Master thesis Wilhelm Coupled Cluster

by

Fredrik Wilhelm Holmen

Thesis

for the degree of

Master of Science

Abstract

This is an abstract text.

To someone

This is a dedication to my cat.

Acknowledgements

I acknowledge my acknowledgements.

Contents

Contents

Chapter 1

Introduction

This is a very nice introduction to my myster thesis. or .. lol

Chapter 2

Quantum Mechanics

2.1   Postulates

2.2   Hermitian Operators

2.3   Pauli's Exclusion Principle

2.4   The Variational Principle

2.5   Slater Determinant

A system composed of a nuclei and electrons moving in accordance to the forces of electromagnetic attraction can be described by assigning each electron a wave function

$$\phi_i(\mathbf{x}_i) \tag{2.1}$$

Where $\mathbf{x}_i$ is the position vector for the electron i. Describing a system of many electrons can be done writing a Slater Determinant

$$|\Phi_0\rangle = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(\mathbf{x}_1) & \phi_2(\mathbf{x}_1) & ... & \phi_N(\mathbf{x}_1) \\ \phi_1(\mathbf{x}_2) & \phi_2(\mathbf{x}_2) & ... & \phi_N(\mathbf{x}_2) \\ ... & & & \\ \phi_1(\mathbf{x}_N) & \phi_2(\mathbf{x}_N) & ... & \phi_N(\mathbf{x}_N) \end{vmatrix} \tag{2.2}$$

This way of writing the many-body wave function will represent linear a combination of products of the one-body wave functions ϕ_i's and all the electronic coordinates $\mathbf{x}_i$ distributed among them in all possible ways. Exchanging two lines will change the sign such that the Slater Determinant will respect the antisymmetry requirement.

We can choose the one-body wave functions that is most rewarding the specified system. When calculating on electrons moving with respect to a nuclei, one can choose the wave functions to be the 1s, 2s, 2p, .. orbitals. This representation will not, however, take into account the Colombic repulsion between two electrons and will only be an approximation to the true wavefunction, $|\Psi\rangle$.

Chapter 3

Second Quantization

Second quantization is a new method of representing states and operators.

3.1 Annihilation and Creation operators

We introduce a new way of writing states using the mathematical technique known as second quantization. The main goal is to treat states without paying attention to individual particle coordinates. We represent the empty space with the symbol for vacuum

$$|0\rangle \tag{3.1}$$

To represent a state, we use a creation operator to add the state to the vacuum.

$$\hat{a}_i^\dagger |0\rangle = |\phi_i\rangle \tag{3.2}$$

And the annihilation operator will remove the particle again.

$$\hat{a}_i |\phi_i\rangle = |0\rangle \tag{3.3}$$

Trying to add a new particle to an already filled state and removing an unoccupied state results in zero.

$$\hat{a}_i^\dagger |\phi_i\rangle = 0 \quad \hat{a}_i |0\rangle = 0 \tag{3.4}$$

We can now write the Slater determinant as a chain of creation operators

$$\hat{a}_1^\dagger \hat{a}_2^\dagger ... \hat{a}_N^\dagger |0\rangle \tag{3.5}$$

Permutations of the operators introduces a sign-change, which is equivalent to interchanging rows in the determinant. This

$$\hat{a}_1^\dagger \hat{a}_2^\dagger \ket{0} = \ket{\phi_1 \phi_2} = -\ket{\phi_2 \phi_1} = -\hat{a}_2^\dagger \hat{a}_1^\dagger \ket{0} \tag{3.6}$$

So we can see that the second quantization respects the antisymmetrization condition. Thus, these operators follow the anti commutation relations

$$\{\hat{a}_i^\dagger \hat{a}_j\} = \delta_{ij} \quad \{\hat{a}_i^\dagger \hat{a}_j^\dagger\} = 0 \quad \{\hat{a}_i \hat{a}_j\} = 0 \tag{3.7}$$

Where δ_{ij} is the Kronecher delta.

3.2   Representation of Operators

3.3   Fermi Vacuum

3.4   Normal Ordering and Wick's Theorem

3.5   Partitioning the Hamiltonian

Chapter 4

Many-Body Methods

We have already justified the use of a Slater Determinant to describe the first approximation of the full wave function, $|\Psi\rangle$. Where

$$|\Psi\rangle \approx |\Phi_0\rangle = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(\mathbf{x}_1) & \phi_2(\mathbf{x}_1) & ... & \phi_N(\mathbf{x}_1) \\ \phi_1(\mathbf{x}_2) & \phi_2(\mathbf{x}_2) & ... & \phi_N(\mathbf{x}_2) \\ ... & & & \\ \phi_1(\mathbf{x}_N) & \phi_2(\mathbf{x}_N) & ... & \phi_N(\mathbf{x}_N) \end{vmatrix} \tag{4.1}$$

This first representation fails to account for the Coulombic interrraction between the electrons, and we need higher-order approximations on top of the Slater Determinant to improve our results.

This chapter will look at three methods, namely the Configuration interraction, Many-body Perturbation theory and Hartree-Fock approximations. The Master thesis is on Coupled Cluster theory, and that will be more elaborately explained in it's own chapter. It is useful to benchmark Coupled Cluster with similar many-body method.

4.1 Configuration Interraction

We can write the configuration interaction wavefunction as

$$|\Psi_{CI}\rangle = (1 + \hat{C})|\Phi_0\rangle \tag{4.2}$$

$$\hat{C} = \hat{C}_1 + \hat{C}_2 + ... = \sum_{ia} c_i^a a_a^\dagger a_i + \frac{1}{4} \sum_{ijab} c_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i + ... \tag{4.3}$$

4.2   Many-body Perturbation Theory

4.3   Hartree-Fock approximations

Chapter 5

Coupled-Cluster Theory

In Coupled Cluster theory, the ansatz we make is to make an expansion in the wave function

$$|\Psi\rangle \approx e^{\hat{T}} |\Psi_0\rangle \tag{5.1}$$

The operator $\hat{T}$ is a linear combination of the cluster operators

$$\hat{T} = \hat{T}_1 + \hat{T}_2 + \hat{T}_3 + ... + \hat{T}_N \tag{5.2}$$

Where the operators represent

$$T_1 = \sum_{ia} t_i^a \hat{a}_a^\dagger \hat{a}_i \tag{5.3}$$

$$T_2 = \frac{1}{2} \sum_{ijab} t_{ij}^{ab} \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i \tag{5.4}$$

$$T_2 = \left(\frac{1}{n!}\right)^2 \sum_{ij..ab..}^{n} t_{ij..n}^{ab..n} \hat{a}_a^\dagger \hat{a}_b^\dagger ... \hat{a}_n^\dagger \hat{a}_n ... \hat{a}_j \hat{a}_i \tag{5.5}$$

$$\tag{5.6}$$

We can write the configuration interaction wavefunction as

$$|\Psi_{CI}\rangle = (1 + \hat{C}) |\Phi_0\rangle \tag{5.7}$$

$$\hat{C} = \hat{C}_1 + \hat{C}_2 + ... = \sum_{ia} c_i^a a_a^\dagger a_i + \frac{1}{4} \sum_{ijab} c_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i + ... \tag{5.8}$$

Comparing this linear expansion to the exponential expansion from Coupled Clus-

9

ter, we can see that

$$\hat{C}_2 = \hat{T}_2 + \frac{1}{2}T_1^2 \tag{5.9}$$

Where we can see that even if we truncate Configuration Interaction and Coupled Cluster at the same level, there are more *disconnected* wave function contributions (REFERENCE page 17 IN C&S) in the Coupled Cluster theory. Both the Coupled Cluster and Configuration Interaction theory provides the exact energy by including the operators to infinite order, i.e. no truncation.

