Week 47, Coupled Cluster theory

Morten Hjorth-Jensen[1]

Department of Physics and Center for Computing in Science Education,
University of Oslo, Norway[1]

November 18-22, 2024

Week 47, November 18-22, 2024

1. Thursday:
   1.1 Introduction to coupled cluster theory and basic equations
2. Friday:
   2.1 Derivation of doubles excitation equation
   2.2 Applications to the pairing model from the second midterm
3. Lecture material: Lecture notes (these notes) and chpater 9 of Shavitt and Bartlett

Introduction

The coupled-cluster method is an efficient tool to compute properties of many-body systems with an effort that grows polynomial with system size. While this might still be expensive, it is now possible to compute for example atomic nuclei with mass numbers about $A \approx 208$ (which corresponds to lead) with this method. Recall that full configuration interaction (FCI) exhibits an exponential cost and is therefore limited to systems with few degrees of freedom.

The normal-ordered Hamiltonian

We start from the reference state

$$|\Phi_0\rangle = \prod_{i=1}^{H} a_i^\dagger |0\rangle \tag{1}$$

for the description of a system with N particles. Usually, this reference is the Hartree-Fock state, but that is not necessary.

Notations again

Here and in what follows, the indices $i, j, k, \ldots$ run over hole states, i.e. orbitals occupied in the reference state (1), while $a, b, c, \ldots$ run over particle states, i.e. unoccupied orbitals. Indices p, q, r, s can identify any orbital. Let n_u be the number of unoccupied states, and N is of course the number of occupied states.

Hamiltonian

We consider the Hamiltonian

$$H = \sum_{pq} \varepsilon_q^p a_p^\dagger a_q + \frac{1}{4} \sum_{pqrs} \langle pq|V|rs\rangle a_p^\dagger a_q^\dagger a_s a_r \tag{2}$$

The reference state

The reference state (1) is a non-trivial vacuum of our theory. We normal order this Hamiltonian with respect to the nontrivial vacuum state given by the Hartree-Fock reference and obtain the normal-ordered Hamiltonian

$$H_N = \sum_{pq} f_{pq} \left\{ a_p^\dagger a_q \right\} + \frac{1}{4} \sum_{pqrs} \langle pq|V|rs\rangle \left\{ a_p^\dagger a_q^\dagger a_s a_r \right\}. \qquad (3)$$

Hartree-Fock basis

Here,

$$f_q^p = \varepsilon_q^p + \sum_i \langle pi|V|qi\rangle \tag{4}$$

is the Fock matrix. We note that the Fock matrix is diagonal in the Hartree-Fock basis. The brackets $\{\cdots\}$ in Eq. (3) denote normal ordering, i.e. all operators that annihilate the nontrivial vaccum (1) are to the right of those operators that create with respect to that vaccum. Normal ordering implies that $\langle\Phi_0|H_N|\Phi_0\rangle = 0$.

Short repetition: Practice in normal ordering

Normal order the expression $\sum_{pq} \varepsilon_q^p a_p^\dagger a_q$.

$$\sum_{pq} \varepsilon_q^p a_p^\dagger a_q = \sum_{ab} \varepsilon_b^a a_a^\dagger a_b + \sum_{ai} \varepsilon_i^a a_a^\dagger a_i + \sum_{ai} \varepsilon_a^i a_i^\dagger a_a + \sum_{ij} \varepsilon_j^i a_i^\dagger a_j \tag{5}$$

Answer

We have to move all operators that annihilate the reference state to the right of those that create on the reference state. Thus,

$$\sum_{pq} \varepsilon_q^p a_p^\dagger a_q = \sum_{ab} \varepsilon_b^a a_a^\dagger a_b + \sum_{ai} \varepsilon_i^a a_a^\dagger a_i + \sum_{ai} \varepsilon_a^i a_i^\dagger a_a + \sum_{ij} \varepsilon_j^i a_i^\dagger a_j \tag{6}$$

$$= \sum_{ab} \varepsilon_b^a a_a^\dagger a_b + \sum_{ai} \varepsilon_i^a a_a^\dagger a_i + \sum_{ai} \varepsilon_a^i a_i^\dagger a_a + \sum_{ij} \varepsilon_j^i \left(-a_j a_i^\dagger + \delta_i^j \right) \tag{7}$$

$$= \sum_{ab} \varepsilon_b^a a_a^\dagger a_b + \sum_{ai} \varepsilon_i^a a_a^\dagger a_i + \sum_{ai} \varepsilon_a^i a_i^\dagger a_a - \sum_{ij} \varepsilon_j^i a_j a_i^\dagger + \sum_i \varepsilon_i^i \tag{8}$$

$$= \sum_{pq} \varepsilon_q^p \left\{ a_p^\dagger a_q \right\} + \sum_i \varepsilon_i^i \tag{9}$$

