COUPLED CLUSTER CALCULATIONS ON NUCLEAR MATTER

by

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Introduction

You have to write about the potentials used in the programs, the potentials that I am supposed to use in the calculations.

Chapter 2

The Second Quantization

Nuclear physics is about many-particle systems, the need for interparticle potentials has to be accounted for when trying to describe such systems. The interparticle potentials have to be implemented in the many-particle Schrödinger equation. A direct solution of the schrödinger equation in configuration space is impractical [1]. It is necessary to resort to other techniques such as the second quantization.

The system studied in this text consists of nucleons which belong to the types of particles called fermions. Fermions are particles with half integer spin. A system of fermions is described by an antisymmetric wave function, these particles obeys the Pauli principle which states that two identical fermions can not occupy the same single particle state.

In most of the cases of interest, as is also the case in this text, the Hamiltonian takes the form

$$H = \sum_{k=1}^{N} T(x_k) + \frac{1}{2} \sum_{k \neq l=1}^{N} V(x_k, x_l). \tag{2.1}$$

Where T is the kinetic energy and V is the potential energy of interaction between the particles, while x_k denotes the coordinates of particle k. The potential energy term represents the interaction between every pair of particles, counted once which account for the factor of $\frac{1}{2}$ [1].

2.1 Creation and annihilation operators

The interpretation of occupation of the antisymmetric many-body fermion states allows to introduce the two operators $a_\alpha^\dagger$ and a_α, which creates and annihilates a particle in the single particle state α.

$$\begin{aligned} a_\alpha^\dagger |0\rangle &= |\alpha\rangle \\ a_\alpha |\alpha\rangle &= |0\rangle \end{aligned} \tag{2.2}$$

The algebra of these operators depends on whether the system under consideration is a system of bosons or a system of fermions. If it consists of bosons the operators obey the commutation relations

$$\begin{aligned} [a_k, a_{k'}^\dagger] &= \delta_{k,k'} \\ [a_k, a_{k'}] &= [a_k^\dagger, a_{k'}^\dagger] = 0. \end{aligned} \tag{2.3}$$

While in the fermion case they obey the anti commutation relations

$$\begin{aligned} \{a_k, a_{k'}^\dagger\} &= \delta_{k,k'} \\ \{a_k, a_{k'}\} &= \{a_k^\dagger, a_{k'}^\dagger\} = 0 \end{aligned} \tag{2.4}$$

With these expressions for the commutations and anti commutations between the creation and annihilation operators the Hamiltonian can be reshaped to the form in Eq. (2.5).

$$H = \sum_{ik} T_{ki} a_k^\dagger a_i + \frac{1}{2} \sum_{ijkl} V_{ijkl} a_i^\dagger a_j^\dagger a_l a_k. \tag{2.5}$$

When the operators in the second quantization are non-relativistic and conserve the particle number, there should be an equal amount of creation and destruction operators in the Hamiltonian. A second quantized one particle operator, an operator that acts on one particle a time is written as in Eq. (2.6)

$$F = \sum_{\alpha,\beta} \langle \alpha | f | \beta \rangle a_\alpha^\dagger a_\beta, \tag{2.6}$$

and a two particle operator is written in the form as in Eq. (2.7)

$$V = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | v | \gamma\delta \rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma. \tag{2.7}$$

2.2 Wicks Theorem

A normal ordered second quantized operator is defined as an operator whose all annihilation operators stands to right of all the creation operators. It is in some manner easier to calculate when the annihilation operators are placed to the right. Wicks theorem describes a fast method to put the annihilation operators to the right of the creation operators, by using the anti commutation rules for these operators. Before introducing Wicks theorem some definitions should be introduced like the normal product of operators and contractions of operators.

Given a product

$$XYZ \cdots W \tag{2.8}$$

of creation and annihilation operators, the normal product is defined as

$$N(XYZ \cdots W), \tag{2.9}$$

where all the destruction operators stand to the right of the creation operators. Thus as an example let us study the cases

$$N(a_\alpha^\dagger a_\beta) = a_\alpha^\dagger a_\beta \tag{2.10}$$

and

$$N(a_\alpha a_\beta^\dagger) = \pm a_\beta^\dagger a_\alpha, \tag{2.11}$$

where the minus sign yields for operators acting only on fermions , and the plus sign yields for operators acting on bosons.

One of the properties of a normalized product of operators is that the ground state expectation value of the product is zero since the destruction operator annihilates the ground state.

A contraction of two operators XY is defined as it's expectation value regarding the ground state.

$$1< 1a_\alpha > 1a_\beta^\dagger = \langle 0|a_\alpha a_\beta^\dagger|0\rangle = \langle 0|\delta_{\alpha\beta} - a_\beta^\dagger a_\alpha|0\rangle = \delta_{\alpha\beta} \tag{2.12}$$

By having defined the normal product and the contraction we are now ready to state Wicks theorem which says that a product of randomly oriented creation and annihilation operators can be written as the normal product of these operators plus the normal product of all possible contractions.

$$XYZ\cdots W = N(XYZ\cdots W) + \sum_{contractions}^{all\ possible} N(XYZ\cdots W) \tag{2.13}$$

As a remark, in this theorem only fermions has been considered.

The proof of this theorem can be found in almost all books that treat quantum field theory or quantum theory of many particles such as [2].

2.3 The Particle-Hole Formalism

In a theory of many particles, there is often more convenient to use another state as reference state rather than the vacuum state. This reference state should be a stable state. The normal ordering will then be altered from the one given above for the true vacuum state. That is our new vacuum state $|\Phi_0\rangle = a_i^\dagger a_j^\dagger \cdots$. A somehow new definition of the creation and destruction operators is needed. The operators will now create and annihilate holes and particles. The definition of a hole is a one particle state that is occupied in the reference state $|\Phi_0\rangle$, while a particle state is one particle state that is not occupied in $|\Phi_0\rangle$. This new nomenclature is easily understood when considering that a "hole" is created when an originally occupied state is acted upon by an annihilation operator such as a_i. A "particle" is created when an unoccupied state is acted upon by a creation operator. These operators that destroy and create holes and particles are called quasiparticle operators. A q-annihilation operator annihilates holes and particles, while a q-creation operator creates holes and particles.

A normal ordered product of quasiparticle operators would then be defined as a product where all the quasiparticle destruction operators stand to the right of all the quasiparticle creation operators. This definition of the normal ordered

product changes the analysis of Wick's theorem a bit. The only contractions that contribute are the ones where a destruction operator stands to the left of a creation operator, there are two ways this can happen

$$
\begin{aligned}
1< 1a_i^\dagger > 1a_j &= a_i^\dagger a_j - N(a_i^\dagger a_j) = a_i^\dagger a_j + a_j a_i^\dagger = \delta_{ij} \\
1< 1a_i > 1a_j^\dagger &= a_i a_j^\dagger - N(a_i a_j^\dagger) = a_i a_j^\dagger + a_j^\dagger a_i = \delta_{ij}
\end{aligned}
\tag{2.14}
$$

That is if i defines a hole state in Eqs. (2.14).

As an example, consider normal ordering of a two particle Hamiltonian, as the one in Eq. (2.15).

$$
\hat{H} = \sum_{pq} \langle p|h|q\rangle a_p^\dagger a_q + \frac{1}{4} \sum_{pqrs} \langle pq|V|rs\rangle a_p^\dagger a_q^\dagger a_s a_r \tag{2.15}
$$

The one particle part can be written as

$$
\sum_{pq} \langle p|h|q\rangle N(a_p^\dagger a_q) + \sum_{i \in hole} \langle i|h|i\rangle \tag{2.16}
$$

While the two particle part would be rewritten as

$$
\begin{aligned}
&\frac{1}{4} \sum_{pqrs} \langle pq|V|rs\rangle a_p^\dagger a_p^\dagger a_s a_r = \\
&\frac{1}{4} \sum_{pqrs} \langle pq|V|rs\rangle N(a_p^\dagger a_q^\dagger a_s a_r) + \sum_{ipq} \langle pi|V|qi\rangle N(a_p^\dagger a_r) + \frac{1}{2} \sum_{ij} \langle ij|V|ij\rangle.
\end{aligned}
\tag{2.17}
$$

After some tedious work, for the entire calculation see [3]. After the equal sign in Eq. (2.17) the letters p, q, r, and s indicate both hole and particle states, while the letters i and j indicate hole states. The entire Hamiltonian is then written as

$$
\begin{aligned}
&\sum_{pq} \langle p|h|q\rangle N(a_p^\dagger a_q) + \sum_{i} \langle i|h|i\rangle + \frac{1}{2} \sum_{ij} \langle ij|V|ij\rangle + \\
&\frac{1}{4} \sum_{pqrs} \langle pq|V|rs\rangle N(a_p^\dagger a_q^\dagger a_s a_r) + \sum_{ipq} \langle pi|V|qi\rangle N(a_p^\dagger a_q)
\end{aligned}
\tag{2.18}
$$

Where p, q, r, and s still run over all states, i and j over hole states only.