5.1   Size Extensivity

It can be important to have a wave function that scales with size. Imagine a two particles, X and Y with infinity separation, they do not interact. This means we should be able to write the total energy as

$$E = E_X + E_Y \tag{5.10}$$

Doing Coupled Cluster

$$\hat{T} = \hat{T}_X + \hat{T}_Y \tag{5.11}$$

$$|\Psi\rangle_{CC} = e^{\hat{T}_X + \hat{T}_Y} |\Phi_0\rangle = e^{\hat{T}_X} e^{\hat{T}_Y} |\Psi_0\rangle \tag{5.12}$$

Since we can write the reference state as a product of the two seperated parts, we are able to write

$$E_{CC} = E_{CC}^X + E_{CC}^Y \tag{5.13}$$

This means Coupled Cluster is size extensive, contrary to the Configuration Interaction.

5.2   The CCD Equations

The Coupled Cluster Doubles equations can be finalized as

$$E_{CCD} = E_{ref} + \Delta E_{CCD} \tag{5.14}$$

With the reference energy defined as

$$E_{ref} = \sum_i \left\langle i \left| \hat{h}_0 \right| j \right\rangle + \sum_{ij} \langle ij|\hat{v}|ij\rangle + \frac{1}{2}Av_0 \tag{5.15}$$

and the corrolation energy given by

$$\Delta E_{CCD} = \frac{1}{4} \sum_{ijab} \langle ij|\hat{v}|ab\rangle \, t_{ij}^{ab} \tag{5.16}$$

v_0 is a constant, nonzero for the finite electron gas. After several applications of Wick's theorem, the amplitude equations can be reduced to

$$(\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b)t_{ij}^{ab} = \langle ab|\hat{v}|ij\rangle + \frac{1}{2}\sum_{cd} \langle ab|\hat{v}|cd\rangle \, t_{ij}^{cd} \tag{5.17}$$

$$+\frac{1}{2}\sum_{kl} \langle kl|\hat{v}|ij\rangle \, t_{kl}^{ab} + \hat{P}\,(ij|ab) \sum_{kc} \langle kb|\hat{v}|cj\rangle \, t_{ik}^{ac} \tag{5.18}$$

$$+\frac{1}{4}\sum_{klcd} \langle kl|\hat{v}|cd\rangle \, t_{ij}^{cd}t_{kl}^{ab} + \frac{1}{2}\hat{P}\,(ij|ab) \sum_{klcd} \langle kl|\hat{v}|cd\rangle \, t_{ik}^{ac}t_{lj}^{db} \tag{5.19}$$

$$-\frac{1}{2}\hat{P}(ij) \sum_{klcd} \langle kl|\hat{v}|cd\rangle \, t_{ik}^{ab}t_{jl}^{cd} - \frac{1}{2}\hat{P}(ab) \sum_{klcd} \langle kl|\hat{v}|cd\rangle \, t_{kl}^{bd}t_{ij}^{ac} \tag{5.20}$$

Where we have defined

$$\hat{P}(ij) = 1 - \hat{P}_{ij} \tag{5.21}$$

Where $\hat{P}_{ij}$ interchanges the two particles occupying the quantum states i and j. Furthermore, we define the operator

$$\hat{P}\,(ij|ab) = (1 - \hat{P}_{ij})(1 - \hat{P}_{ab}) \tag{5.22}$$

We notice that some parts are linear in the amplitude, while some are quadradic. Sorting them into the linear and quadradic parts, L and Q respectably, I get

$$L(t_{ij}^{ab}) = \frac{1}{2}\sum_{cd} \langle ab|\hat{v}|cd\rangle \, t_{ij}^{cd} + \frac{1}{2}\sum_{kl} \langle kl|\hat{v}|ij\rangle \, t_{kl}^{ab} + \hat{P}\,(ij|ab) \sum_{kc} \langle kb|\hat{v}|cj\rangle \, t_{ik}^{ac} \tag{5.23}$$

and

$$Q(t_{ij}^{ab} t_{ij}^{ab}) = \frac{1}{4} \sum_{klcd} \langle kl|\hat{v}|cd\rangle \, t_{ij}^{cd} t_{kl}^{ab} + \frac{1}{2} \hat{P}\,(ij|ab) \sum_{klcd} \langle kl|\hat{v}|cd\rangle \, t_{ik}^{ac} t_{lj}^{db} \tag{5.24}$$

$$-\frac{1}{2} \hat{P}(ij) \sum_{klcd} \langle kl|\hat{v}|cd\rangle \, t_{ik}^{ab} t_{jl}^{cd} - \frac{1}{2} \hat{P}(ab) \sum_{klcd} \langle kl|\hat{v}|cd\rangle \, t_{kl}^{bd} t_{ij}^{ac} \tag{5.25}$$

Labeling each term for practical reasons

$$L_a = \frac{1}{2} \sum_{cd} \langle ab|\hat{v}|cd\rangle \, t_{ij}^{cd} \tag{5.26}$$

$$L_b = \frac{1}{2} \sum_{kl} \langle kl|\hat{v}|ij\rangle \, t_{kl}^{ab} \tag{5.27}$$

$$L_c = \hat{P}\,(ij|ab) \sum_{kc} \langle kb|\hat{v}|cj\rangle \, t_{ik}^{ac} \tag{5.28}$$

$$Q_a = \frac{1}{4} \sum_{klcd} \langle kl|\hat{v}|cd\rangle \, t_{ij}^{cd} t_{kl}^{ab} \tag{5.29}$$

$$Q_b = \frac{1}{2} \hat{P}\,(ij|ab) \sum_{klcd} \langle kl|\hat{v}|cd\rangle \, t_{ik}^{ac} t_{lj}^{db} \tag{5.30}$$

$$Q_c = -\frac{1}{2} \hat{P}(ij) \sum_{klcd} \langle kl|\hat{v}|cd\rangle \, t_{ik}^{ab} t_{jl}^{cd} \tag{5.31}$$

$$Q_d = -\frac{1}{2} \hat{P}(ab) \sum_{klcd} \langle kl|\hat{v}|cd\rangle \, t_{kl}^{bd} t_{ij}^{ac} \tag{5.32}$$

5.3   Intermediates

As Coupled Cluster computations are consume large amounts of computational power, researchers are spending much effort trying to reduce computational cost. One way of reducing the cost is by refactoring the amplitude equations such that we can perform an intermediate computation first and use the result to compute various diagrams later.

Rewriting the equation, (5.20) for CCD amplitudes (Source: Gustav Baardsen

/ Audun):

$$(\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b)t_{ij}^{ab} = \langle ab|\hat{v}|ij\rangle + \frac{1}{2}\sum_{cd}\langle ab|\hat{v}|cd\rangle\, t_{ij}^{cd} \tag{5.33}$$

$$+\frac{1}{2}\sum_{kl} t_{kl}^{ab}\left[\langle kl|\hat{v}|ij\rangle + \frac{1}{2}\sum_{cd}\langle kl|\hat{v}|cd\rangle\, t_{ij}^{cd}\right] \tag{5.34}$$

$$+\hat{P}\,(ij|ab)\sum_{kc} t_{ik}^{ac}\left[\langle kb|\hat{v}|cj\rangle + \frac{1}{2}\sum_{ld}\langle kl|\hat{v}|cd\rangle\, t_{lj}^{db}\right] \tag{5.35}$$

$$-\frac{1}{2}\hat{P}(ij)\sum_{k} t_{ik}^{ab}\left[\sum_{lcd}\langle kl|\hat{v}|cd\rangle\, t_{jl}^{cd}\right] \tag{5.36}$$

$$-\frac{1}{2}\hat{P}(ab)\sum_{c} t_{ij}^{ac}\left[\sum_{kld}\langle kl|\hat{v}|cd\rangle\, t_{kl}^{bd}\right] \tag{5.37}$$