===== =====

Hartree-Fock again

We note that $H = E_{HF} + H_N$, where

$$E_{HF} \equiv \langle \Phi_0 | H | \Phi_0 \rangle = \sum_i \varepsilon_i^i + \frac{1}{2} \sum_{ij} \langle ij | V | ij \rangle \tag{10}$$

is the Hartree-Fock energy. The coupled-cluster method is a very efficient tool to compute nuclei when a "good" reference state is available. Let us assume that the reference state results from a Hartree-Fock calculation.

What does “good” mean?

How do you know whether a Hartree-Fock state is a “good” reference? Which results of the Hartree-Fock computation will inform you?

Answer

Once the Hartree-Fock equations are solved, the Fock matrix (4) becomes diagonal, and its diagonal elements can be viewed as single-particle energies. Hopefully, there is a clear gap in the single-particle spectrum at the Fermi surface, i.e. after N orbitals are filled.
If symmetry-restricted Hartree-Fock is used, one is limited to compute systems with closed subshells for neutrons and for protons. On a first view, this might seem as a severe limitation. But is it?

To nuclear physics aficionadoss: How many nuclei are accessible with the coupled cluster method based on spherical mean fields?

If one limits oneself to nuclei with mass number up to mass number $A = 60$, how many nuclei can potentially be described with the coupled-cluster method? Which of these nuclei are potentially interesting? Why?

Answer

Nuclear shell closures are at $N, Z = 2, 8, 20, 28, 50, 82, 126$, and subshell closures at $N, Z = 2, 6, 8, 14, 16, 20, 28, 32, 34, 40, 50, \ldots$. In the physics of nuclei, the evolution of nuclear structure as neutrons are added (or removed) from an isotope is a key interest. Examples are the rare isotopes of helium (He-8,10) oxygen (O-22,24,28), calcium (Ca-52,54,60), nickel (Ni-78) and tin (Sn-100,132). The coupled-cluster method has the potential to address questions regarding these nuclei, and in a several cases was used to make predictions before experimental data was available. In addition, the method can be used to compute neighbors of nuclei with closed subshells.

The similarity transformed Hamiltonian

There are several ways to view and understand the coupled-cluster method. A first simple view of coupled-cluster theory is that the method induces correlations into the reference state by expressing a correlated state as

$$|\Psi\rangle = e^{T}|\Phi_0\rangle, \tag{11}$$

Clusters of excited states

Here, T is an operator that induces correlations. We can now demand that the correlate state (11) becomes and eigenstate of the Hamiltonian H_N, i.e. $H_N|\Psi\rangle = E|\Psi\rangle$. This view, while correct, is not the most productive one. Instead, we left-multiply the Schroedinger equation with e^{-T} and find

$$\overline{H_N}|\Phi_0\rangle = E_c|\Phi_0\rangle. \tag{12}$$

Here, E_c is the correlation energy, and the total energy is $E = E_c + E_{HF}$.

Similarity transformation

The similarity-transformed Hamiltonian is defined as

$$\overline{H_N} \equiv e^{-T} H_N e^{T}. \tag{13}$$

A more productive view on coupled-cluster theory thus emerges: This method seeks a similarity transformation such that the uncorrelated reference state (1) becomes an exact eigenstate of the similarity-transformed Hamiltonian (13).

What T leads to Hermitian $\overline{H_N}$?

What are the conditions on T such that $\overline{H_N}$ is Hermitian?

Answer

For a Hermitian $\overline{H_N}$, we need a unitary e^T, i.e. an anti-Hermitian T with $T = -T^\dagger$

As we will see below, coupld-cluster theory employs a non-Hermitian Hamiltonian.

Understanding (non-unitary) similarity transformations

Show that $\overline{H_N}$ has the same eigenvalues as H_N for arbitrary T.
What is the spectral decomposition of a non-Hermitian $\overline{H_N}$?