Chapter 3

Perturbation Theory

The many body Schrödinger equation is rather difficult to solve. Even a two body problem is a rather complicated system to solve, that is why we have to come up with approximated methods. Usually the Hamiltonian gets separated in an unperturbed part and a perturbed part, The perturbed part is the one which considers the interactions between the particles.

$$H\Psi = (H_0 + V)\Psi = E\Psi. \tag{3.1}$$

H_0 is the unperturbed Hamiltonian, which is a one particle operator, which in most of the problems governing nuclear physics is a harmonic oscillator Hamiltonian. Then $H_0 = E_{kin} + U_{H.O}$ and $V = V - U_{H.O}$. Where E_{kin} is the kinetic energy and $U_{H.O}$ is the harmonic oscillator potential. Obviously the difference $V - U_{H.O}$ should be small enough so that threating V as a perturbation is valid. The exact result is independent of the one particle potential U, but in an approximated calculation it is possible that the results depend on the one particle potential that is included in the calculations. The eigenfunctions, ϕ_i are taken as a basis for the expansion of the eigenfunction Ψ

$$|\Psi\rangle = \sum_{i=1} a_i |\phi_i\rangle \tag{3.2}$$

It is common practice to divide the space in a model space and an excluded space, to simplify the calculations. By doing this we define two projection operators, that we will meet again later. These projection operators are denoted by a P and a Q. The P operator projects the complete wavefunction onto the model space

$$P|\Psi\rangle = |\Psi_M\rangle. \tag{3.3}$$

While Q is the complimentary projector operator and projects the complete wavefunction to the excluded state $|\Psi_Q\rangle$.

$$\begin{aligned} P &= \sum_{i=1}^{d} |\phi_i\rangle\langle\phi_i| \\ Q &= \sum_{i=d+1}^{N} |\phi_i\rangle\langle\phi_i| \end{aligned} \tag{3.4}$$

The projection operators satisfy the properties

$$\begin{aligned} P^2 &= P \\ Q^2 &= Q \\ PQ = QP &= 0 \\ P + Q &= 1 \end{aligned} \tag{3.5}$$

Since e_k are the eigenvalues of the unperturbed Hamiltonian H_0, we obtain that

$$(E - e_j)a_j = \langle \phi_j | V | \Psi \rangle. \tag{3.6}$$

By using this relation we find that the entire wavefunction $|\Psi\rangle$ can be written as

$$|\Psi\rangle = \sum_{i=1}^{d} a_i |\phi_i\rangle + \sum_{i=d+1}^{N} \frac{|\phi_i\rangle\langle\phi_i|V|\Psi\rangle}{E - e_i} = \sum_{i=1}^{d} a_i |\phi_i\rangle + \frac{QV}{E - H_0}|\Psi\rangle = P|\Psi\rangle + \frac{QV}{E - H_0}|\Psi\rangle \tag{3.7}$$

If we now define a wave operator which projects the model space onto the complete wavefunction $\Omega|\Psi_M\rangle = |\Psi\rangle$ we find it to be

$$\Omega(E) = 1 + \frac{Q}{E - H_0} V \Omega(E) \tag{3.8}$$

If we now use the wave operator in Eq (3.6) we get

$$(E - e_j)a_j = \langle \phi_j | V\Omega | \Psi_M \rangle = \sum_{k=1}^{d} \langle \phi_j | V\Omega | \phi_k \rangle a_k \tag{3.9}$$

which is equivalent to

$$[H_0 + V\Omega(E) - E]\Psi_M = 0. \tag{3.10}$$

If we define an effective interaction

$$\mathcal{V}(E) = V\Omega(E) \tag{3.11}$$

we get an integral equation,

$$\mathcal{V}(E) = V + V\frac{Q}{E - H_0}\mathcal{V}(\Omega), \tag{3.12}$$

for the effective interaction, which is dependent on the energy E. Eq. (3.12) can be solved by iteration, where we by using V as a first guess find that

$$\begin{aligned} \mathcal{V}(E) = V + VQ\frac{1}{E - H_0}QV + VQ\frac{1}{E - H_0}QVQ\frac{1}{E - H_0}QV + \\ VQ\frac{1}{E - H_0}QVQ\frac{1}{E - H_0}QVQ\frac{1}{E - H_0}QV + \cdots \end{aligned} \tag{3.13}$$

This can be solved analytically by observing that the sum resembles a geometric sum.

$$\begin{aligned}\mathcal{V} &= V + VQ\frac{1}{E - H_0 - QVQ}QV \\ &\equiv PVP + PVQ\frac{1}{E - QHQ}QVP\end{aligned} \tag{3.14}$$

3.1 Time dependent perturbation theory

When doing time dependent perturbation theory we have to define the time evolution propagator $U(t,t')$, the time evolution operator evolve a state $\Psi(t')$ at time t' to state $\Psi(t)$ at time t.

$$\Psi(t) = U(t,t')\Psi(t') \tag{3.15}$$

The wavefunctions satisfy the time dependent Schrödinger equation,

$$\begin{aligned}i\hbar\frac{\partial}{\partial t}\Psi(t) &= H\Psi(t) \\ i\hbar\frac{\partial}{\partial t}\Psi(t) &= i\hbar\frac{\partial}{\partial t}U(t,t')\Psi(t'),\end{aligned} \tag{3.16}$$

which yields that the time evolution operator satisfy Schrödinger equation. The solution is

$$U(t,t') = e^{-iH(t-t')/\hbar}. \tag{3.17}$$

This form of the time evolution operator gives right away the properties one would expect of an operator of this kind

$$\begin{aligned}&U(t,t) = 1 \\ &U(t',t)U(t,t') = 1 \\ &U(t,t')U(t,t')^\dagger = U(t,t')^\dagger U(t,t') = 1 \\ &\rightarrow U(t',t) = U(t,t')^\dagger = U(t,t')^{-1} \\ &U(t_1,t_2)U(t_2,t_3) = U(t_1,t_3)\end{aligned} \tag{3.18}$$

By use of Thouless theorem [4], exact eigenstates can be constructed through the action of the time-development operator. In the present approach the time t will be rotated by a small angle ϵ, our time is complex.

The eigenstate can the be written as

$$\frac{|\psi_i\rangle}{\langle\phi|\psi_i\rangle} = \lim_{\epsilon\to 0}\lim_{t'\to -\infty(1-i\epsilon)}\frac{U(t,t')|\phi\rangle}{\langle\phi|U(t,t')|\phi\rangle}, \tag{3.19}$$

where $|\psi_i\rangle$ is the lowest state of H with $\langle\phi|\psi_i\rangle \neq 0$. This relationship is very useful in calculating the ground state energy shift ΔE_0.

If our unperturbed Hamiltonian gives the energy E_0 while acting on the unperturbed state $|\phi\rangle$, and our total energy is E the ground state energy shift is given by

$$\begin{aligned}\Delta E_0 = E - E_0 &= \frac{\langle\phi|V|\psi\rangle}{\langle\phi|\psi\rangle} \\ &= \lim_{\epsilon\to 0^+} \lim_{t'\to -\infty(1-i\epsilon)} \frac{\langle\phi|VU(0,t')|\phi\rangle}{\langle\phi|U(0,t')|\phi\rangle}\end{aligned} \tag{3.20}$$

To evaluate this as a perturbation, we have to expand the time evolution operator $U(t,t')$. This is most conveniently if it is done in the interaction picture. Which will be explained slightly here, [5] and [6] give a more thoroughly explanation of the interaction picture. The interaction picture can be understood as an intermediate between the Schrödinger picture and the Heisenberg picture. In the Schrödinger picture the operators are time independent while the state evolves with time. It is all contrary in the Heisenberg picture where the operators now are time dependent and the state is time independent. In the interaction picture both the state vectors and the operators are time dependent, however their time dependencies are somewhat different.

A state vector in the interaction picture is defined as

$$|\psi_I(t)\rangle = e^{iH_{0,S}t/\hbar}|\psi_s(t)\rangle \tag{3.21}$$

where the letter S stands for the schrödinger picture. The operators in the interaction picture is defined as

$$A_I(t) = e^{iH_{0,S}t/\hbar}A_S(t)e^{-iH_{0,S}t/\hbar}. \tag{3.22}$$

H_0 is still the unperturbed Hamiltonian. The time evolution of the operators is given by

$$i\hbar\frac{d}{dt}A_I(t) = [A_I(t), H_0]\,. \tag{3.23}$$

By using the definition of one particle and two particle operators from chapter 2, our Hamiltonian can be written as in Eq. (2.5)

$$H = \sum_k \epsilon_k a_k^\dagger a_k + \frac{1}{2}\sum_{ijkl} V_{ijkl}a_i^\dagger a_j^\dagger a_l a_k. \tag{3.24}$$

To find the time evolution of the Hamiltonian it suffices to find the time evolution of the creation and annihilation operators $a^\dagger$ and a. Using the commutator we find that

$$\left[a_k^\dagger, H_0\right] = -\epsilon a_k^\dagger(t) \tag{3.25}$$

thus we obtain the time dependence of the creation and destruction operators

$$\begin{aligned}a^\dagger(t)_k &= a_k^\dagger e^{i\epsilon_k t/\hbar} \\ a(t)_k &= a_k e^{-i\epsilon_k t/\hbar}\end{aligned} \tag{3.26}$$

I will now transform the schrödinger equation to the interaction picture

$$\begin{aligned}\psi_I(t) &= e^{iH_0t/\hbar}\psi(t) \\ &= e^{iH_0t/\hbar}U(t,t')e^{-iH_0t'/\hbar}e^{iH_0t'/\hbar}\psi(t') \\ &= U_I(t,t')\psi_I(t')\end{aligned} \tag{3.27}$$

By differentiating Eq. (3.27) with respect to time t we find

$$\frac{\partial}{\partial t}U(t,t') = VU(t,t') \tag{3.28}$$

When we have found how the time evolution operator we may also find the perturbartive expansion of the time evolution operator. The solution to the differential equation is

$$U(t,t') = 1 + \left(\frac{-i}{\hbar}\right)\int_{t'}^{t} dt_1 V(t_1)U(t_1,t') \tag{3.29}$$

The number 1 in Eq. (3.29) is for satisfying $U(t',t') = 1$. Eq. (3.29) can be solved by iteration

$$U(t,t') = 1 + \sum_{n=1}^{\infty}\left(\frac{-i}{\hbar}\right)^n \int_{t'}^{t} dt_1 \int_{t'}^{t_1} dt_2 \cdots \int_{t'}^{t_{n-1}} dt_n V(t_1)V(t_2)\cdots V(t_n) \tag{3.30}$$

Now the above form of the time evolution operator can be inserted into Eq. (3.19), which gives us the perturbative expansion for calculating the interactions.

