $G \geq 0$ and hence $\mathrm{Tr}(G(\gamma - \gamma_{\mathrm{pw}})) \in \mathbf{R}$.
Now we show that

$$\mathrm{Tr}[(-\hbar^2\Delta - \lambda G)(\gamma - \gamma_{\mathrm{pw}})] = tr[A(\gamma - \gamma_{\mathrm{pw}})^2], \tag{4.7}$$

for some operator A.
Since γ and γ_{pw} are projections, we can decompose

$$(\gamma - \gamma_{\mathrm{pw}})^2 = \gamma_{\mathrm{pw}}^{\perp}(\gamma - \gamma_{\mathrm{pw}})\gamma_{\mathrm{pw}}^{\perp} - \gamma_{\mathrm{pw}}(\gamma - \gamma_{\mathrm{pw}})\gamma_{\mathrm{pw}}, \quad \gamma_{\mathrm{pw}}^{\perp} = 1 - \gamma_{\mathrm{pw}}. \tag{4.8}$$

Hence, for any constant $c_0 \in \mathbf{R}$,

$$\begin{aligned} \mathrm{Tr}[A(\gamma - \gamma_{\mathrm{pw}})^2] &= \mathrm{Tr}[(\gamma_{\mathrm{pw}}^{\perp}A\gamma_{\mathrm{pw}} - \gamma_{\mathrm{pw}}A\gamma_{\mathrm{pw}})(\gamma - \gamma_{\mathrm{pw}})] &(4.9)\\ &= \mathrm{Tr}[(\gamma_{\mathrm{pw}}^{\perp}A\gamma_{\mathrm{pw}} - \gamma_{\mathrm{pw}}A\gamma_{\mathrm{pw}} + c_0)(\gamma - \gamma_{\mathrm{pw}})]. &(4.10)\end{aligned}$$

We have used $\mathrm{Tr}(\gamma) = \mathrm{Tr}(\gamma_{\mathrm{pw}}) = N$ in the last equality. Thus the desired equality (4.7) holds true if

$$\gamma_{\mathrm{pw}}^{\perp}A\gamma_{\mathrm{pw}} - \gamma_{\mathrm{pw}}A\gamma_{\mathrm{pw}} + c_0 = -\hbar^2\Delta - \lambda G, \tag{4.11}$$

which is equivalent to

$$A(k)\mathbf{1}(k \in B_f^c) - A(k)\mathbf{1}(k \in B_f) = \hbar^2|k|^2 - \lambda G(k) - c_0. \tag{4.12}$$

This holds true when

$$A(k) = |\hbar^2|k|^2 - \lambda G(k) - c_0|, \tag{4.13}$$

provided that the constant c_0 satisfies

$$\sup_{k\in B_f}(\hbar^2|k|^2 - \lambda G(k)) \leq c_0 \leq \inf_{k\in B_f^c}(\hbar^2|k|^2 - \lambda G(k)). \tag{4.14}$$

We can choose

$$c_0 = \hbar^2 k_f^2 - \lambda G(k_f), \tag{4.15}$$

where k_f is the radius of the fermi ball B_f. Thus, we have

$$\langle\Psi, H_N\Psi\rangle - \langle\Psi_{\mathrm{pw}}, H_N\Psi_{\mathrm{pw}}\rangle \geq tr(A(\gamma - \gamma_{\mathrm{pw}})^2) - \lambda tr(V(\gamma - \gamma_{\mathrm{pw}})^2). \tag{4.16}$$

This is equivalent to finding the lowest eigenvalue of the operator $(A(x)+A(y)-\lambda V(x-y))$. To do this, we need to have some sort of comparison between the operators A and V. As, A is a one-body operator and V is a two-body operator, it is not possible. So, we try to prove the following lemma

Lemma 4.4. *Finding the lowest eigenvalue of the 2 body operator* $(A(x)+A(y)-\lambda V(x-y))$ *is equivalent to finding the lowest eigenvalue of a corresponding 1 body operator.*

Proof. The operator A is given by

$$A = |k^2 - \lambda G(K) - c_0| = |k^2 - k_f^2 - \lambda(G(k) - G(k_f))|. \tag{4.17}$$

We claim

$$A \geq |k^2 - k_f^2| \tag{4.18}$$

We can see that for $|k| \geq k_f$, $k^2 - k_f^2 \geq 0$. We claim that $G(k) - G(k_f) \leq 0$.

$$G(k) = \sum_{p \in B_f} \frac{1}{|k-p|^2} \tag{4.19}$$

If we can show that $\forall p \in B_f$, $\frac{1}{|k-p|^2} \leq \frac{1}{|k_f-p|^2}$, we are done. It is clear that $\forall p \in B_f$ and $|k| \geq k_f$, $|k-p| \geq |k_f-p|$. Thus, our claim is true.
We can see that for $|k| \leq k_f$, $k^2 - k_f^2 \leq 0$. We claim that $G(k) - G(k_f) \geq 0$.