Answer

Let $H_N|E\rangle = E|E\rangle$. Thus

$$\begin{aligned} H_N e^T e^{-T}|E\rangle &= E|E\rangle, \\ \left(e^{-T} H_N e^T\right) e^{-T}|E\rangle &= E e^{-T}|E\rangle, \\ \overline{H_N} e^{-T}|E\rangle &= E e^{-T}|E\rangle. \end{aligned}$$

Thus, if $|E\rangle$ is an eigenstate of H_N with eigenvalue E, then $e^{-T}|E\rangle$ is eigenstate of $\overline{H_N}$ with the same eigenvalue.

Non-hermitian operator

A non-Hermitian $\overline{H_N}$ has eigenvalues E_α corresponding to left $\langle L_\alpha|$ and right $|R_\alpha\rangle$ eigenstates. Thus

$$\overline{H_N} = \sum_\alpha |R_\alpha\rangle E_\alpha \langle L_\alpha| \tag{14}$$

with bi-orthonormal $\langle L_\alpha|R_\beta\rangle = \delta_\alpha^\beta$.

More formalism

To make progress, we have to specify the cluster operator T. In coupled cluster theory, this operator is

$$T \equiv \sum_{ia} t_i^a a_a^\dagger a_i + \frac{1}{4} \sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i + \cdots + \frac{1}{(N!)^2} \sum_{i_1 \ldots i_N a_1 \ldots a_N} t_{i_1 \ldots i_N}^{a_1 \ldots a_N} a_{a_1}^\dagger \cdots a_{a_N}^\dagger \tag{15}$$

Particle-hole excitations

Thus, the operator (15) induces particle-hole (p-h) excitations with respect to the reference. In general, T generates up to $Ap - Ah$ excitations, and the unknown parameters are the cluster amplitides t_i^a, t_{ij}^{ab}, ..., $t_{i_1,\ldots,i_A}^{a_1,\ldots,a_A}$.

How many unknowns?

Show that the number of unknowns is as large as the FCI dimension of the problem, using the numbers A and n_u.

Answer

We have to sum up all $np-nh$ excitations, and there are $\binom{n_u}{n}$ particle states and $\binom{A}{A-n}$ hole states for each n. Thus, we have for the total number

$$\sum_{n=0}^{A}\binom{n_u}{n}\binom{A}{A-n}=\binom{A+n_u}{A}. \tag{16}$$

The right hand side are obviously all ways to distribute A fermions over n_0+A orbitals.

Full clutser operator

Thus, the coupled-cluster method with the full cluster operator (15) is exponentially expensive, just as FCI. To make progress, we need to make an approximation by truncating the operator. Here, we will use the CCSD (coupled clusters singles doubles) approximation, where

$$T \equiv \sum_{ia} t_i^a a_a^\dagger a_i + \frac{1}{4} \sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i. \tag{17}$$

Unknown aplitudes

We need to determine the unknown cluster amplitudes that enter in CCSD. Let

$$|\Phi_i^a\rangle = a_a^\dagger a_i |\Phi_0\rangle, \tag{18}$$

$$|\Phi_{ij}^{ab}\rangle = a_a^\dagger a_b^\dagger a_j a_i |\Phi_0\rangle \tag{19}$$

be 1p-1h and 2p-2h excitations of the reference. Computing matrix elements of the Schroedinger Equation (12) yields

$$\langle \Phi_0 | \overline{H_N} | \Phi_0 \rangle = E_c, \tag{20}$$

$$\langle \Phi_i^a | \overline{H_N} | \Phi_0 \rangle = 0, \tag{21}$$

$$\langle \Phi_{ij}^{ab} | \overline{H_N} | \Phi_0 \rangle = 0. \tag{22}$$

Correlation energy

The first equation states that the coupled-cluster correlation energy is an expectation value of the similarity-transformed Hamiltonian. The second and third equations state that the similarity-transformed Hamiltonian exhibits no 1p-1h and no 2p-2h excitations. These equations have to be solved to find the unknown amplitudes t_i^a and t_{ij}^{ab}. Then one can use these amplitudes and compute the correlation energy from the first line of Eq. (20). We note that in the CCSD approximation the reference state is not an exact eigenstates. Rather, it is decoupled from simple states but $\overline{H}$ still connects this state to 3p-3h, and 4p-4h states etc.