We can now define, and precompute the following values

$$I_1 = \langle kl|\hat{v}|ij\rangle + \frac{1}{2}\sum_{cd}\langle kl|\hat{v}|cd\rangle\, t_{ij}^{cd} \tag{5.38}$$

$$I_2 = \langle kb|\hat{v}|cj\rangle + \frac{1}{2}\sum_{ld}\langle kl|\hat{v}|cd\rangle\, t_{lj}^{db} \tag{5.39}$$

$$I_3 = \sum_{lcd}\langle kl|\hat{v}|cd\rangle\, t_{jl}^{cd} \tag{5.40}$$

$$I_4 = \sum_{kld}\langle kl|\hat{v}|cd\rangle\, t_{kl}^{bd} \tag{5.41}$$

We can now redefine the CCD equation

$$(\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b)t_{ij}^{ab} = \langle ab|\hat{v}|ij\rangle + \frac{1}{2}\sum_{cd}\langle ab|\hat{v}|cd\rangle\, t_{ij}^{cd} + \frac{1}{2}\sum_{kl} t_{kl}^{ab} I_1 \tag{5.42}$$

$$+\hat{P}\,(ij|ab)\sum_{kc} t_{ik}^{ac} I_2 - \frac{1}{2}\hat{P}(ij)\sum_{k} t_{ik}^{ab} I_3 - \frac{1}{2}\hat{P}(ab)\sum_{c} t_{ij}^{ac} I_4 \tag{5.43}$$

Leading to a reduction of computational cost from $\mathcal{O}(h^4 p^4)$ to $\mathcal{O}(h^4 p^2)$

Chapter 6

The Pairing Model

The first system I look at is the pairing model. The pairing model has four energy levels with degeneracy two, one for positive and negative spins. I have used a system consisting of four electrons filling up the four lower-most states up to the Fermi level.
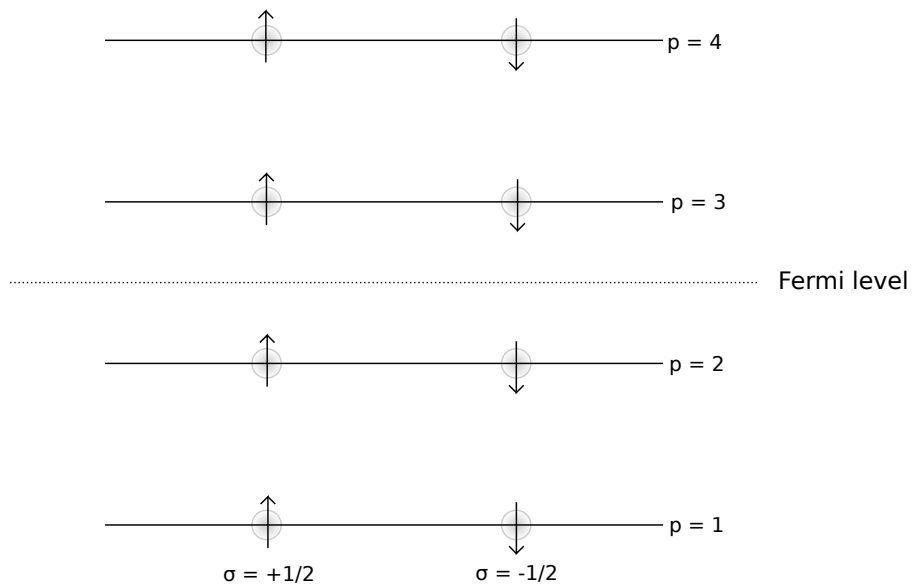

Figure 6.1: A figure depicting a 4 particles-4 holes state. The system consists of occupied particle states below the Fermi level and unoccupied hole states above Fermi level.

6.1   The Hamiltonian

We limit ourselves to a two-body interaction, writing the Hamiltonian as

$$\hat{H} = \sum_{\alpha\beta} \langle \alpha | \hat{h}_0 | \beta \rangle \, \hat{a}_\alpha^\dagger \hat{a}_\beta + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | \hat{v}_0 | \gamma\delta \rangle \, \hat{a}_\alpha^\dagger \hat{a}_\beta^\dagger \hat{a}_\delta \hat{a}_\gamma \tag{6.1}$$

We use the complete basis $|\alpha\rangle$ and define the set as eigenvalues of the one-body operator, $\hat{h}_0$.

The system does require that the total spin is equal to 0. In addition we will not allow spin pairs to be broken, i.e. singly excited states are not allowed.

$$|\Psi_i^a\rangle = 0 \tag{6.2}$$

We introduce the double creation and annihilation operator.

$$\hat{P}_{pq}^\dagger = \hat{a}_{p\sigma}^\dagger \hat{a}_{p-\sigma}^\dagger \tag{6.3}$$

$$\hat{P}_{pq} = a_{q\sigma} a_{q-\sigma} \tag{6.4}$$

We can rewrite the Hamiltonian as an unperterturbed part and a perturbation

$$\hat{H} = \hat{H}_0 + \hat{V} \tag{6.5}$$

$$\hat{H}_0 = \xi \sum_{p\sigma} (p-1)\hat{a}_{p\sigma}^\dagger \hat{a}_{p\sigma} \tag{6.6}$$

$$\hat{V} = -\frac{1}{2}g \sum_{pq} \hat{a}_{p+}^\dagger \hat{a}_{p-}^\dagger \hat{a}_{q-} \hat{a}_{q+} \tag{6.7}$$

The value of ξ determines the spacing between the energy levels, which I have set to 1. This will not impact the insight attained solving this system. p and q determines the energy level. σ is the spin, with value either $+\frac{1}{2}$ or $-\frac{1}{2}$. Both the unperturbed and perturbed Hamiltonian keeps total spin at 0

We can normal order the Hamiltonian by Wicks general theorem.

$$a_p^\dagger a_q = \left\{ a_p^\dagger a_q \right\} + \delta_{pq\in i} \tag{6.8}$$

$$a_p^\dagger a_q^\dagger a_s a_r = \left\{ a_p^\dagger a_q^\dagger a_s a_r \right\} + \left\{ a_p^\dagger a_r \right\} \delta_{qs\in i} - \left\{ a_p^\dagger a_s \right\} \delta_{qr\in i} \tag{6.9}$$
$$+ \left\{ a_q^\dagger a_s \right\} \delta_{pr\in i} - \left\{ a_q^\dagger a_r \right\} \delta_{ps\in i} + \delta_{pr\in i}\delta_{qs\in i} - \delta_{ps\in i}\delta_{qr\in i} \tag{6.10}$$

Which gives the Normal-ordered Hamiltonian

$$\hat{H} = \hat{H}_N + E_{ref} \tag{6.11}$$

$$\hat{H}_N = \hat{F}_N + \hat{W} \tag{6.12}$$

$$\hat{F}_N = \sum_{pq} h_{pq} \left\{ \hat{a}^\dagger_{p\sigma} \hat{a}_{p\sigma} \right\} - \sum_{pqi} \langle pi||qi \rangle \left\{ \hat{a}^\dagger_{p+} \hat{a}_{q-} \right\} \tag{6.13}$$

$$\hat{W} = -\frac{1}{2} \sum_{pqrs} \langle pq||rs \rangle \left\{ \hat{a}^\dagger_{p+} \hat{a}^\dagger_{p-} \hat{a}_{q-} \hat{a}_{q+} \right\} \tag{6.14}$$

$$E_{ref} = \sum_i h_{ii} + \frac{1}{2} \sum_{ij} \langle ij||ij \rangle \tag{6.15}$$