As $G(k)$ is spherically symmetric, we can take the vectors $\mathbf{k}$ and $\mathbf{k_f}$ to be in the same line. We call this line the x-axis. We will now use coordinate representation and express $\mathbf{k}$ and $\mathbf{k_f}$ as $(k,0,0)$ and $(k_f,0,0)$. B_f is a sphere of radius k_f centered at 0. We denote this sphere as S.

Consider the points $\{(a,b,c) \in S | a < k\}$. Lets denote the set of these points by C. The contribution of sum in G(k) from these points is greater than that from $G(k_f)$ i.e.

$$\sum_{p \in C} \frac{1}{|k_f - p|^2} < \sum_{p \in C} \frac{1}{|k-p|^2}. \tag{4.20}$$

Now, we consider the set $A = \{(a,b,c) \in S | a \geq \frac{k_f+k}{2}\}$. The points in set A are closer to k_f

than k. Hence, they give a larger contribution for $G(k_f)$ than $G(k)$ i.e.

$$\sum_{p\in A}\frac{1}{|k_f-p|^2}>\sum_{p\in A}\frac{1}{|k-p|^2}. \tag{4.21}$$

We consider a bijective mapping $F:A\to B$ given by $F((a,b,c))=(k+k_f-a,b,c)$. Note that $B\subset S$ and the contribution of sum in G(k) from the set B is equal to the contribution of sum in $G(k_f)$ from the set A i.e.

$$\sum_{p\in A}\frac{1}{|k_f-p|^2}=\sum_{p\in B}\frac{1}{|k-p|^2}, \tag{4.22}$$

$$\sum_{p\in B}\frac{1}{|k_f-p|^2}=\sum_{p\in A}\frac{1}{|k-p|^2}. \tag{4.23}$$

The remaining points are closer to (k,0,0) than $(k_f,0,0)$. Lets denote the set of remaining points by D. Hence, they result in a larger contribution to G(k) than $G(k_f)$ i.e.

$$\sum_{p\in D}\frac{1}{|k_f-p|^2}<\sum_{p\in D}\frac{1}{|k-p|^2}. \tag{4.24}$$

Thus, we get $A(k)=|k^2-k_f^2|+|\lambda(G(k)-G(k_f))|\geq|k^2-k_f^2|$. Hence for the lower bound, we can take operator A to be $k^2-k_f^2$. In the position space, operator A is given by

$$A=-\Delta-k_f^2. \tag{4.25}$$

We do a coordinate transformation given by

$$r=x-y, l=\frac{x+y}{2}. \tag{4.26}$$

In the new coordinates, we have

$$\frac{\partial^2}{\partial r^2}=\frac{1}{4}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)-\frac{1}{2}\frac{\partial^2}{\partial x\partial y}, \tag{4.27}$$

$$\frac{\partial^2}{\partial r^2}=\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+\frac{\partial^2}{\partial x\partial y}. \tag{4.28}$$

So, we get the form of A as

$$A = \frac{1}{2}\left| -i\nabla_r + \frac{-i\nabla_l}{2}\right|^2 + \frac{1}{2}\left| -i\nabla_r - \frac{-i\nabla_l}{2}\right|^2 - k_f^2. \tag{4.29}$$

This can also be written as

$$A = \frac{1}{2}\left| -i\nabla_r + \frac{l}{2}\right|^2 + \frac{1}{2}\left| -i\nabla_r - \frac{l}{2}\right|^2 - k_f^2, \tag{4.30}$$

where l is the fourier variable. We can see that the minimum is attained for $l = 0$ and we get

$$\lambda_1(A(x) + A(y) - \lambda V(x-y)) = \lambda_1(A(r) - \lambda V(r)). \tag{4.31}$$

□

We now have to find a bound on V in terms of A so that we can compare the two terms.

$$\sum_r V(r)|\Psi(r)|^2 = \sum_{k,l} |\hat{\Psi}(k)| \frac{1}{|k-l|^2} |\hat{\Psi}(l)|. \tag{4.32}$$

We use the generalised Cauchy Schwarz theorem to get

$$\begin{aligned}\sum_r V(r)|\Psi(r)|^2 &= 2\sum_{k,l} \frac{|\hat{\Psi}(k)|^2 A(k)}{A(l)|l-k|^2} \\ &= 2\sum_k |\hat{\Psi}(k)|^2 A(k) \sum_l \frac{1}{(l^2-k_f^2)|l-k|^2}.\end{aligned} \tag{4.33}$$