Good reference state

At this point, it is important to recall that we assumed starting from a "good" reference state. In such a case, we might reasonably expect that the inclusion of 1p-1h and 2p-2h excitations could result in an accurate approximation. Indeed, empirically one finds that CCSD accounts for about 90% of the corelation energy, i.e. of the difference between the exact energy and the Hartree-Fock energy. The inclusion of triples (3p-3h excitations) typically yields 99% of the correlation energy.

We see that the coupled-cluster method in its CCSD approximation yields a similarity-transformed Hamiltonian that is of a two-body structure with respect to a non-trivial vacuum. When viewed in this light, the coupled-cluster method "transforms" an A-body problem (in CCSD) into a two-body problem, albeit with respect to a nontrivial vacuum.

Above we argued that a similarity transformation preserves all eigenvalues. Nevertheless, the CCD correlation energy is not the exact correlation energy. Explain!
The CCD approximation does not make $|\Phi_0\rangle$ an exact eigenstate of $\overline{H_N}$; it is only an eigenstate when the similarity-transformed Hamiltonian is truncated to at most 2p-2h states. The full $\overline{H_N}$, with $T = T_2$, would involve six-body terms (do you understand this?), and this full Hamiltonian would reproduce the exact correlation energy. Thus CCD is a similarity transformation plus a truncation, which decouples the ground state only from 2p-2h states.

Computing the similarity-transformed Hamiltonian

The solution of the CCSD equations, i.e. the second and third line of Eq. (20), and the computation of the correlation energy requires us to compute matrix elements of the similarity-transformed Hamiltonian (13). This can be done with the Baker-Campbell-Hausdorff expansion

$$\overline{H_N} = e^{-T} H_N e^{T} \tag{23}$$

$$= H_N + [H_N, T] + \frac{1}{2!}[[H_N, T], T] + \frac{1}{3!}[[[H_N, T], T], T] + \ldots. \tag{24}$$

The cluster operator

We now come to a key element of coupled-cluster theory: the cluster operator (15) consists of sums of terms that consist of particle creation and hole annihilation operators (but no particle annihilation or hole creation operators). Thus, all terms that enter T commute with each other. This means that the commutators in the Baker-Campbell-Hausdorff expansion (23) can only be non-zero because each T must connect to H_N (but no T with another T). Thus, the expansion is finite.

When does CCSD truncate?

In CCSD and for two-body Hamiltonians, how many nested commutators yield nonzero results? Where does the Baker-Campbell-Hausdorff expansion terminate? What is the (many-body) rank of the resulting $\overline{H_N}$?
CCSD truncates for two-body operators at four-fold nested commutators, because each of the four annihilation and creation operators in $\overline{H_N}$ can be knocked out with one term of T.

Non-hermitian Hamiltonian

We see that the (disadvantage of having a) non-Hermitian Hamiltonian $\overline{H_N}$ leads to the advantage that the Baker-Campbell-Hausdorff expansion is finite, thus leading to the possibility to compute $\overline{H_N}$ exactly. In contrast, the IMSRG deals with a Hermitian Hamiltonian throughout, and the infinite Baker-Campbell-Hausdorff expansion is truncated at a high order when terms become very small.

Similarity transformed Hamiltonian

We write the similarity-transformed Hamiltonian as

$$\overline{H_N} = \sum_{pq} \overline{H}_q^p a_q^\dagger a_p + \frac{1}{4} \sum_{pqrs} \overline{H}_{rs}^{pq} a_p^\dagger a_q^\dagger a_s a_r + \dots \tag{25}$$

with

$$\overline{H}_q^p \equiv \langle p|\overline{H_N}|q\rangle, \tag{26}$$

$$\overline{H}_{rs}^{pq} \equiv \langle pq|\overline{H_N}|rs\rangle. \tag{27}$$

Thus, the CCSD Eqs. (20) for the amplitudes can be written as $\overline{H}_i^a = 0$ and $\overline{H}_{ij}^{ab} = 0$.

Compute the matrix element $\overline{H}^{ij}_{ab} \equiv \langle ij|\overline{H_N}|ab\rangle$

This is a simple task. This matrix element is part of the operator $\overline{H}^{ij}_{ab} a_i^\dagger a_j^\dagger a_b a_a$, i.e. particles are annihilated and holes are created. Thus, no contraction of the Hamiltonian H with any cluster operator T (remember that T annihilates holes and creates particles) can happen, and we simply have $\overline{H}^{ij}_{ab} = \langle ij|V|ab\rangle$.