6.2 Configuration Interaction theory

This system is a good way to benchmark various methods as we can compute the exact solution using Full Configuration Interaction.
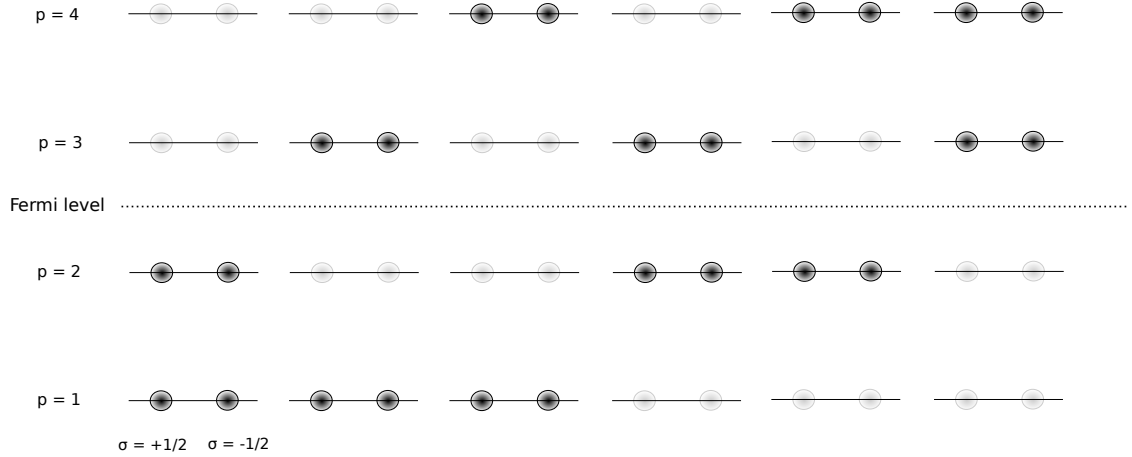

Figure 6.2: Configuration space for given pairing model showing all possible distributions of electrons

We need to diagonalize the Hamiltonian matrix looking at the linear combination of all different compinations of

$$
\hat{\mathcal{H}} = \begin{pmatrix}
 & |\Phi_0\rangle & |\Phi_{12}^{56}\rangle & |\Phi_{12}^{78}\rangle & |\Phi_{34}^{56}\rangle & |\Phi_{34}^{78}\rangle & |\Phi_{1234}^{5678}\rangle \\
\langle\Phi_0| & & & & & & \\
\langle\Phi_{12}^{56}| & & & & & & \\
\langle\Phi_{12}^{78}| & & & & & & \\
\langle\Phi_{34}^{56}| & & & & & & \\
\langle\Phi_{34}^{78}| & & & & & & \\
\langle\Phi_{1234}^{5678}| & & & & & &
\end{pmatrix}
\tag{6.16}
$$

Excluding the 4p-4h excitations one does not diagonalize the exact matrix, but rather the approximated matrix known from Configuration Interaction.

The diagonal elements are calculated using Wick's theorem. Looking first at the ground state calculation with the unperturbed Hamiltonian part

$$
\left\langle \Phi_0 \middle| \hat{\mathbf{H}}_0 \middle| \Phi_0 \right\rangle
\tag{6.17}
$$

$$
\langle| \, a_{2\downarrow}a_{2\uparrow}a_{1\downarrow}a_{1\uparrow} \sum_{p\sigma} \delta(p-1) a_{p\sigma}^\dagger a_{p\sigma} a_{1\uparrow}^\dagger a_{1\downarrow}^\dagger a_{2\uparrow}^\dagger a_{2\downarrow}^\dagger \, |\rangle
\tag{6.18}
$$

Which we see can contract in four different ways, resulting in

$$
2\delta(1-1) + 2\delta(2-1) = 2\delta
\tag{6.19}
$$

And the perturbation part

$$
\left\langle \Phi_0 \middle| \hat{\mathbf{V}} \middle| \Phi_0 \right\rangle
\tag{6.20}
$$

$$
\langle| \, a_{2\downarrow}a_{2\uparrow}a_{1\downarrow}a_{1\uparrow} \left(-g/2 \sum_{pq} a_{p\uparrow}^\dagger a_{q\downarrow}^\dagger a_{q\downarrow} a_{p\uparrow} \right) a_{1\uparrow}^\dagger a_{1\downarrow}^\dagger a_{2\uparrow}^\dagger a_{2\downarrow}^\dagger \, |\rangle
\tag{6.21}
$$

As we can see, there are two ways this can contract, each contributing with the constant factor, $-g/2$ Resulting in the final Hamiltonian matrix

$$
\hat{\mathcal{H}} = \begin{pmatrix}
2\delta - g & -g/2 & -g/2 & -g/2 & -g/2 & 0 \\
-g/2 & 4\delta - g & -g/2 & -g/2 & 0 & -g/2 \\
-g/2 & -g/2 & 6\delta - g & 0 & -g/2 & -g/2 \\
-g/2 & -g/2 & 0 & 6\delta - g & -g/2 & -g/2 \\
-g/2 & 0 & -g/2 & -g/2 & 8\delta - g & -g/2 \\
0 & -g/2 & -g/2 & -g/2 & -g/2 & 10\delta - g
\end{pmatrix}
\tag{6.22}
$$

6.3   Diagrammatic Rules

One can visualize many-body quantum physics by using diagrams.

6.4   Many-Body Perturbation Theory

The Perturbation theory presents a non-iterative approach to approximating the ground state energy. The approach is similar to previous methods. We start by splitting the Hamiltonian into a solvable part and a perturbation.

$$\hat{H} = \hat{H}_0 + \hat{V} \tag{6.23}$$

Where we have chosen our basis such that

$$\hat{H}_0 \left| \Psi_0 \right\rangle = W_0 \left| \Psi_0 \right\rangle \tag{6.24}$$

We split the basis aswell

$$\left| \Psi_0 \right\rangle = \left| \Phi_0 \right\rangle + \sum_i^\infty c_i \left| \phi_i \right\rangle \tag{6.25}$$

Assuming intermediate normalization

$$\left\langle \Phi_0 | \Psi_0 \right\rangle = 1 \tag{6.26}$$

We can calculate the total exact energy

$$E = \left\langle \Phi_0 \right| \hat{H}_0 \left| \Psi_0 \right\rangle + \left\langle \Phi_0 \right| \hat{V} \left| \Psi_0 \right\rangle \tag{6.27}$$

Where we know that

$$\left\langle \Phi_0 \right| \hat{H}_0 \left| \Psi_0 \right\rangle = W_0 \tag{6.28}$$

And we get the corrolation energy

$$E - W_0 = \Delta E = \left\langle \Phi_0 \right| \hat{V} \left| \Psi_0 \right\rangle \tag{6.29}$$

We will usually aim to compute this energy when doing MBPT.