Lemma 4.5. *We claim that for every $k \in Z^3$,*

$$\sum_l \frac{1}{(l^2-k_f^2)|l-k|^2} \leq Ck_f. \tag{4.34}$$

Proof. We divide the sum into 3 cases
Case 1: $|l-k| \leq 4k_f$. Then

$$\sum_{l\in Z^3, l\neq k, |l-k|\leq 4k_f} \frac{1}{|l^2-k_f^2||l-k|^2} \leq \sum_{l\in Z^3, l\neq k, |l-k|\leq 4k_f} \frac{1}{|l-k|^2} \leq \sum_{l\in Z^3, 1\leq |l'|\leq 4k_f} \frac{1}{|l'|^2} \leq Ck_f. \tag{4.35}$$

Case 2: $|l-k| > 4k_f$ and $|l| \leq 2k_f$. Then,

$$\sum_{l\in Z^3, l\neq k, |l-k|>4k_f, |l|\leq 2k_f} \frac{1}{|l^2-k_f^2||l-k|^2} \leq \sum_{l\in Z^3, |l|\leq 2k_f} \frac{1}{k_f^2} \leq Ck_f. \tag{4.36}$$

Case 3: $|l-k| > 4k_f$ and $|l| \geq 2k_f$. Then,

$$\sum_{l\in Z^3, l\neq k, |l-k|>4k_f, |l|\geq 2k_f} \frac{1}{|l^2-k_f^2||l-k|^2} \leq \sum_{l\in Z^3, l\neq k, |l-k|>4k_f, |l|\geq 2k_f} \frac{1}{l^2|l-k|^2}. \tag{4.37}$$

We further divide the sum into 3 parts: $|l| > 2|k|$, $\frac{|k|}{2} \leq |l| \leq 2|k|$ and $|l| < \frac{|k|}{2}$. Then we have,

$$\sum_{l\in Z^3, |l-k|>4k_f, |l|\geq 2k_f, |l|>2|k|} \frac{1}{l^2|l-k|^2} \leq \sum_{l\in Z^3, |l|\geq 2k_f} \frac{C}{l^4} \leq C \tag{4.38}$$

for the first part,

$$\begin{aligned}\sum_{l\in Z^3, l\neq k, |l-k|>4k_f, |l|\geq 2k_f, |k|/2\leq |l|\leq 2|k|} \frac{1}{l^2|l-k|^2} &\leq \sum_{l\in Z^3, l\neq k, |l-k|>4k_f, |l|\geq 2k_f, |k|/2\leq |l|\leq 2|k|} \frac{C}{k^2|l-k|^2} \\ &\leq \sum_{l'\in Z^3, 1\leq |l'|\leq 3|k|} \frac{C}{k^2 l'^2} \leq C \end{aligned} \tag{4.39}$$

for the second part, and

$$\sum_{l\in Z^3, |l-k|>4k_f, |l|\geq 2k_f, |l|<\frac{|k|}{2}} \frac{1}{l^2|l-k|^2} \leq \sum_{l\in Z^3, 1\leq |l|\leq \frac{|k|}{2}} \frac{C}{l^2k^2} \leq C \tag{4.40}$$

for the last part. □

So, we get

$$\langle \Psi, H_N \Psi\rangle - \langle \Psi_{\text{pw}}, H_N \Psi_{\text{pw}}\rangle \geq \text{Tr}[(A - Ck_f\kappa\lambda A)(\gamma-\gamma_{\text{pw}})^2]. \tag{4.41}$$

From this, we can see that for $\kappa \leq \frac{1}{C}$, $\langle \Psi, H_N \Psi\rangle - \langle \Psi_{\text{pw}}, H_N \Psi_{\text{pw}}\rangle \geq 0$. □

4.2 Theorem 2

Proof. Let us first show that for $\kappa = 1$, free fermi gas is not the HF ground state [10, 11, 12]. To show this, we will deform the fermi sphere and introduce spin density waves and we will find that the resultant energy is less than free fermi gas energy.
The free fermi gas state is given by

$$\Psi = (\bigwedge_{k\in B_f} f_{k,\uparrow}) \wedge (\bigwedge_{k\in B_f} f_{k,\downarrow}). \tag{4.42}$$

In step 1, we deform the fermi surface and get state to be

$$\Psi = (\bigwedge_{k\in \mathcal{F}_\uparrow} f_{k,\uparrow}) \wedge (\bigwedge_{k\in \mathcal{F}_\downarrow} f_{k,\downarrow}). \tag{4.43}$$

The 1 particle density matrix can be given by

$$\gamma_D = \sum_{k\in\mathcal{F}_\uparrow} |f_{k\uparrow}\rangle\langle f_{k\uparrow}| + \sum_{k\in F_{k\downarrow}} |f_{k\downarrow}\rangle\langle f_{k\downarrow}|. \tag{4.44}$$