3.2 Feynman-Goldstone diagrams

To evaluate Eq. (3.19) we had to define a new operator, called the time ordering operator. The effect of operating this operator on a product of operators is to order the operators so the operators with a larger time argument are placed to the left to those of smaller time arguments. Since we in nuclear physics are dealing with fermions which obey the Pauli exclusion principle there will be a sign dependency on the number of permutations needed in making the arrangement. As an example

$$\begin{aligned}&T\left[A_1(t_1)A_2(t_2)\cdots A_n(t_n)\right] \\ &= (-1)^p A_\alpha(t_\alpha)A_\beta(t_\beta)\cdots A_\gamma(t_\gamma)\end{aligned} \tag{3.31}$$

If we use time ordering together with the particle hole formalism from section 2.3, we will find a new definition of the contraction. A contraction of two operators will now be defined as

$$1< 1A > 1B = T[AB] - N[AB], \tag{3.32}$$

Where $N[AB]$ is the normal ordering operator. As an example I will derive a contraction of two hole operators and a contraction of two particle operators. I will first start with a contraction of two hole operators where both particles have momenta below k_F, and with $t < t'$.

$$
\begin{aligned}
&1\!<1a_h(t)>1a^\dagger_{h'}(t') = T\left[a_h(t)a^\dagger_{h'}(t')\right] - N\left[a_h(t)a^\dagger_{h'}(t')\right] \\
&= -a^\dagger_{h'}(t')a_h(t) - a_h(t)a^\dagger_{h'}(t') \\
&= -\left(a^\dagger_{h'}(t')a_h(t) + a_h(t)a^\dagger_{h'}(t')\right)e^{-\frac{i}{\hbar}(\epsilon_h t - \epsilon_{h'}t')} \\
&= -\delta_{h,h'}e^{-\frac{i}{\hbar}(\epsilon_h t - \epsilon_{h'}t')}.
\end{aligned}
\tag{3.33}
$$

Similarly for particles with momenta above k_F and $t < t'$

$$
1\!<*a_p(t)>*a_{p'}(t') = \delta_{p,p'}e^{-\frac{i}{\hbar}\epsilon_p(t-t')} \tag{3.34}
$$

We have

$$
1\!<*a_\alpha(t)>*a^\dagger_\beta(t') = -1\!<*a^\dagger_\beta(t')>*a_\alpha(t) \tag{3.35}
$$

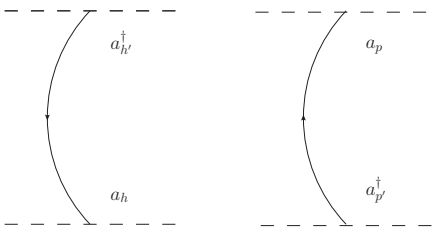

Figure 3.1: Diagrammatic representation of the contractions in Eqs. (3.33) and (3.34) The time is going upward.

In Fig (3.1) the two contractions in Eqs (3.33) and (3.34) are represented diagrammatically, the annihilation operator a_α destroys the particle line $a^\dagger_\beta$ creates. The time is upward.

With the above definitions of time ordering and contractions we are ready to go back to the time evolution operator, it is already in a time ordered form.

$$
U(t,t') = \sum_{n=0}^{\infty}\left(\frac{-i}{\hbar}\right)^n \int_{t'}^{t} dt_1 \int_{t'}^{t_1} dt_2 \cdots \int_{t'}^{t_{n-1}} dt_n T\left[V(t_1)V(t_2)\cdots V(t_n)\right] \tag{3.36}
$$

From Eq. (3.36) we see that the integral with respect to the time $t_1, t_2 \cdots t_n$ and that there are $n!$ ways to order them, we can again rewrite the time evolution operator in the form

$$
U(t,t') = \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{-i}{\hbar}\right)^n \int_{t'}^{t} dt_1 \int_{t'}^{t} dt_2 \cdots \int_{t'}^{t} dt_n T\left[V(t_1)V(t_2)\cdots V(t_n)\right] \tag{3.37}
$$

If we recall that it is the energy shift we want to calculate, we can rewrite Eq. (3.20)

$$\Delta E_0 = \lim_{\epsilon\to 0^+} \lim_{t'\to -\infty(1-i\epsilon)} \frac{\langle\phi|VU(0,t')|\phi\rangle}{\langle\phi|U(0,t')|\phi\rangle}$$
$$= \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{-i}{\hbar}\right)^n \int_{t'}^{t} dt_1 \int_{t'}^{t} dt_2 \cdots \int_{t'}^{t} dt_n \langle\phi|T\left[V(t)V(t_1)V(t_2)\cdots V(t_n)\right]|\phi\rangle$$
$$\times \frac{1}{\sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{-i}{\hbar}\right)^n \int_{t'}^{t} dt_1 \int_{t'}^{t} dt_2 \cdots \int_{t'}^{t} dt_n \langle\phi|T\left[V(t_1)V(t_2)\cdots V(t_n)\right]|\phi\rangle}. \tag{3.38}$$

Where $V(t)$ in the numerator in Eq. (3.38) is put into to the time ordering operator. To evaluate the integrals in the numerator and the denominator we have to use wicks theorem, wicks theorem with time ordering will be slightly modified from the first version in section 2.2. Wicks theorem states now that

$$T\left[A(t_1)B(t_2)C(t_3)\cdots Z(t_n)\right] = N\left[A(t_1)B(t_2)C(T_3)\cdots Z(t_n)\right]$$
$$+ \sum_{1\,contraction} N\left[A(t_1)B(t_2)C(T_3)\cdots Z(t_n)\right] + \sum_{2\,contractions} N\left[A(t_1)B(t_2)C(T_3)\cdots Z(t_n)\right]$$
$$+ \cdots + \sum_{\substack{contractions\,with\\ all\,operators}} N\left[A(t_1)B(t_2)C(T_3)\cdots Z(t_n)\right] \tag{3.39}$$

Since our unperturbed state is the groundstate, which is our reference vacuum state, only the last term in Eq. (3.39) survive. We are left with the term where all operators are participating in the contractions.

Let us now evaluate the first order contribution to the energy shift in Eq. (3.38). The only contributing term is $V(t)$ which in a second quantized form is $V_{\alpha\beta\gamma\delta}a^\dagger_\alpha(t)a^\dagger_\beta(t)a_\delta(t)a_\gamma(t)$. From wicks theorem we will then have two terms contributing to the energy shift.

$$21{<}*a^\dagger_\alpha(t) < 2a^\dagger_\beta(t) > 2a_\delta(t) > *a_\gamma(t) + 21{<}*a^\dagger_\alpha(t) < 2a^\dagger_\beta(t) > *a_\delta(t) > 2a_\gamma(t) \tag{3.40}$$

The terms in Eq. (3.40) can be depicted diagrammatically as seen in Fig (3.2).

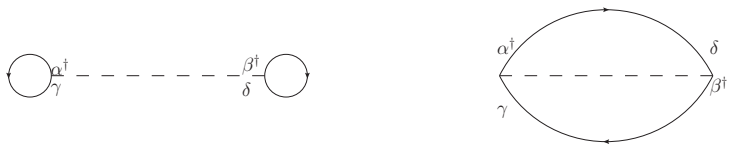

Figure 3.2: Diagrammatic representation of the first order diagram, the diagram to the left depicts the first term in Eq. (3.40), the diagram to the right depicts the second term in Eq. (3.40).

α, β, γ and δ must all be holes, since they are all equal time operators and hence the only contractions which contribute. The energy shift can now be written as

$$\Delta E_0 = \frac{1}{2} \sum_{\alpha\beta<k_f} \frac{1}{2}(V_{\alpha\beta\alpha\beta} - V_{\alpha\beta\beta\alpha}) \tag{3.41}$$

The minus sign comes in, by the "rule" that for every contraction that cross another contributes with a factor (-1).

With the clever invention of the diagrams that depicts the contractions, we are able to describe every term in the expansion of the time evolution operator as diagrams. These diagrams are usually called Feynman diagrams or Feynman-Goldstone diagrams, to honor the inventor. When presenting all the terms as diagrams we need some rules to keep track of them. The idea is that we find a term in the expansion by studying the corresponding diagram. A nice derivation of the diagram rules can be found in [7]. The rules are described in appendix A.