Algebraic manipulations

We need to work out the similarity-transformed Hamiltonian of Eq. (23). To do this, we write $T = T_1 + T_2$ and $H_N = F + V$, where T_1 and F are one-body operators, and T_2 and V are two-body operators.

Example: The contribution of $[F, T_2]$ to $\overline{H_N}$

The commutator $[F, T_2]$ consists of two-body and one-body terms. Let us compute first the two-body term, as it results from a single contraction (i.e. a single application of $[a_p, a_q^\dagger] = \delta_p^q$). We denote this as $[F, T_2]_{2b}$ and find

$$
\begin{aligned}
[F, T_2]_{2b} &= \frac{1}{4} \sum_{pq} \sum_{rsuv} f_p^q t_{ij}^{ab} \left[a_q^\dagger a_p, a_a^\dagger a_b^\dagger a_j a_i \right]_{2b} \\
&= \frac{1}{4} \sum_{pq} \sum_{abij} f_p^q t_{ij}^{ab} \delta_p^a a_q^\dagger a_b^\dagger a_j a_i \\
&- \frac{1}{4} \sum_{pq} \sum_{abij} f_p^q t_{ij}^{ab} \delta_p^b a_q^\dagger a_a^\dagger a_j a_i \\
&- \frac{1}{4} \sum_{pq} \sum_{abij} f_p^q t_{ij}^{ab} \delta_q^j a_a^\dagger a_b^\dagger a_p a_i \\
&+ \frac{1}{4} \sum_{pq} \sum_{abij} f_p^q t_{ij}^{ab} \delta_q^i a_a^\dagger a_b^\dagger a_p a_j \\
&- \frac{1}{4} \left(\sum_{pq} \sum_{abij} \right) \\
&+
\end{aligned}
$$

Antisymmetry

Here we exploited the antisymmetry $t_{ij}^{ab} = -t_{ji}^{ab} = -t_{ij}^{ba} = t_{ji}^{ba}$ in the last step. Using $a_q^\dagger a_b^\dagger a_j a_i = -a_b^\dagger a_q^\dagger a_j a_i$ and $a_a^\dagger a_b^\dagger a_p a_i = a_a^\dagger a_b^\dagger a_i a_p$, we can make the expression manifest antisymmetric, i.e.

$$[F, T_2]_{2b} = \frac{1}{4} \sum_{qbij} \left[\sum_a \left(f_a^q t_{ij}^{ab} - f_a^b t_{ij}^{qa} \right) \right] a_q^\dagger a_b^\dagger a_j a_i$$
$$- \frac{1}{4} \sum_{pabi} \left[\sum_j \left(f_p^j t_{ij}^{ab} - f_i^j t_{pj}^{ab} \right) \right] a_a^\dagger a_b^\dagger a_p a_i .$$

Final contribution

Thus, the contribution of $[F, T_2]_{2b}$ to the matrix element $\overline{H}_{ij}^{ab}$ is

$$\overline{H}_{ij}^{ab} \leftarrow \sum_c \left(f_c^a t_{ij}^{cb} - f_c^b t_{ij}^{ac} \right) - \sum_k \left(f_j^k t_{ik}^{ab} - f_i^k t_{jk}^{ab} \right)$$

Here we used an arrow to indicate that this is just one contribution to this matrix element. We see that the derivation straight forward, but somewhat tedious. As no one likes to commute too much (neither in this example nor when going to and from work), and so we need a better approach. This is where diagramms come in handy.

Assign the correct matrix element $\langle pq|V|rs\rangle$ to each of the following diagrams of the interaction

Remember: $\langle \mathrm{left-out, right-out|V|left-in, right-in}\rangle$.

$\langle ab|V|cd\rangle + \langle ij|V|kl\rangle + \langle ia|V|bj\rangle$

$\langle ai|V|bc\rangle + \langle ij|V|ka\rangle + \langle ab|V|ci\rangle$

$\langle ia|V|jk\rangle + \langle ab|V|ij\rangle + \langle ij|V|ab\rangle$

CCD Approximation

In what follows, we will consider the coupled cluster doubles (CCD) approximation. This approximation is valid in cases where the system cannot exhibit any particle-hole excitations (such as nuclear matter when formulated on a momentum-space grid) or for the pairing model (as the pairing interactions only excites pairs of particles). In this case $t_i^a = 0$ for all i, a, and $\overline{H}_i^a = 0$. The CCD approximation is also of some sort of leading order approximation in the Hartree-Fock basis (as the Hartree-Fock Hamiltonian exhibits no particle-hole excitations).