In step 2, we introduce spin density waves by the transformation $|k,\uparrow\rangle \mapsto a_k|k,\uparrow\rangle + b_k|k+Q_k,\downarrow\rangle$. After this transformation, state is given by

$$\Psi = (\bigwedge_{k\in\mathcal{F}_\uparrow} (a_k f_{k,\uparrow} + b_k f_{k+Q_k,\downarrow})) \wedge (\bigwedge_{k\in\mathcal{F}_\downarrow} (a'_k f_{k,\downarrow} + b'_k f_{k+Q_k,\uparrow})). \tag{4.45}$$

The 1 particle density matrix is given by

$$\begin{aligned}\gamma_H &= \sum_{k\in F_\uparrow} |a_k f_{k,\uparrow} + b_k f_{k+Q_k,\downarrow}\rangle\langle a_k f_{k,\uparrow} + b_k f_{k+Q_k,\downarrow}| \\ &+ \sum_{k\in F_\downarrow} |a'_k f_{k,\downarrow} + b'_k f_{k+Q_k,\uparrow}\rangle\langle a'_k f_{k,\downarrow} + b'_k f_{k+Q_k,\uparrow}| \qquad (4.46)\\ \gamma(x,y) &= \sum_{k\in F_\uparrow} (a_k e^{ikx}|\uparrow\rangle + b_k e^{i(k+Q_k)x}|\downarrow\rangle)(a_k e^{-iky}|\uparrow\rangle + b_k e^{-i(k+Q_k)y}|\downarrow\rangle) \\ &+ \sum_{k\in F_\downarrow} (a'_k e^{ikx}|\downarrow\rangle + b'_k e^{i(k+Q_k)x}|\uparrow\rangle)(a'_k e^{-iky}|\downarrow\rangle + b'_k e^{-i(k+Q_k)y}|\uparrow\rangle). \qquad (4.47)\end{aligned}$$

The Hartree Fock energy functional can be written as

$$\varepsilon_{HF}(\gamma) = tr(-\Delta\gamma) + \int\int \underline{dx}\underline{dy}\frac{\rho(x)\rho(y)}{|x-y|} - \int \underline{dx}\underline{dy}\frac{|\gamma(x,y)|^2}{|x-y|}, \tag{4.48}$$

where $\int \underline{dx} = \int dx \sum_{\sigma\in\{\uparrow,\downarrow\}}$ and $\rho(x) = \gamma(x,x)$.
We have to calculate the difference in energy between the SDW state and free fermi gas state. We can write the difference as

$$\Delta\varepsilon_{HF} = \varepsilon_{HF}(\gamma_H) - \varepsilon_{HF}(\gamma_{FFG}) = \varepsilon_{HF}(\gamma_H) - \varepsilon_{HF}(\gamma_D) + \varepsilon_{HF}(\gamma_D) - \varepsilon_{HF}(\gamma_{FFG}). \tag{4.49}$$

Let us first handle the kinetic part.

$$\begin{aligned}
tr(-\Delta\gamma_H) - tr(-\Delta\gamma_D) &= 2\sum_{k\in\mathcal{F}_\uparrow} \langle a_k f_{k\uparrow} + b_k f_{(k+Q_k)\downarrow}| - \Delta|a_k f_{k\uparrow} + b_k f_{(k+Q_k)\downarrow}\rangle - tr(-\Delta\gamma_D) \\
&= 2\sum_{k\in\mathcal{F}_\uparrow} |a_k|^2\langle f_k, -\Delta f_k\rangle + |b_k|^2\langle f_{(k+Q_k)}, -\Delta f_{k+Q_k}\rangle - tr(-\Delta\gamma_D) \\
&= 2\sum_{k\in\mathcal{F}_\uparrow} |a_k|^2 k^2 + |b_k|^2(k+Q_k)^2 - tr(-\Delta\gamma_D) \\
&= 2\sum_{k\in\mathcal{F}_\uparrow} k^2 + 2\sum_{k\in\mathcal{F}_\uparrow} -|b_k|^2 k^2 + |b_k|^2(k+Q_k)^2 - tr(-\Delta\gamma_D) \\
&= 2\sum_{k\in\mathcal{F}_\uparrow} -|b_k|^2 k^2 + |b_k|^2(k+Q_k)^2.
\end{aligned} \tag{4.50}$$

For the first part of interaction energy, we have

$$\begin{aligned}
\int dxdy\frac{\rho_H(x)\rho_H(y)}{|x-y|} - \int dxdy\frac{\rho_D(x)\rho_D(y)}{|x-y|} & \\
\rho_H(x) &= 2\sum_k tr_{C^2}|a_k|^2|f_k(x)|^2|\uparrow\rangle\langle\uparrow| \\
&\quad + 2\sum_k tr_{C^2}|b_k|^2|f_{k+Q_k}(x)|^2|\downarrow\rangle\langle\downarrow| \\
&= 2\sum_k(|a_k|^2 + |b_k|^2) = 2\sum_k 1 = 2N \\
\rho_D(x) &= 2N \\
\int dxdy\frac{\rho_H(x)\rho_H(y)}{|x-y|} - \int dxdy\frac{\rho_D(x)\rho_D(y)}{|x-y|} &= 0.
\end{aligned} \tag{4.51}$$