Chapter 4

The nucleon-nucleon potential

Since Chadwick discovered the neutron in 1932, understanding the nucleon-nucleon interaction has been a main focus for nuclear physicists. Yukawa [8] proposed the first significant theory of the nuclear force, where a meson is exchanged in the nucleon-nucleon interaction. This meson were later to be identified with the pion. The one pion exchange model turned out to be very useful in explaining nucleon-nucleon scattering data and the properties of the deuteron [9]. Problems arose when multipion exchange were included, and the "pion theories" of the 1950's are generally judged to be failures [9]. The reasons for the failure of the theories in the 50's is because of the then unknown pion dynamics understood by QCD and chiral symmetries, which were not to be used by the nuclear physicists until the 80's. The problem of the nuclear force seemed to have been solved by using QCD, however there are still remaining problems such as the nonperturabtive character in the low energy regime, where nuclear physicists are working in.

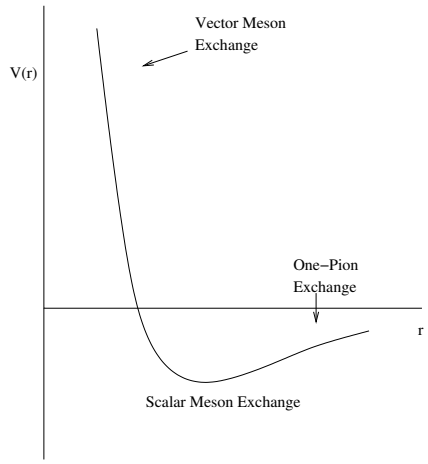

Figure 4.1: The behavior of the nucleon-nucleon interaction

4.1 Chiral Perturbation Theory

The discovery of QCD and the understanding of effective field theory was a breakthrough for understanding the nucleon-nucleon potential.
QCD is the theory of the strong interaction, where the quarks and gluons are treated as the degrees of freedom. The principles behind the theory are really simple and elegant, the interactions are derived by demanding that the Lagrangian is gauge invariant under SU(3). QCD is a non-Abelian field theory which is a consequence of the discovery of the three quantum numbers of color. The underlying gauge group is the SU(3) group. QCD is also known for "asymptotic freedom", the force is weak at short distances but strong, at long distances or at low energies. The consequences of the asymptotic freedom is that the quarks are confined into "colorless" objects, called hadrons, and that perturbation theory in the low energy regime is strictly forbidden. As noted earlier nuclear physics is in this limit, and diffiulties arise when treating quarks and gluons in the nuclear force. The solution is to identify the relevant degrees of freedom, which in the nuclear case are the nucleons, we treat the nucleons as "elementary" particles and not a composite of quarks. When identifying the nucleons as the degrees of freedom we have to take in consideration the properties of the quarks, they will be considered, but hidden in the coupling constants.

When constructing an effective field theory from QCD, all the symmetries of the Lagrangian should be manifest in the effective Lagrangian. In the case of QCD, the Lagrangian is invariant under SU(3) transformation.
In the limit where the quark masses are zero, the chiral limit, the Lagrangian may be separated into a Lagrangian of left and right handed fields. The Lagrangian is invariant under left and right handed SU(3) transformations in the chiral limit.

We know that the quarks are not massless, but it is not a bad approximation in the nuclear scale since $m_{u,d,s} \ll m_N$, where u, d, s denotes the up, down and the strange quark, while m_N stands for the nucleon mass. The remarkable theorem by Emma Noether states that for each symmetry of the Lagrangian there exists a conserved current. In the case of chiral invariance the conserved currents are the left handed and the right handed ones. However these two currents can combine to a vector current $J_V^{\mu,b}$ and an axial current $J_A^{\mu,b}$. Where

$$\begin{aligned} J_V^{\mu,b} &= R^{\mu,b} + L^{\mu,b} = \overline{q}\gamma^\mu \frac{\lambda^b}{2} q \\ J_A^{\mu,b} &= R^{\mu,b} - L^{\mu,b} = \overline{q}\gamma^\mu \gamma_5 \frac{\lambda^b}{2} q \end{aligned} \tag{4.1}$$

For each current there is a corresponding charge, Q, which is a generator of $SU(3)_V \times SU(3)_A$, that is conserved.

The conserved charges will in this case be

$$\begin{aligned} Q_V^b &= \int d^3x J^{0,b} \\ Q_A^b &= \int d^3x J_A^{0,b} \end{aligned} \tag{4.2}$$

When a mass term for the quarks are included in the Lagrangian, the symmetry will break down, let us look at the QCD Lagrangian

$$\mathcal{L}_{QCD} = \overline{q}(i\gamma^{\mu}D_{\mu} - M)q - \frac{1}{4}G^{a}_{\mu\nu}G^{\mu\nu,a}. \tag{4.3}$$

By introducing explicitly the symmetry breaking mass term the currents will generally not be conserved, their divergences will satisfy

$$\begin{aligned} \partial_{\mu}J^{\mu,a}_{V} &= i\overline{q}[M, \frac{\lambda^{a}}{2}]q \\ \partial_{\mu}J^{\mu,a}_{A} &= i\overline{q}\{\frac{\lambda^{a}}{2}, M\}\gamma_{5}q. \end{aligned} \tag{4.4}$$

For equal quark masses, the vector currents are conserved since all matrices commute with a multiple of the identity matrix. The axial currents are not conserved. The symmetry breaks down to $SU(3)_V$, in the case where the quarks have equal mass.

If the symmetry is spontaneously broken, the ground state is not invariant under a certain symmetry, the theory will be enriched by new particles, called goldstone bosons. These particles will be massless and have the same quantum numbers as the generators that break the symmetry [10].
There are reasons to believe that the ground state is not annihilated by the generators of the axial symmetry. If there were an exact axial symmetry we would expect the existence of a degenerate hadron multiplet of opposite parity [11]. For each hadron there should exist a hadron of opposite parity. These multiplets are not observed. There exist a multiplet of particles in different isospin charges, the ρ meson comes in three charge states, $\rho^{\pm}$ and ρ^{0} which is equivalent to three isospin states. The $SU(3)_V$ is still a valid symmetry, but the $SU(3)_A$ is broken. As said earlier for each broken symmetry we will expect a massless goldstone boson. It is here the problem comes in, the standard model doesn't account for any extra massless particles. This dilemma is solved by using the fact that the quarks are not massless, this implies that the goldstone bosons acquire a small effective mass. The goldstone bosons are then identified as the pions, kaons and the η particle, which have the same quantum numbers as the broken generators. These goldstone bosons are then interpreted as the mediators in the nuclear interactions.

4.2 V_{low-k}

During the search for convergence of the two particle interaction diagrams in the laboratory system, I used V_{low-k} to renormalize the nucleon-nucleon interaction. The method separates the Hilbert space in a low momentum part and a high momentum part [12]. This is done by introducing a momentum cutoff in the momentum space, where all states with momenta higher than the cutoff belongs to the high momentum space.

As explained above, the nuclear potential is non perturbative in the nuclear limit, at high energies, or short distances the nucleon-nucleon interaction becomes highly repulsive. By renormalizing the potential the repulsive and the

non perturbative part of it "get swept under the carpet" as Zee in ref. [13] says it.There are many ways to renormalize the potential , or to get "rid off" the high momentum part, all of them, must have one thing in common. The renormalized potential should give an accurate description of the low energy nucleon-nucleon scattering data.

The cut off in V_{low-k} is done on the momentum. The cut off is based on two steps [14]. Diagonalization of the momentum space for the relative momentum. The transformation of $k \in [0, \infty)$ to $k \in [0, \Lambda]$. A typical value of Λ is approximately $2fm^{-1}$, the renormalized potential, V_{low-k}, is dependent on the cutoff.

For deriving the effective potential we first have to consider the full many body system described by Schrödinger's equation

$$H|\Psi\rangle = E|\Psi\rangle. \tag{4.5}$$

The Hamiltonian is separated in an unperturbed part and a perturbed part

$$H = H_0 + H_I. \tag{4.6}$$

Where H_I denotes the perturbed Hamiltonian and describes the interaction part. The first part of constructing an effective Hamiltonian, is to define two projector operators that projects onto the low energy state. Usually the projector operator that projects onto the low energy state is symbolized with P and the complement is denoted by Q. The projection operators satisfy the properties

$$\begin{aligned} &P^2 = P \\ &Q^2 = Q \\ &P + Q = 1 \\ &PQ = QP = 0 \\ &[H_0, P] = [H_0, Q] = 0 \\ &QH_0P = PH_0Q = 0. \end{aligned} \tag{4.7}$$

By using the projection operators the Hamiltonian may be written as

$$H = (P+Q)H(P+Q) = PHP + PHQ + QHP + QHQ \tag{4.8}$$

The Schrödinger equation can then be written in a matrix form

$$\begin{pmatrix} PHP & PHQ \\ QHP & QHQ \end{pmatrix} \begin{pmatrix} P|\Psi\rangle \\ Q|\Psi\rangle \end{pmatrix} = E \begin{pmatrix} P|\Psi\rangle \\ Q|\Psi\rangle \end{pmatrix}. \tag{4.9}$$

There exists two main methods for solving the effective Hamiltonian, the first is the Bloch-Horowitz [15],[16] where the effective Hamiltonian turns out to be dependent on the exact energy eigenvalue one is solving for, and the Lee-Suzuki method [17],[18]. The two methods are thoroughly compared in [19]. Both of the methods want the effective Hamiltonian to be of the form

$$H_{eff} = PHP \tag{4.10}$$

The solution of the Bloch-Horowitz effective Hamiltonian is

$$\mathcal{H}_{eff}^{BH} = P(H + H\frac{1}{E - QHQ}H)P \tag{4.11}$$

The corresponding eigenvalue problem

$$P(H + H\frac{1}{E - QHQ}H)PP|\Psi\rangle = EP|\Psi\rangle \tag{4.12}$$

has to be solved by a self consistent treatment.