Deriving the CCD equations

Let us consider the matrix element $\overline{H}_{ij}^{ab}$. Clearly, it consists of all diagrams (i.e. all combinations of T_2, and a single F or V that have two incoming hole lines and two outgoing particle lines. Write down all these diagrams.
We start systematically and consider all combinations of F and V diagrams with 0, 1, and 2 cluster amplitudes T_2.

The algebraic expression

$$
\begin{aligned}
\overline{H}_{ij}^{ab} &= \langle ab|V|ij\rangle + P(ab)\sum_{c} f_c^b\, t_{ij}^{ac} - P(ij)\sum_{k} f_j^k\, t_{ik}^{ab} \\
&+ \frac{1}{2}\sum_{cd}\langle ab|V|cd\rangle\, t_{ij}^{cd} + \frac{1}{2}\sum_{kl}\langle kl|V|ij\rangle\, t_{kl}^{ab} + P(ab)P(ij)\sum_{kc}\langle kb|V|cj\rangle \\
&+ \frac{1}{2}P(ij)P(ab)\sum_{kcld}\langle kl|V|cd\rangle\, t_{ik}^{ac}\, t_{lj}^{db} + \frac{1}{2}P(ij)\sum_{kcld}\langle kl|V|cd\rangle\, t_{ik}^{cd}\, t_{lj}^{ab} \\
&+ \frac{1}{2}P(ab)\sum_{kcld}\langle kl|V|cd\rangle\, t_{kl}^{ac}\, t_{ij}^{db} + \frac{1}{4}\sum_{kcld}\langle kl|V|cd\rangle\, t_{ij}^{cd}\, t_{kl}^{ab}.
\end{aligned}
$$

Computational cost of a CCD computation

For each of the diagrams in (add fig) write down the computational cost in terms of the number of occupied A and the number of unoccupied n_u orbitals.
The cost is $A^2 n_u^2$, $A^2 n_u^3$, $A^3 n_u^2$, $A^2 n_u^4$, $A^4 n_u^2$, $A^3 n_u^3$, $A^4 n_u^4$, $A^4 n_u^4$, $A^4 n_u^4$, and $A^4 n_u^4$ for the respective diagrams.

Additional details

Note that $n_u \gg A$ in general. In textbooks, one reads that CCD (and CCSD) cost only $A^2 n_u^4$. Our most expensive diagrams, however are $A^4 n_u^4$. What is going on?
To understand this puzzle, let us consider the last diagram of Figure xx . We break up the computation into two steps, computing first the intermediate

$$\chi_{ij}^{kl} \equiv \frac{1}{2} \sum_{cd} \langle kl|V|cd\rangle t_{ij}^{cd} \tag{28}$$

at a cost of $A^4 n_u^2$, and then

$$\frac{1}{2} \sum_{kl} \chi_{ij}^{kl} t_{kl}^{ab} \tag{29}$$

at a cost of $A^4 n_u^2$. This is affordable. The price to pay is the storage of the intermediate χ_{ij}^{kl}, i.e. we traded memory for computational cycles. This trick is known as **factorization**.

Factorizing the remaining diagrams of the CCD equation

Diagrams 7, 8, and 9 of Fig. xx also need to be factorized.
For diagram number 7, we compute

$$\chi_{id}^{al} \equiv \sum_{kc} \langle kl|V|cd\rangle t_{ik}^{ac} \tag{30}$$

at a cost of $A^3 n_u^3$ and then compute

$$\frac{1}{2} P(ij)P(ab) \sum_{ld} \chi_{id}^{al} t_{lj}^{db} \tag{31}$$

at the cost of $A^3 n_u^3$.

Diagram 8

For diagram number 8, we compute

$$\chi_i^l \equiv -\frac{1}{2}\sum_{kcd}\langle kl|V|cd\rangle\, t_{ik}^{cd} \tag{32}$$

at a cost of $A^3 n_u^2$, and then compute

$$-P(ij)\sum_{l}\chi_i^l t_{lj}^{ab} \tag{33}$$

at the cost of $A^3 n_u^2$.

Diagram 9

For diagram number 9, we compute

$$\chi_d^a \equiv \frac{1}{2} \sum_{kcl} \langle kl|V|cd\rangle t_{kl}^{ac} \tag{34}$$

at a cost of $A^2 n_u^3$ and then compute

$$P(ab) \sum_d \chi_d^a t_{ij}^{db} \tag{35}$$

at the cost of $A^3 n_u^3$.