6.4.1 General derivation of Many Body Particle Theory equations

Looking at the equation

$$\hat{V}\ket{\Psi_0} = \hat{H}\ket{\Psi_0} + \hat{H}_0\ket{\Psi_0} \tag{6.30}$$

We reorganize and add the term $\omega\ket{\Psi_0}$ on both sides

$$\hat{V}\ket{\Psi_0} + \omega\ket{\Psi_0} - \hat{H}\ket{\Psi_0} = \omega\ket{\Psi_0} - \hat{H}_0\ket{\Psi_0} \tag{6.31}$$

Remembering that $\hat{H}\ket{\Psi_0} = E\ket{\Psi_0}$, we get

$$\ket{\Psi_0} = \frac{\hat{V} + \omega - E}{\omega - \hat{H}_0}\ket{\Psi_0} \tag{6.32}$$

Before continuing, we introduce the operators $\hat{P}$ and $\hat{Q}$, such that

$$\ket{\Psi_0} = \hat{P}\ket{\Psi_0} + \hat{Q}\ket{\Psi_0} = \ket{\Phi_0}\braket{\Phi_0|\Psi_0} + \sum_i \ket{\Phi_i}\braket{\Phi_i|\Psi_0} \tag{6.33}$$

$$= \ket{\Phi_0} + \chi \tag{6.34}$$

Giving

$$\ket{\Phi_0} = \hat{P}\ket{\Psi_0} \quad \chi = \hat{Q}\ket{\Psi_0} \tag{6.35}$$

Using $\hat{R}(\omega) = \frac{\hat{Q}}{(\omega - \hat{H}_0)}$ and multiplying both sides with $\hat{Q}$ from the left in equation (6.32) we attain

$$\hat{Q}\ket{\Psi_0} = \hat{R}(\omega)\left(\hat{V} + \omega - E\right)\ket{\Psi_0} \tag{6.36}$$

Using equations (6.33) and (6.35), we get

$$\ket{\Psi_0} = \ket{\Phi_0} + \hat{R}(\omega)\left(\hat{V} + \omega - E\right)\ket{\Psi_0} \tag{6.37}$$

This is an iterative scheme. We can substitute $\ket{\Psi_0}$ on the right hand side with the entire right hand side. This results in an infinite sum provided the series converges

$$\ket{\Psi_0} = \sum_0^\infty \left\{ \hat{R}(\omega)(\hat{V} + \omega - E) \right\}^m \ket{\Phi_0} \tag{6.38}$$

The right hand side does include the energy, E, which must be computed using $E = W_0 + \Delta E$, and

$$\Delta E = \langle \Phi_0 | \hat{V} | \Psi_0 \rangle = \sum_0^\infty \langle \Phi_0 | \hat{V} \left[\hat{R}(\omega)(\hat{V} - E + \omega) \right]^m | \Phi_0 \rangle \qquad (6.39)$$

6.4.2   Equations for Reileigh-Schrodinger Perturbation Theory

We can interpret ω different ways. I here present the Reileigh-Schrodinger Perturbation Theory which postulates that

$$\omega = W_0 \qquad (6.40)$$

Such that

$$|\Psi_0\rangle = \frac{\hat{V} - \Delta E}{\omega - \hat{H}_0} |\Psi_0\rangle \qquad (6.41)$$

and we get the final equations

$$|\Psi_0\rangle = \sum_0^\infty \left\{ \hat{R}(\omega)(\hat{V} + -\Delta E) \right\}^m |\Phi_0\rangle \qquad (6.42)$$

and

$$\Delta E = \sum_0^\infty \langle \Phi_0 | \hat{V} \left[\hat{R}(\omega)(\hat{V} - \Delta E) \right]^m |\Phi_0\rangle \qquad (6.43)$$

Taking a closer look at the energy-equations, we find that we can write the first orders as

$$E^{(1)} = \langle \Phi_0 | \hat{V} | \Phi_0 \rangle = V_{00}$$
$$E^{(2)} = \langle \Phi_0 | \hat{V} \hat{R}_0 \hat{V} | \Phi_0 \rangle$$
$$E^{(3)} = \langle \Phi_0 | \hat{V} \hat{R}_0 (\hat{V} - E^{(1)}) \hat{R}_0 \hat{V} | \Phi_0 \rangle$$
$$E^{(4)} = \langle \Phi_0 | \hat{V} \hat{R}_0 (\hat{V} - E^{(1)}) \hat{R}_0 (\hat{V} - E^{(1)}) \hat{R}_0 \hat{V} | \Phi_0 \rangle - E^{(2)} \langle \Phi_0 | \hat{V} \hat{R}_0^2 \hat{V} | \Phi_0 \rangle$$

Because of the frequent appearance, we can rewrite $\hat{V} - E^{(1)}$ as

$$\hat{\Omega} = \hat{V} - E^{(1)} \qquad (6.44)$$

We name this new variable the wave operator

6.4.3   Canonical Hartree-Fock

In the pairing model, we work with the Normal-ordered Hamiltonian

$$\hat{H}_N = \hat{F}_N^d + \hat{F}_N^0 + \hat{W} \tag{6.45}$$

Which is part of the total Hamiltonian by

$$\hat{H} = \hat{H}_N + E_{\text{ref}} \tag{6.46}$$

Where

$$\hat{H}_N \left| \Psi \right\rangle = \Delta E \left| \Psi \right\rangle \tag{6.47}$$

If we use a Canonical Hartree-Fock basis, the Fock matrix will be diagonal, meaning

$$\hat{F}_N^o = 0 \quad \text{and} \quad f_{pq} = \epsilon_p \delta_{pq} \tag{6.48}$$

A noncanonical Hartree-Fock will be block diagonal with

$$f_{ia} = \left\langle i \right| \hat{f} \left| a \right\rangle = 0 \tag{6.49}$$

6.4.4   Hartree-Fock calculations

When doing Hartree-Fock calculation, we do a change of basis and instead of expanding our Hamiltonian, we vary the wavefunction to minimize the energy. We name the original basis by greek letters and the new basis by latin letters. The original basis should be chosen such that we can calculate the its expectation value.

$$\left\langle \Phi_0 \right| \hat{H} \left| \Phi_0 \right\rangle = E^{\text{HF}} \tag{6.50}$$

Variational principle ensures that

$$E^{\text{HF}} > 0 \tag{6.51}$$

We now introduce a change of basis

$$\left| \psi_a \right\rangle = \sum_\lambda C_{a\lambda} \left| \psi_\lambda \right\rangle \tag{6.52}$$

Varying $C_{p\lambda}$, we can look for the basis providing the lowest energy. We start by rewriting E^{HF} as a functional

$$E\left[\psi\right] = \sum_{a=1}^{N} \langle a| \, h \, |a\rangle + \frac{1}{2} \sum_{ab}^{N} \langle ab| \, v \, |ab\rangle \tag{6.53}$$

In terms of the original greek basis

$$E\left[\psi\right] = \sum_{a=1}^{N} \sum_{\alpha\beta} C_{a\alpha}^{*} C_{a\beta} \langle \alpha| \, h \, |\beta\rangle + \frac{1}{2} \sum_{ab}^{N} \sum_{\alpha\beta\gamma\delta} C_{a\alpha}^{*} C_{b\beta}^{*} C_{a\gamma} C_{b\delta} \langle \alpha\beta| \, v \, |\gamma\delta\rangle \tag{6.54}$$

To find the minima, we introduce a Lagrange multiplier before differentiating with respect to $C_{a\alpha}^{*}$. This will give N equations, one for each state, a. The equations are given by

$$\sum_{\beta} C_{a\beta} \langle \alpha| \, h \, |\beta\rangle + \sum_{b}^{N} \sum_{\beta\gamma\delta} C_{b\beta}^{*} C_{b\delta} C_{a\gamma} \langle \alpha\beta| \, v \, |\gamma\delta\rangle = \epsilon_a C_{a\alpha} \tag{6.55}$$

Defining

$$h_{\alpha\gamma}^{\mathrm{HF}} = \langle \alpha| \, h \, |\gamma\rangle + \sum_{b=1}^{N} \sum_{\beta\delta} C_{b\beta}^{*} C_{b\delta} \langle \alpha\beta| \, v \, |\gamma\delta\rangle \tag{6.56}$$

We get the short hand iterative equations to be solved

$$\sum_{\gamma} h_{\alpha\gamma}^{\mathrm{HF}} C_{a\gamma} = \epsilon_a C_{a\alpha} \tag{6.57}$$

6.4.5   RSPT to for Pairing model

Given that our Hartree-Fock basis is canonical, $\hat{F}_N^0 = 0$, and $f_{pq} = \epsilon_p \delta_{pq}$, we can

Chapter 7

Infinite Matter

A study of infinite matter is the most comprehensible way of studying nuclear material. This thesis will study the infinite electron gas before the final study of nuclear material. This is done because of pedagogical reasons and because the electron gas has closed form solutions that provide important benchmarking for the code.