The Lee-Suzuki method avoids the difficulties with the energy eigenvalue in the effective Hamiltonian by constructing a similarity transformation of the Hamiltonian in Eq. (4.9) to the structure

$$H^{LS} = \begin{pmatrix} P\mathcal{H}P & P\mathcal{H}Q \\ 0 & Q\mathcal{H}Q \end{pmatrix} = X^{-1}HX \tag{4.13}$$

The condition for $P\mathcal{H}P$ to be the P space effective Hamiltonian is that

$$QX^{-1}HXP = 0 \tag{4.14}$$

The choice of X is crucial, different choice of X leads to different many body theory, Lee and Suzuki [17] made the ansatz of

$$\begin{aligned} X &= e^{\omega} \\ \mathcal{H} &= e^{-\omega}He^{\omega}. \end{aligned} \tag{4.15}$$

Where ω is the so called wave operator it connects the P and Q space in the sense that it transform the state $P|\Psi\rangle$ to the state $Q|\Psi\rangle$. With the wave operator on the form $\omega = Q\omega P$ the condition (4.14) is satisfied. This will also constrain the matrix X by the following properties of the wave operator

$$\begin{aligned} P\omega P &= PQ\omega PP = 0 \\ Q\omega Q &= QQ\omega PQ = 0 \\ P\omega Q &= PQ\omega QQ = 0 \\ \omega^2 &= Q\omega PQ\omega P = 0 \end{aligned} \tag{4.16}$$

The expansion of X will then consist of just two terms

$$X = e^{\omega} = 1 + \omega = 1 + Q\omega P \tag{4.17}$$

The four parts of of the Hamiltonian matrix in (4.9) will then be expressed as

$$\begin{aligned} P\mathcal{H}P &= PHP + PH_IQ\omega P \\ P\mathcal{H}Q &= PH_IQ \\ Q\mathcal{H}Q &= QHQ - \omega PH_IQ \\ Q\mathcal{H}P &= QH_IP + QHQ\omega - \omega PHP - \omega PH_IQ\omega \end{aligned} \tag{4.18}$$

With Eq. (4.16) and Eq. (4.18) we get an equation for the waveoperator.

$$QH_IP + QHQ\omega - \omega PHP - \omega PH_IQ\omega = 0 \tag{4.19}$$

If we have a solution for ω it is then just to replace it for ω in our effective Hamiltonian

$$H_{eff} = PHP + PH_IQ\omega P \tag{4.20}$$

By defining the P space effective interaction operator

$$V_{eff} = H_{eff} - PH_0P = PH_IP + PH_IQ\omega. \tag{4.21}$$

The P space eigenvalue problem can be written as

$$H_{eff}|\psi_\mu\rangle = (PH_0P + V_{eff})|\psi_\mu\rangle = E_\mu|\psi_\mu\rangle \tag{4.22}$$

The wave operator can be solved in terms of the eigenvalue and eigenstates E_μ and $|\psi_\mu\rangle$.

$$\omega(E_\mu) = \sum_{\mu=1}^{d} \frac{1}{E_\mu - QHQ} QH_IP|\psi_\mu\rangle\langle\tilde{\psi}_\mu|. \tag{4.23}$$

$\langle\tilde{\psi}_\mu|$ is the bi orthogonal state corresponding to $|\psi_\mu\rangle$. There are various methods to solve the non-linear equation for the wave operator. For the two body problem the exact solutions for the eigenstates can be used, and the effective interaction can be calculated directly by using Eq. (4.23). For more complex applications the equation has to be solved iteratively.

Chapter 5

Coupled Cluster Theory

The coupled cluster theory was developed by Fritz Coester and Hermann Kümmel. It is a numerical technique used to describe many body systems. The method starts with a ground state Slater determinant, as the Slater determinant below, Eq. 5.1, corresponding to a system consisting of four particles.

$$\frac{1}{4!}\begin{vmatrix} \phi_i(x_1) & \phi_j(x_1) & \phi_k(x_1) & \phi_l(x_1) \\ \phi_i(x_2) & \phi_j(x_2) & \phi_k(x_2) & \phi_l(x_2) \\ \phi_i(x_3) & \phi_j(x_3) & \phi_k(x_3) & \phi_l(x_3) \\ \phi_i(x_4) & \phi_j(x_4) & \phi_k(x_4) & \phi_l(x_4) \end{vmatrix} \tag{5.1}$$

A convenient shorthand notation for the Slater determinant consists of a Dirac-notation ket containing only the diagonal elements of the Slater determinant [3]. The ket vector corresponding to Eq. 5.1 would be

$$|\phi_i(x_1)\phi_j(x_2)\phi_k(x_3)\phi_l(x_4)\rangle. \tag{5.2}$$

When there are more orbitals available than particles occupying them, the ground state Slater determinant fails to account for the total state. The wavefunction would then be a linear combination of various Slater determinants where the other Slater determinants are excitations of the ground state.

The ansatz is that the total wavefunction can be written as

$$\psi = e^T \phi_0 \tag{5.3}$$

where T, called the cluster operator, consists of cluster coefficients, which are to be determined via the Schrödinger equation [3]. The cluster operator is written in the form

$$T = T_1 + T_2 + T_3 + \cdots \tag{5.4}$$

T_1 is a operator of all single excitations, and T_2 the operator of all double excitations, and so on. By the formalism of the second quantization the excitation operators are expressed as

$$T_1 = \sum_{ia} t_i^a a_a^\dagger a_i \tag{5.5}$$

$$T_2 = \frac{1}{4} \sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i \tag{5.6}$$

More generally an $n-$orbital cluster operator may be defined as

$$T_n = \left(\frac{1}{n!}\right)^2 \sum_{ij\ldots ab\ldots} t_{ij\ldots}^{ab\ldots} a_a^\dagger a_b^\dagger \ldots a_j a_i \tag{5.7}$$

.

The energy expectation value is then computed by the relation

$$E = \langle \phi_0 | e^{-T} H e^T | \phi_0 \rangle \tag{5.8}$$

By using the Campbell-Baker-Hausdorff formula on $e^{-T}He^T$ Eq. (5.8) transforms to

$$E = \langle \phi_0 | H + [H, T_1] + [H, T_2] + \frac{1}{2}[[H, T_1], T_1] + \frac{1}{2}[[H, T_2], T_2] + [[H, T_1], T_2] + \cdots | \phi_0 \rangle. \tag{5.9}$$

This expansion may appear more complicated than in Eq. (5.8). However there is an advantage with this new expansion, it terminates exactly at four nested commutators when the Hamiltonian consists at most of a two-body term and at six nested commutators when three-body potentials are present.

The amplitudes t_i^a etc, can be found by the equations

$$\begin{aligned} \langle \phi_i^a | e^{-T} H e^T | \phi_0 \rangle &= 0 \\ \langle \phi_{ij}^{ab} | e^{-T} H e^T | \phi_0 \rangle &= 0 \end{aligned} \tag{5.10}$$

In this work the cluster operator is truncated at T_2, the equations in Eq. (5.10) are then the only equations needed to determine the cluster amplitudes t_i^a and t_{ij}^{ab}.

5.1 The CCSD energy equation

The energy problem simplifies a lot when the normalized Hamiltonian, according to the quasiparticle formalism, is used. When our Hamiltonian is at most a two particle operator, the exact expression will be truncated at

$$\begin{aligned} e^{-T} H_N e^T = H_N + [H_N, T_1] + [H_N, T_2] + \\ \frac{1}{2}[[H_N, T_1], T_1] + \frac{1}{2}[[H_N, T_2], T_2] + [[H_N, T_1], T_2] \end{aligned} \tag{5.11}$$

Where

$$H_N = \sum_{\alpha\beta} f_{\alpha\beta} N(a^\dagger_\alpha a_\beta) + \frac{1}{4}\sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta} N(a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma). \tag{5.12}$$

By taking the expectation value of the expanded Hamiltonian, Eq. (5.11), we see that the first term doesn't contribute.
I will now go thoroughly through the anti commutators. I start with the anti commutator of H_1 and T_1.

$$\{H_N, T_1\} = H_N T_1 + T_1 H_N \tag{5.13}$$

Let us first calculate $\langle\Phi_0|H_N T_1|\Phi_0\rangle$,

$$\sum_{\substack{\alpha\beta\gamma\delta,\\ i\in holes,\\ a\in particles}} f_{\alpha\beta} t^a_i \langle\Phi_0|21< 1a^\dagger_\alpha < 2a_\beta > 2a^\dagger_a > 1a_i|\Phi_0\rangle + V_{\alpha\beta\gamma\delta} t^a_i \sum_{all\ contractions} \langle\Phi_0|a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma a^\dagger_a a_i|\Phi_0\rangle$$
$$= \sum_{\substack{a\in particles,\\ i\in holes}} f_{ia} t^a_i.$$
(5.14)

The term $\langle\Phi_0|T_1 H_N|\Phi_0\rangle$ is zero.