Solving the CCD equations

The CCD equations, depicted in Fig xx, are nonlinear in the cluster amplitudes. How do we solve $\overline{H}_{ij}^{ab} = 0$? We subtract $(f_a^a + f_b^b - f_i^i - f_j^j)t_{ij}^{ab}$ from both sides of $\overline{H}_{ij}^{ab} = 0$ (because this term is contained in $\overline{H}_{ij}^{ab}$) and find

$$(f_i^i + f_j^j - f_a^a - f_b^b)t_{ij}^{ab} = (f_i^i + f_j^j - f_a^a - f_b^b)t_{ij}^{ab} + \overline{H}_{ij}^{ab}$$

More manipulations

Dividing by $(f_i^i + f_j^j - f_a^a - f_b^b)$ yields

$$t_{ij}^{ab} = t_{ij}^{ab} + \frac{\overline{H}_{ij}^{ab}}{f_i^i + f_j^j - f_a^a - f_b^b} \tag{36}$$

This equation is of the type $t = f(t)$, and we solve it by iteration, i.e. we start with a guess t_0 and iterate $t_{n+1} = f(t_n)$, and hope that this will converge to a solution. We take the perturbative result

$$\left(t_{ij}^{ab}\right)_0 = \frac{\langle ab|V|ij\rangle}{f_i^i + f_j^j - f_a^a - f_b^b} \tag{37}$$

as a starting point, compute $\overline{H}_{ij}^{ab}$, and find a new t_{ij}^{ab} from the right-hand side of Eq. (36). We repeat this process until the amplitudes (or the CCD energy) converge.

CCD for the pairing Hamiltonian

You learned about the pairing Hamiltonian earlier in this school. Convince yourself that this Hamiltonian does not induce any 1p-1h excitations. Let us solve the CCD equations for this problem. This consists of the following steps

1. Write a function that compute the potential, i.e. it returns a four-indexed array (or tensor). We need $\langle ab|V|cd\rangle$, $\langle ij|V|kl\rangle$, and $\langle ab|V|ij\rangle$. Why is there no $\langle ab|V|id\rangle$ or $\langle ai|V|jb\rangle$?
2. Write a function that computes the Fock matrix, i.e. a two-indexed array. We only need f_a^b and f_i^j. Why?
3. Initialize the cluster amplitudes according to Eq. (37), and solve Eq. (36) by iteration. The cluster amplitudes T_1 and T_2 are two- and four-indexed arrays, respectively.

Please note that the contraction of tensors (i.e. the summation over common indices in products of tensors) is very user friendly and elegant in python when `numpy.einsum` is used.

Solving the CCD equations for the pairing problem

The Hamiltonian is

$$H = \delta \sum_{p=1}^{\Omega} (p-1) \left(a_{p+}^{\dagger} a_{p+} + a_{p-}^{\dagger} a_{p-} \right) - \frac{g}{2} \sum_{p,q=1}^{\Omega} a_{p+}^{\dagger} a_{p-}^{\dagger} a_{q-} a_{q+}. \tag{38}$$

Python code

```
## Coupled clusters in CCD approximation
## Implemented for the pairing model of Lecture Notes in Physics 936,
import numpy as np


def init_pairing_v(g,pnum,hnum):
    """
    returns potential matrices of the pairing model in three relevant

    param g: strength of the pairing interaction, as in Eq. (8.42)
    param pnum: number of particle states
    param hnum: number of hole states

    return v_pppp, v_pphh, v_hhhh: np.array(pnum,pnum,pnum,pnum),
                                   np.array(pnum,pnum,hnum,hnum),
                                   np.array(hnum,hnum,hnum,hnum),
                                   The interaction as a 4-indexed tens
    """
    v_pppp=np.zeros((pnum,pnum,pnum,pnum))
    v_pphh=np.zeros((pnum,pnum,hnum,hnum))
    v_hhhh=np.zeros((hnum,hnum,hnum,hnum))

    gval=-0.5*g
    for a in range(0,pnum,2):
        for b in range(0,pnum,2):
            v_pppp[a,a+1,b,b+1]=gval
            v_pppp[a+1,a,b,b+1]=-gval
            v_pppp[a,a+1,b+1,b]=-gval
```