7.1 The Infinate Electron Gas

The infinite electron gas gives a good approximation to valence electrons in metal. The gas consist only of interacting electrons with a uniform background of charged ions. The whole system is charge neutral. We assume a cubic box, length L and volume $\Omega = L^3$, with N_e as the number of electrons with a charge density $\rho = N_e/\Omega$.

We regard the system as homogenic, using the free particle normalized wave function

$$\psi_{\mathbf{k}\sigma}(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} e^{i\mathbf{k}\mathbf{r}} \xi_\sigma \qquad (7.1)$$

Where $\mathbf{k}$ is the wave number and ξ_σ is a spin function.

$$\xi_{+\frac{1}{2}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \xi_{-\frac{1}{2}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \qquad (7.2)$$

Assuming periodic boundary conditions, we acquire the following wave numbers

$$k_i = \frac{2\pi n_i}{L} \quad i = x, y, z \quad n_i = 0, \pm 1, \pm 2, \dots \qquad (7.3)$$

The electrons interact with the sentral symmetric Colomb potential, $\hat{V}(\mathbf{r}_1, \mathbf{r}_2)$ depending only on the distance $|\mathbf{r}_1 - \mathbf{r}_2|$.

The Hamiltonian for infinite electron gas is

$$\hat{H} = \hat{T} + \hat{V} \tag{7.4}$$

Where we have the kinetic energy, $\hat{T}$ as

$$\hat{T} = \sum_p \frac{\hbar^2 k^2}{2m} a_{k\sigma}^\dagger a_{k\sigma} \tag{7.5}$$

7.2   Infinite Nuclear Matter

Central to my thesis, is the study of infinite nuclear matter. I look at baryonic matter similar to the dense baryonic matter found in neutron stars. I limit the study to temperatures far below Fermi level. The matter is mostly made up of an equilibrium of baryons and leptons. In neutron star matter, we assume the equilibrium consist of protons, neutrons, electrons and muons with densities larger than 0.1fm^-3. The equilibrium conditions are specified by weak interactions

$$b_1 \rightarrow b_2 + l + \bar{\nu}_l \quad b_2 + l \rightarrow b_1 + \nu_l \tag{7.6}$$

Where b represent either neutron or proton and l is either an electron or muon. ν_l is the corresponding neutrino.

Nuclear matter is a hypothetical system filling all of space at a uniform density. Symmetric nuclear matter (SNM) consist of equal numbers of protons of neutrons, while pure nuclear matter (PNM) consist only of neutrons. For finite-nucleus systems, the most difficult part is calculating the single particle wave function. For nuclear matter we can use plane wave basis and similar to electron gas, the difficult part is calculating the energy and the effective interaction between particles [2]. In my calculations, I have looked at pure nuclear matter.

7.3   Nuclear Interaction

Nuclear matter is composed of baryons, which interacts through the strong force.

7.3.1   The Minnesota Potential

The Minnesota Potential is given as

$$v(r) = (v_R + (1 + P_{12}^\sigma)v_T/2 + (1 - P_{12}^\sigma)v_S/2) \tag{7.7}$$

$$\cdot (\alpha + (2 - \alpha)P_{12}^r)/2 + (1 + m_{t,1})(1 + m_{t,2})\frac{e^2}{4r} \tag{7.8}$$

where r is given as $|\mathbf{r_1} - \mathbf{r_2}|$ and m_t is the isospin projection of particle 1 or 2. $m_t = \pm 1$. P_{12}^σ and P_{12}^r are exchange operators for spin and position, respectively [1]. Furthermore, we have used

$$v_R = v_{0R}e^{-k_R r^2}, \quad v_T = -v_{0T}e^{-k_T r^2}, \quad v_S = -v_{0S}e^{-k_s r^2} \tag{7.9}$$

Where the constants v_{0R}, v_{0T}, v_{0S}, k_R, k_T and k_S are given by [3]

1. $v_{0R} = 200\text{MeV}$, $k_R = 0.1487\text{fm}^{-2}$

2. $v_{0T} = 178\text{MeV}$, $k_T = 0.649\text{fm}^{-2}$

3. $v_{0S} = 91.85\text{MeV}$, $k_S = 0.465\text{fm}^{-2}$

Written by second quantisation, we want to calculate the two-body interaction

$$\langle k_p k_q | v | k_r k_s \rangle = \frac{V_0}{L^3} \left(\frac{\pi}{\alpha} \right)^{3/2} e^{-q^2/4\alpha} \delta_{\mathbf{k}_p+\mathbf{k}_q, \mathbf{k}_r+\mathbf{k}_s} \tag{7.10}$$

Where q is the relative momentum transfer

$$\mathbf{q} = \mathbf{p} - \mathbf{p}' \tag{7.11}$$

$$\mathbf{p} = \frac{1}{2}(\mathbf{k}_p - \mathbf{k}_q) \quad \mathbf{p}' = \frac{1}{2}(\mathbf{k}_r - \mathbf{k}_s) \tag{7.12}$$

We can now set up the two-body Matrix-elements for the Minnesota Potential

$$\langle \mathbf{k}_p \mathbf{k}_q | v | \mathbf{k}_r \mathbf{k}_s \rangle = \langle \mathbf{k}_p \mathbf{k}_q | \frac{1}{2} \left(V_R + \frac{1}{2}V_T + \frac{1}{2}V_S \right) | \mathbf{k}_r \mathbf{k}_s \rangle \tag{7.13}$$

$$+ \langle \mathbf{k}_p \mathbf{k}_q | \frac{1}{4}(V_T - V_S) P_{12}^\sigma | \mathbf{k}_r \mathbf{k}_s \rangle \tag{7.14}$$

$$- \langle \mathbf{k}_p \mathbf{k}_q | \frac{1}{2} \left(V_R + \frac{1}{2}V_T + \frac{1}{2}V_S \right) P_{12}^\sigma P_{12}^\tau | \mathbf{k}_r \mathbf{k}_s \rangle \tag{7.15}$$

$$- \langle \mathbf{k}_p \mathbf{k}_q | \frac{1}{4}(V_T - V_S) P_{12}^\tau | \mathbf{k}_r \mathbf{k}_s \rangle \tag{7.16}$$

Matrix elements for the spin and isospin exchange operators are

$$\langle \sigma_p \sigma_q | P_{12}^\sigma | \sigma_r \sigma_s \rangle = \delta_{\sigma_p, \sigma_s} \delta_{\sigma_q, \sigma_r} \tag{7.17}$$

One can see that these matrix elements come at a far greater computational cost than for electron-electron interaction in the electron gas. Therefore it is necessary to compute and store all elements instead of computing them "on the fly". Source: Lecture 1-2 infinite matter.