The second part of interaction energy is given by

$$\int dxdy \frac{|\gamma_H(x,y)|^2}{|x-y|} - \int dxdy \frac{|\gamma_D(x,y)|^2}{|x-y|} \tag{4.52}$$

$$\begin{aligned}
|\gamma_H(x,y)|^2 = & \sum_{k\in F_\uparrow, k'\in F_\uparrow} a_k^2 a_{k'}^2 e^{ik(x-y)} e^{-ik'(x-y)} \\
& + \sum_{k\in F_\uparrow, k'\in F_\uparrow} a_k b_k a_{k'} b_{k'} e^{i(k-k')(x-y)} e^{-i(Q_k - Q_{k'})y} \\
& + \sum_{k\in F_\uparrow, k'\in F_\uparrow} a_k b_k a_{k'} b_{k'} e^{i(k-k')(x-y)} e^{i(Q_k - Q_{k'})x} \\
& + \sum_{k\in F_\uparrow, k'\in F_\uparrow} b_k^2 b_{k'}^2 e^{i(k+Q_k)(x-y)} e^{-i(k'+Q_{k'})(x-y)} \\
& + \sum_{k\in F_\uparrow, k'\in F_\downarrow} b_k^2 a_{k'}'^2 e^{(k+Q_k-k')(x-y)} \\
& + \sum_{k\in F_\uparrow, k'\in F_\downarrow} a_k^2 b_{k'}'^2 e^{(k-Q_{k'}-k')(x-y)} \\
& + \sum_{k\in F_\uparrow, k'\in F_\downarrow} a_k b_k a_{k'}' b_{k'}' e^{i(k-k')(x-y)} e^{iQ_k x} e^{iQ_{k'} y} \\
& + \sum_{k\in F_\uparrow, k'\in F_\downarrow} a_k b_k a_{k'}' b_{k'}' e^{i(k-k')(x-y)} e^{-iQ_k y} e^{-iQ_{k'} x} \\
& + \sum_{k\in F_\downarrow, k'\in F_\uparrow} a_k'^2 b_{k'}^2 e^{(k+Q_k-k')(x-y)} \\
& + \sum_{k\in F_\downarrow, k'\in F_\uparrow} a_k'^2 b_{k'}^2 e^{(k-Q_{k'}-k')(x-y)} \\
& + \sum_{k\in F_\downarrow, k'\in F_\uparrow} a_k' b_k' a_{k'}' b_{k'}' e^{i(k-k')(x-y)} e^{iQ_k x} e^{iQ_{k'} y} \\
& + \sum_{k\in F_\downarrow, k'\in F_\uparrow} a_k' b_k' a_{k'}' b_{k'}' e^{i(k-k')(x-y)} e^{-iQ_k y} e^{-iQ_{k'} x} \\
& + \sum_{k\in F_\downarrow, k'\in F_\downarrow} a_k'^2 a_{k'}'^2 e^{ik(x-y)} e^{-ik'(x-y)} \\
& + \sum_{k\in F_\downarrow, k'\in F_\downarrow} a_k' b_k' a_{k'}' b_{k'}' e^{i(k-k')(x-y)} e^{-i(Q_k - Q_{k'})y} \\
& + \sum_{k\in F_\downarrow, k'\in F_\downarrow} a_k' b_k' a_{k'}' b_{k'}' e^{i(k-k')(x-y)} e^{i(Q_k - Q_{k'})x} \\
& + \sum_{k\in F_\downarrow, k'\in F_\downarrow} b_k'^2 b_{k'}'^2 e^{i(k+Q_k)(x-y)} e^{-i(k'+Q_{k'})(x-y)}.
\end{aligned} \tag{4.53}$$

Define

$$(T^{\pm}f)(k) = \int_{F_\uparrow} dk' \left(\frac{1}{||k-k'||^2} \pm \frac{1}{||\tilde{k}-k'||^2} \right) f(k'). \tag{4.54}$$

We can rewrite ΔE as

$$\Delta E = \frac{4a_V R^4}{r_s}(2(\kappa, b^2) + (T^- a^2, b^2) - (T^- ab, ab)), \tag{4.55}$$

where a,b are understood as functions of k (a_k, b_k) and (f, g) is the scalar product $\int_{F_\uparrow} fg$ and $\kappa = \frac{a_K R}{4a_V r_s} Q(Q - 2k_z) \geq 0$. We set $R = 1$. We have to find maximum value of ΔE. For this, we take the derivative of the expression for ΔE wrt b. We get

$$2b\kappa + bT^-(a^2 - b^2) = \frac{a^2 - b^2}{a} T^+ ab. \tag{4.56}$$

Setting $\Xi = ab$, we can rewrite the above expression as $J(\Xi) = \Xi$, where

$$J(\Xi) = \frac{1}{2} \frac{T^+\Xi}{\sqrt{(\kappa + T^-\sqrt{1/4 - \Xi^2})^2 + (T^+\Xi)^2}}. \tag{4.57}$$