All the terms with a cluster operator to the left of the normalized Hamiltonian become zero when taking the expectation value. By using these relations, we can write down the energy equation to a somewhat less tedious form.

$$E = \langle\Phi_0|H_N + H_N T_1 + H_N T_2 + \frac{1}{2} H_N T_1^2 + \ldots|\Phi_0\rangle \tag{5.15}$$

The other terms to calculate are

$$\begin{aligned} &H_N T_2 \\ &\frac{1}{2} H_N T_1^2 \end{aligned} \tag{5.16}$$

Since the other terms in Eq. (5.15) will be zero, for calculations of the non contributing terms, I will again refer to [3].

For the terms in Eq. (5.16) it's only the two particle operator of the Hamiltonian that contributes.

The first term to be considered is $H_N T_2$

$$\langle\Phi_0|H_N T_2|\Phi_0\rangle = \frac{1}{16}\Big(\sum_{\substack{\alpha\beta\gamma\delta,\\ ab\in particles\\ ij\in holes}} V_{\alpha\beta\gamma\delta} t^{ab}_{ij} \langle\Phi_0|4321< 1a^\dagger_\alpha < 2a^\dagger_\beta < 3a_\delta < 4a_\gamma > 4a^\dagger_a > 3a^\dagger_b > 2a_j > 1a_i|\Phi_0\rangle$$
$$+ V_{\alpha\beta\gamma\delta} t^{ab}_{ij} \langle\Phi_0|4321< 1a^\dagger_\alpha < 2a^\dagger_\beta < 3a_\delta < 4a_\gamma > 4a^\dagger_a > 3a^\dagger_b > 1a_j > 2a_i|\Phi_0\rangle + V_{\alpha\beta\gamma\delta} t^{ab}_{ij} \langle\Phi_0|4321< 1a^\dagger_\alpha < 2a^\dagger_\beta$$
$$+ V_{\alpha\beta\gamma\delta} t^{ab}_{ij} \langle\Phi_0|4321< 1a^\dagger_\alpha < 2a^\dagger_\beta < 4a_\delta < 3a_\gamma > 4a^\dagger_a > 3a^\dagger_b > 1a_j > 2a_i|\Phi_0\rangle\Big)$$
$$= \frac{1}{4} \sum_{\substack{ab\in particles\\ ij\in holes}} V_{ijab} t^{ab}_{ij}$$
(5.17)

The last expectation value is calculated by the same method,

$$\frac{1}{2}\langle\Phi_0|H_N T_1^2|\Phi_0\rangle = \frac{1}{2}\sum_{\substack{a,b\in particles,\\ i,j\in holes}} V_{ijab}t_i^a t_j^b. \tag{5.18}$$

We sum the terms contributing to the energy, in the coupled cluster single and doubly excited approximation, CCSD;

$$E_{CC} = E_{CCSD} - E_0 = \sum_{i,a} f_{ia}t_i^a + \frac{1}{4}\sum_{\substack{i,j\\a,b}} V_{ijab}t_{ij}^{ab} + \frac{1}{2}\sum_{\substack{i,j,\\a,b}} V_{ijab}t_i^a t_j^b. \tag{5.19}$$

Where i, j act only in the hole space and a, b act in the particle space.
This energy relation is valid even if the cluster operator is not truncated at T_2, when the Hamiltonian is a twobody operator. The cluster operators such as T_3 would contribute indirectly through the amplitude equations.

5.2 The CCSD amplitude equations

The amplitude equations in Eq. (5.10), has to be solved to compute the energy. The single excitation amplitudes t_i^a is computed from Eq.(5.20).

$$\langle\Phi_i^a|e^{-T}He^T|\Phi_0\rangle. \tag{5.20}$$

The double excitation amplitude, t_{ij}^{ab}, is determined from Eq.(5.21).

$$\langle\Phi_{ij}^{ab}|e^{-T}He^T|\Phi_0\rangle. \tag{5.21}$$

Computing these ones is much more tedious, and will require much more terms than the energy problem since they are not an expectation value of the reference vacuum, but they combine an excited state and the vacuum state. There are more creation and destruction operators to handle. The singly excited state is written as

$$\langle\Phi_i^a| = \langle\Phi_0|a_i^\dagger a_a \tag{5.22}$$

The leading term in the equation for the singly excited state is just H. Only the one particle part of the Hamiltonian contributes to the first leading term of the singly excited amplitude, $\langle\Phi_i^a|e^{-T}He^T|\Phi_0\rangle$.

$$\langle\Phi_i^a| = \langle\Phi_0|a_i^\dagger a_a e^{-T}He^T|\Phi_0\rangle = f_{ai} \tag{5.23}$$

The first leading term in $\langle\Phi_{ij}^{ab}|e^{-T}He^T|\Phi_0\rangle$ is

$$\langle\Phi_0|a_i^\dagger a_j^\dagger a_b a_a e^{-T}He^T|\Phi_0\rangle = V_{abij}. \tag{5.24}$$

The tedious work arises when trying to calculate parts including the cluster operators. Doing the entire calculations would be to boring to follow for the reader, since they are already calculated in other papers, it will be skipped. However the interested reader may take a look at [3].

The resulting equation for the T_1 amplitude is

$$0 = f_{ai} + \sum_c f_{ac} t_i^c - \sum_k f_{ki} t_k^a + \sum_{kc} \langle ka|V|ci\rangle t_k^c + \sum_{kc} f_{kc} t_{ik}^{ac} + \frac{1}{2} \sum \langle ka|V|cd\rangle t_{ki}^{cd} -$$
$$\frac{1}{2} \sum_{klc} \langle kl|V|ci\rangle t_{kl}^{ca} - \sum_{kc} f_{kc} t_i^c t_k^a - \sum_{klc} \langle kl|V|ci\rangle t_k^c t_l^a + \sum_{kcd} \langle ka|V|cd\rangle t_k^c t_i^d -$$
$$\sum_{klcd} \langle kl|V|cd\rangle t_k^c t_i^d t_l^a + \sum_{klcd} \langle kl|V|cd\rangle t_k^c t_{li}^{da} - \frac{1}{2} \sum_{klcd} \langle kl|V|cd\rangle t_{ki}^{cd} t_l^a - \frac{1}{2} \sum_{klcd} \langle kl|V|cd\rangle t_{kl}^{ca} t_i^d \tag{5.25}$$

While the amplitude equation for T_2 is

$$0 = \langle ab|V|ij\rangle + \sum_c (f_{bc} t_{ij}^{ac} - f_{ac} t_{ij}^{bc}) - \sum_k (f_{kj} t_{ik}^{ab} - f_{ki} t_{jk}^{ab}) +$$
$$\frac{1}{2} \sum_{kl} \langle kl|V|ij\rangle t_{kl}^{ab} + \frac{1}{2} \sum_{cd} \langle ab|V|cd\rangle t_{ij}^{cd} + P(ij)P(ab) \sum_{kc} \langle kb|V|cj\rangle t_{ik}^{ac} +$$
$$P(ij) \sum_c \langle ab|V|cj\rangle t_i^c - P(ab) \sum_k \langle kb|V|ij\rangle t_k^a +$$
$$\frac{1}{2} P(ij)P(ab) \sum_{klcd} \langle kl|V|cd\rangle t_{ik}^{ac} t_{lj}^{db} + \frac{1}{4} \sum_{klcd} \langle kl|V|cd\rangle t_{ij}^{cd} t_{kl}^{ab} -$$
$$P(ab) \frac{1}{2} \sum_{kl} \langle kl|V|cd\rangle t_{ij}^{ac} t_{kl}^{bd} - P(ij) \frac{1}{2} \sum_{klcd} \langle kl|V|cd\rangle t_{ik}^{ab} t_{jl}^{cd} +$$
$$P(ab) \frac{1}{2} \sum_{kl} \langle kl|V|ij\rangle t_k^a t_l^b + P(ij) \frac{1}{2} \sum_{cd} \langle ab|V|cd\rangle t_i^c t_j^d - P(ij)P(ab) \sum_{kc} \langle kb|V|ic\rangle t_k^a t_j^c +$$
$$P(ab) \sum_{kc} f_{kc} t_k^a t_{ij}^{bc} + P(ij) \sum_{kc} f_{kc} t_i^c t_{jk}^{ab} -$$
$$P(ij) \sum_{klc} \langle kl|V|ci\rangle t_k^c t_{lj}^{ab} + P(ab) \sum_{kcd} \langle ka|V|cd\rangle t_k^c t_{ij}^{db} +$$
$$P(ij)P(ab) \sum_{kcd} \langle ak|V|dc\rangle t_i^d t_{jk}^{bc} + P(ij)P(ab) \sum_{klc} \langle kl|V|ic\rangle t_l^a t_{jk}^{bc} +$$
$$P(ij) \frac{1}{2} \sum_{klc} \langle kl|V|cj\rangle t_i^c t_{kl}^{ab} - P(ab) \frac{1}{2} \sum_{kcd} \langle kb|V|cd\rangle t_k^a t_{ij}^{cd} -$$
$$P(ij)P(ab) \frac{1}{2} \sum_{kcd} \langle kb|V|cd\rangle t_i^c t_k^a t_j^d + P(ij)P(ab) \frac{1}{2} \sum_{klc} \langle kl|V|cj\rangle t_i^c t_k^a t_l^b -$$
$$P(ij) \sum_{klcd} \langle kl|V|cd\rangle t_k^c t_i^d t_{lj}^{ab} - P(ab) \sum_{klcd} \langle kl|V|cd\rangle t_k^c t_l^a t_{ij}^{db} +$$
$$P(ij) \frac{1}{4} \sum_{klcd} \langle kl|V|cd\rangle t_i^c t_j^d t_{kl}^{ab} + P(ab) \frac{1}{4} \sum_{klcd} \langle kl|V|cd\rangle t_k^a t_l^b t_{ij}^{cd} +$$
$$P(ij)P(ab) \sum_{klcd} \langle kl|V|cd\rangle t_i^c t_l^b t_{kj}^{ad} + P(ij)P(ab) \frac{1}{4} \sum_{klcd} \langle kl|V|cd\rangle t_i^c t_k^a t_j^d t_l^b . \tag{5.26}$$