Chapter 8

Implementation

8.1 Matrix Representation of Contractions

Diagrams can be viewed as contractions of tensors of varying degree. An example is the matrix-matrix multiplication product

$$(MN)^{\alpha}_{\gamma} = \sum_{\beta} M^{\alpha}_{\beta} N^{\beta}_{\gamma} \tag{8.1}$$

As our goal is to rewrite the Coupled Cluster equations as matrix-matrix products. We will need to map tensors of rank ≥ 2 onto matrices. One mapping that provides systematic and unique matrix elements can be

$$\langle pq|\hat{v}|rs\rangle = V_{\alpha(p,q),\beta(r,s)} \tag{8.2}$$

Where

$$\alpha(p,q) = p + qN_p \quad \beta(r,s) = r + sN_r \tag{8.3}$$

We need to be careful when mapping tensors this way. Consider first the calculation of the perfectly aligned L_a term

$$L_a = \sum_{cd} \langle ab|\hat{v}|cd\rangle \, t^{cd}_{ij} \tag{8.4}$$

Mapping this equation using equation (8.3)

$$\langle ab|\hat{v}|cd\rangle = v^{cd}_{ab} \rightarrow V^{\alpha(a,b)}_{\beta(c,d)} \tag{8.5}$$

and

$$t^{cd}_{ij} \rightarrow T^{\beta(c,d)}_{\delta(i,j)} \tag{8.6}$$

As we are mapping to unique elements

$$\beta(c,d) = \beta(c,d) \tag{8.7}$$

We can now rewrite the equation

$$(L_a)_\delta^\alpha = \sum_\beta V_\beta^\alpha T_\delta^\beta \tag{8.8}$$

Implying by regarding equation (8.1) that we can rewrite the product as matrix-matrix multiplication

$$L_a = VT \tag{8.9}$$

8.1.1   Aligning elements

Unfortunately, not all product are perfectly aligned like L_a. Consider, for example, the term, L_c

$$L_c = -P\left(ij|ab\right)\sum_{kc}\langle kb|\hat{v}|cj\rangle\, t_{ik}^{ac} \tag{8.10}$$

Using the same mapping scheme

$$\langle kb|\hat{v}|cj\rangle = v_{cj}^{kb} \rightarrow V_{\beta(cj)}^{\alpha(kb)} \tag{8.11}$$

and

$$t_{ik}^{ac} \rightarrow T_{\delta(ik)}^{\gamma(ac)} \tag{8.12}$$

This matrix multiplication is misaligned, and if the number of particles is unequal to the number of holes, the matrices' size will uncompatible.

$$(L_c)_\delta^\alpha \neq -P\left(ij|ab\right)\sum_\beta V_{\beta(cj)}^{\alpha(kb)} T_{\delta(ik)}^{\gamma(ac)} \tag{8.13}$$

We need to find another mapping, such that

$$v_{cj}^{kb} \rightarrow \tilde{V}_{\beta(ck)}^{\alpha(bj)} \tag{8.14}$$

and

$$t_{ik}^{ac} \rightarrow \tilde{T}_{\delta(ia)}^{\gamma(ck)} \tag{8.15}$$

Now, the matrix multiplication is aligned

$$(\tilde{L}_c)_\delta^\alpha = -P\,(ij|ab) \sum_\beta \tilde{V}_{\beta(ck)}^{\alpha(bj)} \tilde{T}_{\delta(ia)}^{\gamma(ck)} \tag{8.16}$$

Note, however, that

$$L_c \neq \tilde{L}_c \tag{8.17}$$

We must "realigne" $\tilde{L}_c$ to match the correct diagram

$$(\tilde{L}_c)_{\delta(i,a)}^{\alpha(b,j)} \rightarrow (L_c)_{\delta(i,k)}^{\alpha(k,b)} \tag{8.18}$$

8.2 Block Implementation

We can exploit symmetries in the homogeneous electron gas to optimize performance. Due to kroenecker delta's in the interaction, one such symmetry is the conservation of momentum

$$\delta_{\mathbf{k}_p+\mathbf{k}_q, \mathbf{k}_r+\mathbf{k}_s} \rightarrow \mathbf{k}_p + \mathbf{k}_q = \mathbf{k}_r + \mathbf{k}_s \tag{8.19}$$

We also conserve spin

$$m_{s_p} + m_{s_q} = m_{s_r} + m_{s_s} \tag{8.20}$$

The amplitudes will be subject to the same restrictions, vizualised by the first order amplitude generated by perturbation theory

$$(t_{ij}^{ab})^{t=0} = \frac{\langle ab|\hat{v}|ij\rangle}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b} \tag{8.21}$$

Looking at the L_a term

$$L_a = \sum_{cd} \langle ab|\hat{v}|cd\rangle\, t_{ij}^{ab} \tag{8.22}$$

We see that

$$\mathbf{k}_a + \mathbf{k}_b = \mathbf{k}_c + \mathbf{k}_d = \mathbf{k}_i + \mathbf{k}_j \tag{8.23}$$

And the same for spin

$$m_{s_a} + m_{s_b} = m_{s_c} + m_{s_d} = m_{s_i} + m_{s_j} \tag{8.24}$$

When summing over all variations of contractions, only the quantum numbers preserving the symmetry requirements are nonzero. When storing the interactions in a matrix, most of it will have zero-elements. The blocking method will store the nonzero parts in blocks inside the matrix. By keeping track of the blocks, we can reduce the full matrix-matrix multiplication to a series of multiplications of the blocks.

We need a unique identifier when sorting states into boxes. One can apply the same logic as in equation (8.3) and set up

$$k_{\text{unique}} = k_x + k_y \Delta k + k_z \Delta k^2 2 \tag{8.25}$$

where we have defined

$$\Delta k = k_{\text{max}} + 1 \tag{8.26}$$

Chapter 9

Results

9.1 The Pairing Model

The Pairing Model serve as a valuable benchmark for implemented solvers. As I have looked at a 4p4h configuration, a full configuration interaction solver can be implemented giving the exact solution. One can also calculate the exact solution for second order perturbation theory by hand [4].

$$\Delta E_{MBPT2} = \frac{1}{4} \sum_{abij} \frac{\langle ij||ab \rangle \langle ab||ij \rangle}{\epsilon_{ij}^{ab}} = \sum_{a<b,i<j} \frac{\langle ij||ab \rangle \langle ab||ij \rangle}{\epsilon_{ij}^{ab}} \tag{9.1}$$

Where

$$\epsilon_{ij}^{ab} = \epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b \tag{9.2}$$

and

$$\epsilon_p = h_{pp} + \sum_i \langle pi||pi \rangle \tag{9.3}$$

This results in

$$\Delta E_{MBPT2} = \frac{\langle 01||45 \rangle^2}{\epsilon_{01}^{45}} + \frac{\langle 01||67 \rangle^2}{\epsilon_{01}^{67}} + \frac{\langle 23||45 \rangle^2}{\epsilon_{23}^{45}} \frac{\langle 23||67 \rangle^2}{\epsilon_{23}^{67}} \tag{9.4}$$

$$\Delta E_{MBPT2} = -\frac{g^2}{4} \left(\frac{1}{4+g} + \frac{1}{6+g} + \frac{1}{2+g} + \frac{1}{4+g} \right) \tag{9.5}$$

Where g represents the interaction strength. The table below shows my results for various g's both using the exact mbpt2 calculations and my numerically computed results. All results can be accessed on github [5]

g	E_0	exact ΔE_{MBPT2}	ΔE_{MBPT2}
-1	3	-0.466667	-0.466667
-0.5	2.5	-0.0887446	-0.0887446
0	2	0	0
0.5	1.5	-0.0623932	-0.0623932
1	1	-0.219048	-0.219048

Table 9.1: A table showing corrolation energies for Pairing model with 4 particle-states and 4 hole-states.

g	ΔE_{MBPT2}	$\Delta E_{CCD}^{(1)}$
-1	-0.466667	-0.466667
-0.5	-0.0887446	-0.0887446
0	0	0
0.5	-0.0623932	-0.0623932
1	-0.219048	-0.219048

Table 9.2: A table comparing corrolation energies for Pairing model with 4 particle-states and 4 hole-states. This table show that CCD solver used with only a single iteration produces results exactly equal to mbpt2. This was done with the naive implementation of CCD equations

As one can see, the corrolation energies computed perfectly matches which both tells us that the basis set is set up correctly and that the MBPT2 solver is set up correctly. The results presented also match the results found in [4]

The second order perturbation theory is valuble for benchmarking my implementation of Coupled Cluster Doubles. By initializing the first set of amplitudes, t, as zero, I get

$$t_{ij}^{ab(0)} = 0 \tag{9.6}$$

$$t_{ij}^{ab(1)} = \frac{1}{4} \sum_{ijab} \frac{\langle ab||ij\rangle}{\epsilon_{ij}^{ab}} \tag{9.7}$$

Which is equal to second order pertubation theory.