The problem now reduces to find the solutions of equation $J(\Xi) = \Xi$. The fermi gas($\Xi = 0$) is a trivial fixed point. By definition, $0 \leq \Xi \leq 1/2$ and $0 \leq J(\Xi) \leq \frac{1}{2}$.
We can clearly see that $T^{\pm}$ are positivity preserving linear opeartors. If $\Xi \geq \Xi'$, then $T^+\Xi \geq T^+\Xi'$ and $T^-\sqrt{1/4 - \Xi^2} \leq T^-\sqrt{1/4 - \Xi'^2}$ and $J(\Xi) \geq J(\Xi')$.
Starting with $\Xi_0 = 1/2$, we have $J(\Xi_0) \leq \Xi_0$ and setting $\Xi_n = J(\Xi_{n-1})$, Ξ_n is a decreasing sequence of positive functions and thus converges to a fixed point Ξ_∞.

Taking the 1D approximation:

Now we impose that b_k is non zero only in the region given by $C = \{k : k_x^2 + k_y^2 \leq r^2 = 1 - (1-\epsilon)^2 \approx 2\epsilon, 0 \leq k_z \leq Q\}$.
The second term of the expression for ΔE can be written as

$$(a^2, T^- b^2) = (b^2, T^- a^2) = (b^2, T^- 1) - (b^2, T^- b^2). \tag{4.58}$$

We get $T^{-1} = v_F(k) - v_F(\tilde{k})$ where v_F is the potential induced by the truncated sphere. In spherical case, potential of unit sphere is given by

$$v(k) = 2\pi + \pi \frac{1-k^2}{k} ln \frac{1+k}{|1-k|}. \tag{4.59}$$

In this case, for k close to 1 (k and $\tilde{k}$ are close and near unit sphere), $v(k) - v(\tilde{k}) \approx -4\pi(1-k)\ln(\frac{1-k}{2})$. For the truncated sphere, we get the same expression except that we replace $1-k$ by $Q/2-k$.

$$T^{-}1 \approx -4\pi(Q/2 - k_z)\ln(\frac{|Q/2-k_z|}{2}), \tag{4.60}$$

if $|Q/2 - k_z| \ll 1$. For $h > 0$, this equation holds except in a small neighbourhood of the edge of the top disk.

We will use the scaled distance $x = (Q/2 - k_z)/r$ and we get

$$2\kappa + T^{-}1 = 2\pi r(\gamma x - 2x\ln(x)). \tag{4.61}$$

After integrating over $q = (k_x, k_y)$, we get

$$\Delta E^F_{SDW} = \frac{4\pi a_V r^4}{r_s} \delta E^F_{SDW} \tag{4.62}$$

$$\delta E^F_{SDW} = 2\pi(\gamma x - 2x\ln(x), b^2) - (T^{-}b^2, b^2) - (T^{+}\Xi, \Xi), \tag{4.63}$$

where the scalar product is now given by $(f,g) = \int_{x>0} dx f(x)g(x)$ and $T^{\pm}$ becomes

$$(T^{\pm}f)(x) = \pi \int_0^{1/r} dx'(G(x-x') \pm G(x+x'))f(x') \tag{4.64}$$

$$\begin{aligned} G(x) &= \frac{1}{\pi^2 r^2} \int_{q^2, q'^2 < r^2} dq dq' \frac{1}{r^2 x^2 + (q-q')^2} \\ &= 2ln\left[1 + \frac{2}{|x|u}\right] - \frac{4}{u^2}, \quad u = |x| + \sqrt{x^2+4}. \end{aligned} \tag{4.65}$$

In the above, we have just evaluated the integral as shown in [10].
We have that T^{-} is a positive operator. So, we can ignore the term $(T^{-}b^2, b^2)$ for the upper bound of energy. If we do a variation of the upper bound with respect to b, we can get the

equation $\Xi = J(\Xi)$ for the 1d case where

$$J(\Xi) = \frac{1}{2}\frac{T^+\Xi}{\sqrt{\pi^2(\gamma x - 2x\ln(x))^2 + (T^+\Xi)^2}}. \tag{4.66}$$