The notation $P(ab)$ indicates a permutation operator whose action on a

function, f, is defined as

$$P(pq)f(p,q) = f(p,q) - f(q,p) \tag{5.27}$$

5.3 Coupled cluster diagrams

As a relief there exists easier ways to construct the coupled cluster energy and amplitude equations, that is with a diagrammatic approach. The equations can be represented by some sort of Feynman diagrams, the rules are not quite the same as in ordinary many body physics, somehow distorted because of the cluster operators. New rules are needed, and they are as follow

1. As in ordinary many body perturbation, holes are represented by downward pointing lines and particles by upward pointing lines.

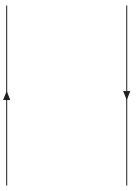

Figure 5.1: Diagrammatic representation of holes and particles, holes with an downward pointing arrow and particles with and upward pointing arrow.

2. The reference wavefunction, Φ_0, is represented by empty space.
3. Dynamical operators such as the one particle and two particle part of the Hamiltonian are depicted by horizontal dashed lines.
4. The cluster operators are depicted by solid horizontal lines.
5. The one particle component of the Hamiltonian is represented by a dashed interaction line capped by an X.
6. Representation of the cluster operators is seen in Fig (5.2). In the diagram representing the T_1 amplitude there is one incoming hole line and one outgoing particle line meeting at a solid horizontal line.

   The diagram representing T_2 consists of two incoming hole lines and two outgoing particle lines.
7. For each hole line, multiply with a factor of -1.
8. For each loop, multiply with a factor of -1
9. If there are n equivalent vertices's in the diagram, multiply with the factor $\frac{1}{n!}$.
10. For each pair of unique external hole or particle lines, multiply with the permutation operator $P(pq)$.

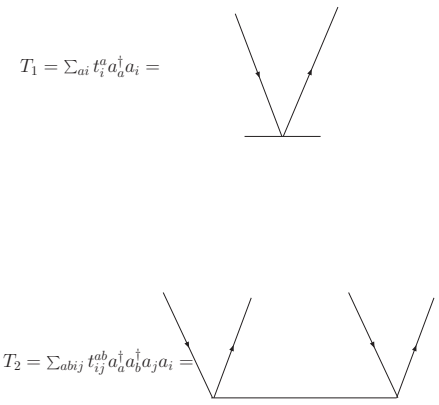

Figure 5.2: Diagrammatic representation of the cluster operators T_1 and T_2.

By using the above diagram rules it is possible to write diagrams corresponding to the energy equation and amplitude equations.

Like the diagrams for the energy equation in Eq. (5.15),

$$E = \langle \Phi_0 | H_N + H_N T_1 + H_N t_2 + \frac{1}{2} H_N T_1^2 + \ldots | \Phi_0 \rangle \tag{5.28}$$

can be evaluated with the above rules. The first term will not contribute since the operator is normalized and therefore will annihilate the vacuum state and give zero contribution.

Lets now study the second term

$$\langle \Phi_0 | H_N T_1 | \Phi_0 \rangle \tag{5.29}$$

Since both the incoming and outgoing states are the same there should be now external lines, meaning that there shouldn't be any lines neither below or above the two horizontal operator lines. The T_1 operator stands to the right, and it's corresponding interaction line should then be in the bottom of the diagram. Only the one particle operator contributes since with a two particle operator it is impossible to draw a diagram with just internal lines. See Fig. (5.3).

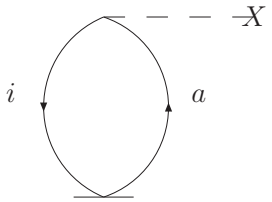

Figure 5.3: Diagrammatic representation of the first term in the ECCSD energy equation.

The second contributing part

$$\langle \Phi_0 | H_N T_2 | \Phi_0 \rangle, \tag{5.30}$$

has also the same ingoing as outgoing state, the same reasoning, with none external lines still yields. Since the cluster operator is the rightmost one, the interaction line representing it should again be at the bottom. However to this part only the two-particle operator of the Hamiltonian is contributing, something which should be reflected in the diagram. Fig. 5.4 shows the diagram representing Eq. (5.30).

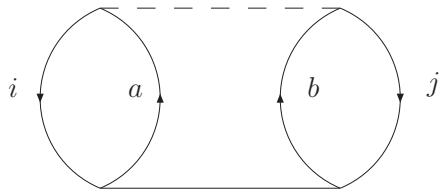

Figure 5.4: Diagrammatic representation of the second term in the ECCSD energy equation.

The last part contributing to the $ECCSD$ energy equation is the term

$$\frac{1}{2}\langle\Phi_0|H_N T_1^2|\Phi_0\rangle \tag{5.31}$$

The interaction lines corresponding to the two cluster operators will again have to be drawn at the bottom of the diagram, the difference in this diagram, Fig. (5.5), from Fig. (5.4) is that the interaction line corresponding to the cluster operator is split since there are two one excitation cluster operators to the right in Eq. (5.31)

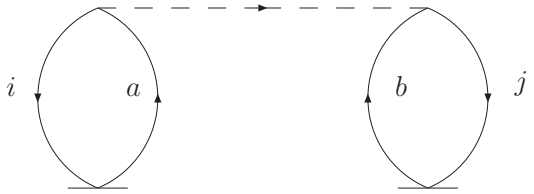

Figure 5.5: Diagrammatic representation of the last term in the ECCSD energy equation.

The cluster diagrams is computed by the same reasoning, keeping in mind that for the $T1$ equation there should be one incoming hole line and one outgoing particle line. The diagrams corresponding to the $T2$ equation all have two incoming hole lines and two outgoing particle lines. The first leading term in the equation corresponding to $T1$ consists just of the Hamiltonian, and only the one particle part of it contributes. It's corresponding diagram is depicted in Fig. (5.6).

The other diagrams corresponding to $T1$ is made with the same reasoning. All diagrams contributing to the T_1 equation can be seen in Fig. (5.7).

In the $T2$ amplitude diagrams there should be two incoming hole lines and two outgoing particle lines. The first leading term consists just of the twoparticle operator. All the diagrams contributing to $T2$ are depicted in Fig. (5.9).

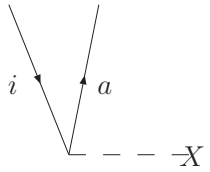

Figure 5.6: The diagram representing the first leading term in the T_1 amplitude equation.

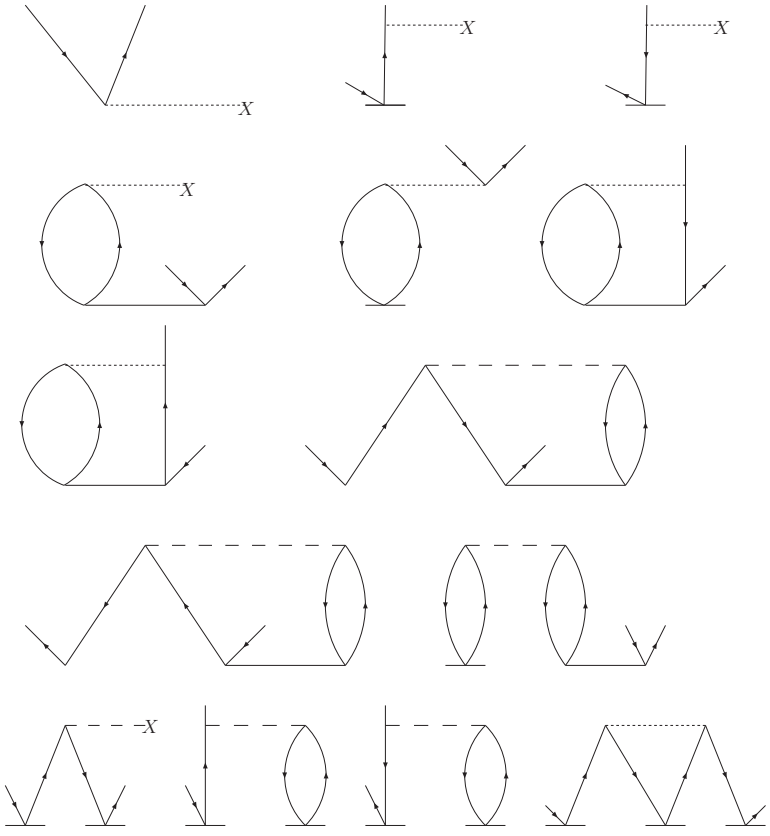

Figure 5.7: All diagrams contributing to the equation for solving the T_1 amplitude.