9.1.1   Comparison of CCD solvers

In this thesis I have created three different solvers for Coupled Cluster Doubles equations.

g	ΔE_{CCD} Naive	ΔE_{CCD} Intermediates
0	x	x
-0.5	-0.0630564	-0.0630562
0	0	0
0.5	-0.0833621	-0.0833623
1	-0.369557	-0.369557

Table 9.3: A table comparing corrolation energies for Pairing model with 4 particle-states and 4 hole-states. This table compare results from Naive and Intermediate implementation of CCD equations. A relaxing factor of $w = 0.3$ has been used because of divergence around $g = -1$

1. A naive brute force implementation of the equations summing over all variables.

2. A naive brute force implementation of intermediate equations summing over all variables.

3. Rewriting summations as matrix-matrix multiplications and exploiting various symmetry arguments one can set up a block implementation.

As shown in table (9.2), the naive implementation reproduces the mbpt2 energies as expected. I have used both the naive and intermediate CCD solver to compute corrolation energies for the Pairing model and again, [4] provides us with a good benchmark for the CCD equations.

As one can see, my solvers reproduce results presented in [4]. For values of g close to -1, one will see a divergence for CCD equations. By introducing a relaxing factor of $w = 0.3$, this problem was solved.

9.1.2   Comparison of various solvers

The full configuration interaction provides us with the exact solution for the 4p4h Pairing model. It can therefore be useful to compare the performance of Perturbation theory to second, third and fourth order with Coupled Cluster Doubles and configuration interaction without the four-particle excitation.
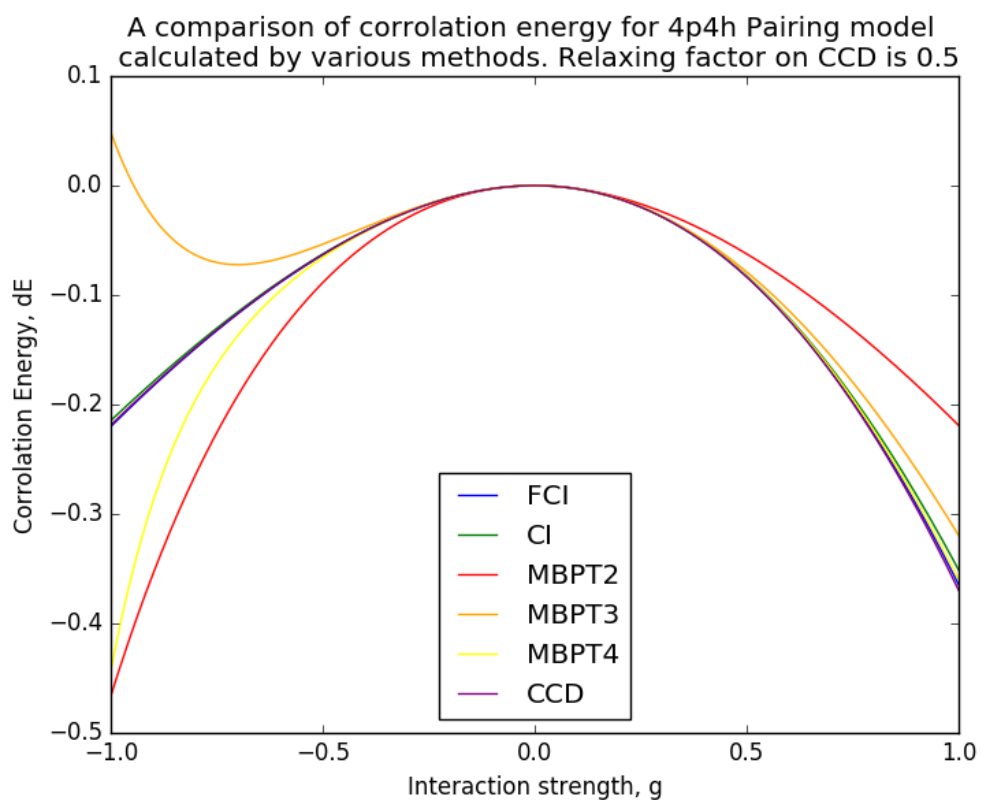
H

Figure 9.1: Comparing
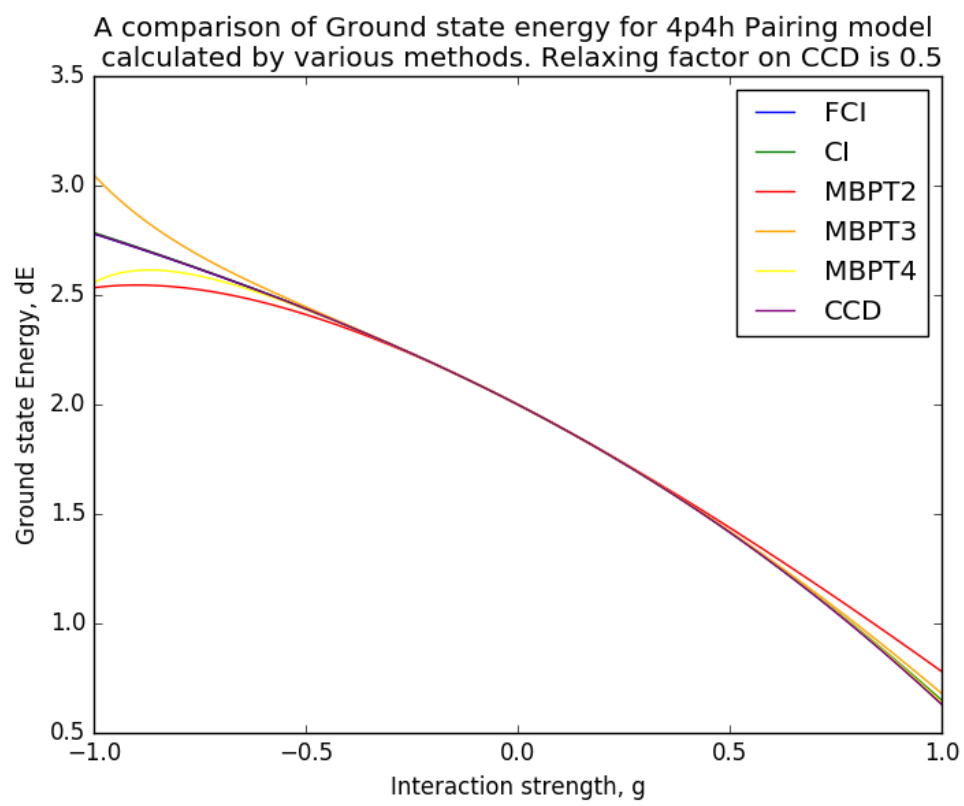
Figure 9.2

Chapter 10

Appendix

Bibliography

[1] Gustav Baardsen *Coupled-cluster theory for infinite matter* 2014

[2] B. D. Day *Rev. Mod. Phys.,* 39:719, 1967.

[3] D. R. Thompson, M. Lemere and Y.C. Tang. *Nucl. Phys. A,* 286:53 1977.

[4] Morten Hjorth-Jensen, Maria Paola Lombardo and Ubiraja van Kolck *An Advanced Course in Computational Nuclear Physics* 2016

[5] Fredrik Wilhelm Holmen *https://github.com/wholmen/Master*