We can find the fixed point of this equation by iteration. After getting the fixed point, we can substitute and get the value of ΔE.
We can also get an analytical solution for small r_s. As we are working in the high density regime, this is a valid assumption for us.
Let us consider the simple problem where we consider

$$J_0(\Xi) = \frac{1}{2}\frac{T^+\Xi}{\sqrt{(\pi x\gamma')^2 + (T^+\Xi)^2}}, \tag{4.67}$$

where we have replaced γ by γ' which is a constant and a large parameter of the problem. As J, J_0 are monotonous, we can get the fixed point of J by taking limit of the sequence $\Xi_n = J_0(\Xi_{n-1})$, starting with $\Xi_0 = \frac{1}{2}$. We can check that if $\Xi' \leq 0$ then $(T^+\Xi') \leq 0$ and $J(\Xi)' < 0$. Starting with $\Xi_0 = 1/2$, we have $\Xi_0' \leq 0$ and by induction $\Xi_n' \leq 0$ and $T^+\Xi_n \leq 0$. Thus setting $\eta = \lim \Xi_n$, η and $T^+\eta$ are decreasing functions.
We have $(T^+\Xi)'(0) = 0$. So, for small x, fixed point of J_0 behaves like

$$\eta_0(x) = \frac{1}{2}\frac{1}{\sqrt{(x/x_0)^2 + 1}} \tag{4.68}$$

$$x_0 = \frac{(T^+\eta)(0)}{\pi\gamma'}. \tag{4.69}$$

And since $(T^+\eta)' \leq 0$, we have

$$\eta_0(x) \geq \eta(x) \geq \eta_0(x)\frac{T^+\eta(x)}{T^+\eta(0)}. \tag{4.70}$$

We have that J_0 is an increasing function of $T^+\Xi$ and $T^+\eta \geq T^+\eta(0)$. This gives the first inequality and we can obtain the second inequality by replacing $T^+\eta$ by $T^+\eta(0)$ in the expression of J_0.

For non zero finite x, η_0 is narrowed near 0 and G(x) is continuous which gives

$$T^+\eta(x) \approx 2\pi G(x) \int_0^\infty \eta(x')dx' \tag{4.71}$$

$$\eta(x) \approx \frac{2G(x)}{\gamma' x_0}\eta_0(x) \int_0^\infty \eta(x')dx'. \tag{4.72}$$

The behaviour of η mainly depends on what happens at small x. So, the above expression is not very useful.

So, we look for the solution for $x < 1$. We assume that the denominator in the expression of J_0 is equivalent to $\sqrt{(\pi x\gamma')^2 + (T^+\eta(0))^2}$ for large γ'. We now look for the solution of

$$\eta(x) = \frac{1}{2}\frac{T^+\eta(x)}{\sqrt{(\pi x\gamma')^2 + (T^+\eta(0))^2}} = \eta_0\frac{T^+\eta(x)}{T^+\eta(0)}. \tag{4.73}$$

After setting $\eta = \eta_0 H$, we can rewrite the above expression as

$$H = \frac{T^+ H\eta_0}{T^+\eta(0)}. \tag{4.74}$$

We now assume that the tail of η is not relevant. So, we can approximate G(x) by $-ln(x^2)-1$ in the definition of T^+. Set $x = x_0 sinh\phi$. This reduces the problem to finding a solution $H(\phi)$ for $\phi \in [0, \phi_0]$ and $H(\phi_0) \approx 0$. We have

$$\gamma' H(\phi) = \int_0^{\phi_0} F(\phi, \phi')H(\phi')d\phi' \tag{4.75}$$

$$F(\phi, \phi') \approx -ln(|sinh(\phi) - sinh(\phi')|) - ln(|sinh(\phi) + sinh(\phi')|) - 2lnx_0 - 1. \tag{4.76}$$

$$H(0) = 1,\ H(\phi_0) = 0 \tag{4.77}$$

We can make the approximation

$$ln(|sinh(\phi) \pm sinh(\phi')|) \approx max(\phi, \phi') - ln2, \tag{4.78}$$

except on the finite ranges $\phi' \approx \phi$ and $\phi' \approx \phi_0$. Thus

$$F(\phi, \phi') \approx F_0(\phi, \phi') = 2(\phi_M - max(\phi, \phi') \tag{4.79}$$

$$\phi_M = -lnx_0 + ln2 - \frac{1}{2}. \tag{4.80}$$

We get

$$\gamma' \frac{dH(\phi)}{d\phi} = -2 \int_0^{\phi} H(\phi') d\phi' \tag{4.81}$$

$$H(0) = 1, \ H(\phi_0) = 0. \tag{4.82}$$

We can solve this to get

$$H(\phi) = cos\left(\sqrt{\frac{2}{\gamma}}\phi\right) \tag{4.83}$$

$$\phi_0 = \frac{\pi}{2\sqrt{2}}\sqrt{\gamma'}. \tag{4.84}$$

We can find x_0 using

$$\begin{aligned} \gamma' &= \frac{T^+\eta(0)}{\pi x_0} \\ &= \int_0^{\phi_0} F(0,\phi) H(\phi) d\phi \\ &= \int_0^{\phi_0} 2(\phi_M - \phi) H(\phi) d\phi \\ &= 2(\phi_M - \phi_0)\sqrt{\frac{\gamma'}{2}} + \gamma'. \end{aligned} \tag{4.85}$$