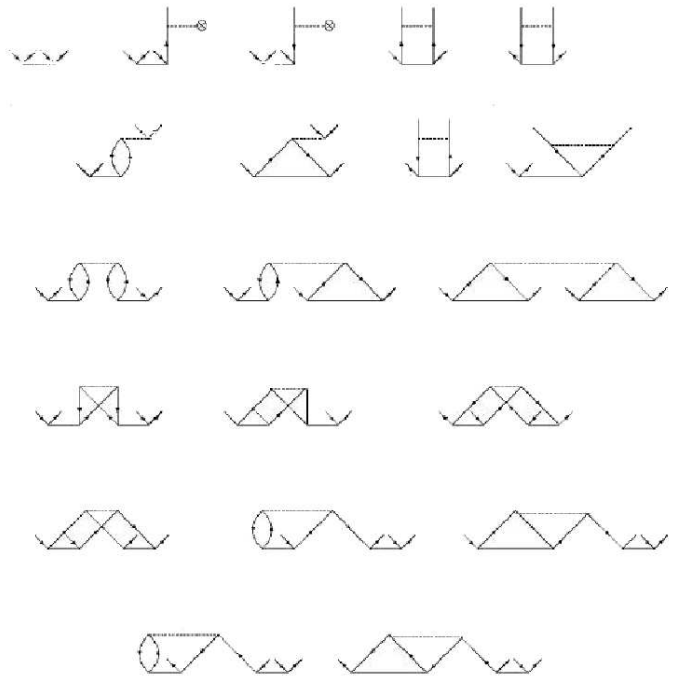

Figure 5.8: All diagrams contributing to the equation for solving the T_2 amplitude.

To see the benefit with the diagrams, the $CCSD$ energy equation will now be computed from the diagrams. The total energy can be depicted as in Fig.(5.10)

The way to interpret the diagrams is from the bottom to the upper part, the time is upward. The ingoing states are represented by a ket vector and the outgoing by the dual, bra vector. The first figure in Fig. (5.10), corresponding to the one particle operator should then be understood as

$$\sum_{ia} \langle i|F_N|a\rangle t_i^a = \sum_{ai} f_{ia} t_i^a, \tag{5.32}$$

where $f_{ia} = \langle i|F_N|a\rangle$. By using the above diagram rules to the second diagram in Fig. (5.10), it's matrix elements become

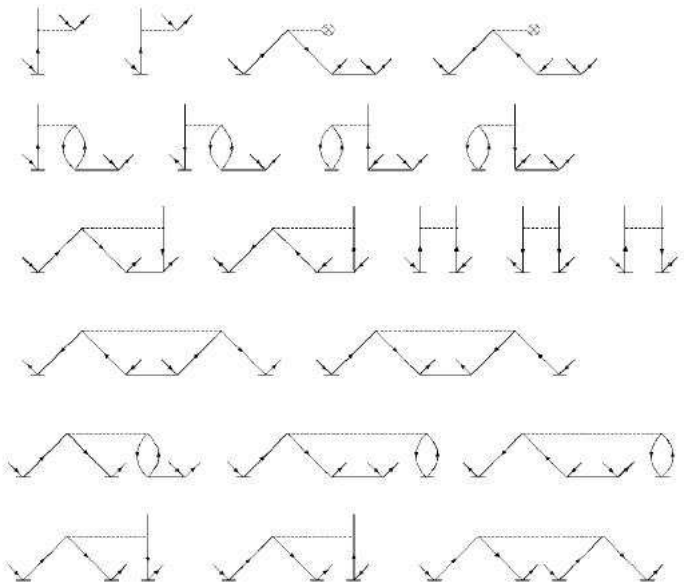

Figure 5.9: All diagrams contributing to the equation for solving the T_2 amplitude.

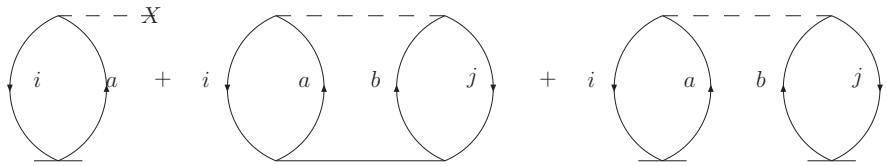

Figure 5.10: The diagrams representing the total $CCSD$ energy.

$$\frac{1}{4}\sum_{ijab}\langle ij|V_N|ab\rangle t_{ij}^{ab} = \frac{1}{4}\sum_{ijab} V_{ijab}t_{ij}^{ab}, \tag{5.33}$$

where $V_{ijab} = \langle ij|V_N|ab\rangle$. The last part is written as

$$\frac{1}{2}\sum_{ijab}\langle ij|V_N|ab\rangle t_i^a t_j^b = \frac{1}{2}\sum_{ijab} V_{ijab}t_i^a t_j^b. \tag{5.34}$$

After summing up the energy, the total equation becomes

$$\sum_{ia} f_{ia}t_i^a + \frac{1}{4}\sum_{ijab} V_{ijab}t_{ij}^{ab} + \frac{1}{2}\sum_{ijab} V_{ijab}t_i^a t_j^b, \tag{5.35}$$

which is exactly the same as the equation got by using Wicks theorem.

5.4 Computation of the equations

This section will treat the computational approach for solving the amplitude equations as Eqs. (5.25) and (5.26). It is not always clear how one should approach the equations for the amplitudes. A first approach could be to rearrange the equations to provide a more handier form. As an example the first few terms of Eq. (5.25), could be written as

$$0 = f_{ai} + f_{aa} - f_{ii}t_i^a + \sum_c (1-\delta_{ca})f_{ac}t_i^c - \sum_k (1-\delta_{ik})f_{ik}t_k^a + \cdots \tag{5.36}$$

By defining

$$D_i^a = f_{ii} - f_{aa} \tag{5.37}$$

Eq. (5.36) would be rewritten as

$$D_i^a t_i^a = f_{ai} + \sum_c (1-\delta_{ca})f_{ac}t_i^c - \sum_k (1-\delta_{ik})f_{ik}t_k^a + \cdots . \tag{5.38}$$

By also defining

$$D_{ij}^{ab} = f_{ii} + f_{jj} - f_{aa} - f_{bb} \tag{5.39}$$

the T_2 amplitude can be rewritten as

$$D_{ij}^{ab}t_{ij}^{ab} = \langle ab|V|ij\rangle + P(ab)\sum_c (1-\delta_{bc})f_{bc}t_{ij}^{ac} - P(ij)\sum_k (1-\delta_{kj})f_{kj}t_{ik}^{ab} + \cdots \tag{5.40}$$

The equations above have to be solved iteratively. A starting point for t_i^a and t_{ij}^{ab} may be obtained by setting all of the amplitudes on the right-hand side to zero. The initial guess for the amplitudes are then

$$t_i^a = f_{ai}/D_i^a, \tag{5.41}$$

for the T_1 amplitude and

$$t_{ij}^{ab} = \langle ab|V|ij\rangle / D_{ij}^{ab} \tag{5.42}$$

for the T_2 amplitude.

These initial guesses have to be inserted on the right-hand side of the equations and then subsequently used to obtain new amplitudes. This process is continued until an explicit convergence is reached.

We saw in Eqs. (5.25) and (5.26) that there are many diagrams contributing to the amplitude equations, as many diagrams as terms in the equations. It requires a lot of time computing all these diagrams separately. By saving a great amount of computing time the amplitude diagrams are factorized. The coupled cluster diagrams can be factorized in contrast to the diagrams in perturbation theory since the first ones do not have any denominators in their's expressions. By notice that some diagrams are similar in the sense that they have the same factors. Instead of computing the same factors several times, we compute it once and multiply it with the corresponding terms, as explained by [20]. In this work the factorization used is the same as the one used by [21].

Appendix A

Diagram rules

1. There are $n+1$ vertices, one vertice for each time, with the ordring $t < t_1 < t_2 < \cdots < t_n$. Each vertex/interaction is represented by a dashed line, as in Fig.(3.2).

2. Lines with upward pointing arrows are particles and lines with downward pointing arrows are holes. Lines starting and ending at the same vertex ate holes.

3. Each vertex gives a factor $\frac{1}{2}V_{\alpha\beta\gamma\delta}$.

4. There is an overall sign $(-1)^{n_h+n_l}$, where n_h is the number of hole lines and n_l is the number of fermion loops.

5. For each interval between two successive vertices there are an energy factor

$$\left[\sum_h \epsilon_h - \sum_p \epsilon_p\right]^{-1} \tag{A.1}$$

   Where the sum over h is over all hole lines in the intervall and the sum over p is over all particle lines in the intervall.

6. For each pair of lines that begins at the same interaction line and end at the same interaction line gives a factor $\frac{1}{2}$.

7. All the above factors have to be multiplied. Sum over all the labels of fermion lines.

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