Thus $\phi_M = \phi_0$ and

$$x_0 = 2exp\left(- \frac{\pi}{2\sqrt{2}}\sqrt{\gamma'} - \frac{1}{2}\right). \tag{4.86}$$

So, we can get the solution for η

$$\eta(x) = \frac{1}{2\sqrt{\frac{x^2}{x_0^2} + 1}} cos\left(\sqrt{\frac{2}{\gamma'}} arcsinh(\frac{x}{x_0})\right). \tag{4.87}$$

This solution satisfies the above 2 assumptions.

The final step is to calculate δE^F_{SDW}. We get

$$\frac{\delta E^F_{SDW}(\eta)}{\pi x_0^2} = \frac{\pi^2 - 4}{32}\gamma' + \frac{\pi}{8\sqrt{2}}(\gamma - \gamma')\sqrt{\gamma'} + O(\sqrt{\gamma'}). \tag{4.88}$$

The minimum of above expression with respect to γ' is for $2\pi\sqrt{2}(\gamma'-\gamma)=\sqrt{\gamma}(\pi^2+4)$

$$\delta E^F_{SDW} \approx -\frac{\pi}{8} C\gamma e^{-\frac{\pi}{\sqrt{2}}\sqrt{\gamma}}, \tag{4.89}$$

with $C = 8e^{-3/2-\pi^2/8}$.

$$\Delta E^F_{SDW} \leq -\frac{2\pi^2 a_V}{r_s} C\epsilon^2\gamma exp(-\frac{\pi}{\sqrt{2}}\sqrt{\gamma}). \tag{4.90}$$

The total change in energy is given by

$$\begin{aligned}\Delta E &= \Delta E^F_{SDW} + \Delta E^F_{FG} \\ &= \frac{2\pi^2 a_V}{r_s}\delta E,\end{aligned} \tag{4.91}$$

$$\delta E = \epsilon^3\gamma\alpha - C\epsilon^2\gamma exp\bigg(-\frac{\pi}{\sqrt{2}}\sqrt{\gamma}\bigg). \tag{4.92}$$

The behaviour of δE is asymptotically dominated by the powers of ϵ and the minimum occurs for

$$3\epsilon^2\gamma\alpha - 2C\epsilon\gamma exp\bigg(-\frac{\pi}{\sqrt{2}}\sqrt{\gamma}\bigg) \approx 0. \tag{4.93}$$

We get the value of ΔE as

$$\Delta E \approx -0.69\alpha\frac{\epsilon^3}{r_s^2}. \tag{4.94}$$

□

Bibliography

[1] J. J. Sir Thomson. Xl. cathode rays. *Philosophical Magazine Series 1*, 44:293–316, 1897.

[2] A. Sommerfeld. Zur elektronentheorie der metalle auf grund der fermischen statistik. *Zeitschrift für Physik*, 47(1):1–32, Jan 1928.

[3] Douglas Rayner Hartree and W. Hartree. Self-consistent field, with exchange, for beryllium. *Proceedings of the Royal Society of London. Series A - Mathematical and Physical Sciences*, 150(869):9–33, 1935.

[4] Gabriele Giuliani and Giovanni Vignale. *Quantum Theory of the Electron Liquid*. Cambridge University Press, 2005.

[5] David Gontier, Christian Hainzl, and Mathieu Lewin. Lower bound on the hartree-fock energy of the electron gas. *Physical Review A*, 99(5), 2019.

[6] Niels Benedikter, Marcello Porta, Benjamin Schlein, and Robert Seiringer. Correlation energy of a weakly interacting fermi gas with large interaction potential. *Archive for Rational Mechanics and Analysis*, 247(4):65, Jul 2023.

[7] Phan Thanh Nam. Functional analysis 2.

[8] Jan Phillip Solovej. Many body quantum mechanics.

[9] Niels Benedikter, Phan Thành Nam, Marcello Porta, Benjamin Schlein, and Robert Seiringer. Correlation energy of a weakly interacting fermi gas. *Inventiones mathematicae*, 225(3):885–979, 2021.

[10] F. Delyon, B. Bernu, L. Baguet, and M. Holzmann. Upper bounds of spin-density wave energies in the homogeneous electron gas. *Physical Review B*, 92(23), 2015.

[11] A. W. Overhauser. Spin density waves in an electron gas. *Phys. Rev.*, 128:1437–1452, 1962.

[12] Peter A. Fedders and Paul C. Martin. Itinerant antiferromagnetism. *Phys. Rev.*, 143:245–259, 1966.