

Many-body theory and nuclear few- and many-body systems

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Classical many-body methods and quantum computing

Classical many-body methods in quantum mechanics often trade computational complexity for accuracy when solving for the ground state energy of a system. The recent advances in quantum computing have shown promise in approximating the ground state energy without such a large trade-off. In classical computing, the basic unit of information is called a bit. The bit is represented by a binary digit, either a 1 or a 0. A collection of bits provides a binary string with information, and this information can be manipulated with what we call logic gates. Logic gates are operations on one or more bits and produce a single output, 1 or 0. A collection of such logic gates is called a circuit and an example of such a circuit could be outputting a 1 if all input bits are put to 1 and output 0 otherwise. The behaviour of all circuits on classical computers is deterministic in the sense that a given input binary string will always produce the same output.

Quantum computing

How quantum computing differs from classical computing can partly be illustrated by looking at the surface of the unit Bloch sphere discussed in earlier lectures. A classical bit must either be in the $|0\rangle$ state at the surface on the north pole, or in the $|1\rangle$ state at the surface on the south pole; the quantum bit, namely a qubit, can be in a state located anywhere on the surface of the Bloch sphere. The qubit state $|\psi\rangle$ can be in superposition,

$$|\psi\rangle = c_0|0\rangle + c_1|1\rangle,$$

where a measurement of the qubit will collapse the state, resulting in the state $|0\rangle$ or $|1\rangle$ with probability $|c_0|^2$ or $|c_1|^2$ respectively. These coefficients are referred to as amplitudes and could be any complex number as long as the measurement probabilities are normalized, that is $|c_0|^2 + |c_1|^2 = 1$.

Slater determinants as basis states, Fermionic problems

The simplest possible choice for many-body wavefunctions are **product** wavefunctions. That is

$$\Psi(x_1, x_2, x_3, \dots, x_A) \approx \phi_1(x_1)\phi_2(x_2)\phi_3(x_3)\dots$$

because we are really only good at thinking about one particle at a time. Such product wavefunctions, without correlations, are easy to work with; for example, if the single-particle states $\phi_i(x)$ are orthonormal, then the product wavefunctions are easy to orthonormalize.

Similarly, computing matrix elements of operators are relatively easy, because the integrals factorize.

The price we pay is the lack of correlations, which we must build up by using many, many product wavefunctions. (Thus we have a trade-off: compact representation of correlations but difficult integrals versus easy integrals but many states required.)

Slater determinants as basis states, repetition

Because we have fermions, we are required to have antisymmetric wavefunctions, e.g.

$$\Psi(x_1, x_2, x_3, \dots, x_A) = -\Psi(x_2, x_1, x_3, \dots, x_A)$$

etc. This is accomplished formally by using the determinantal formalism

$$\Psi(x_1, x_2, \dots, x_A) = \frac{1}{\sqrt{A!}} \det \begin{vmatrix} \phi_1(x_1) & \phi_1(x_2) & \dots & \phi_1(x_A) \\ \phi_2(x_1) & \phi_2(x_2) & \dots & \phi_2(x_A) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_A(x_1) & \phi_A(x_2) & \dots & \phi_A(x_A) \end{vmatrix}$$

Product wavefunction + antisymmetry = Slater determinant.

Slater determinants as basis states

$$\Psi(x_1, x_2, \dots, x_A) = \frac{1}{\sqrt{A!}} \det \begin{vmatrix} \phi_1(x_1) & \phi_1(x_2) & \dots & \phi_1(x_A) \\ \phi_2(x_1) & \phi_2(x_2) & \dots & \phi_2(x_A) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_A(x_1) & \phi_A(x_2) & \dots & \phi_A(x_A) \end{vmatrix}$$

Properties of the determinant (interchange of any two rows or any two columns yields a change in sign; thus no two rows and no two columns can be the same) lead to the Pauli principle:

- No two particles can be at the same place (two columns the same); and
- No two particles can be in the same state (two rows the same).

Slater determinants as basis states

As a practical matter, however, Slater determinants beyond $N = 4$ quickly become unwieldy. Thus we turn to the **occupation representation** or **second quantization** to simplify calculations.

The occupation representation or number representation, using fermion **creation** and **annihilation** operators, is compact and efficient. It is also abstract and, at first encounter, not easy to internalize. It is inspired by other operator formalism, such as the ladder operators for the harmonic oscillator or for angular momentum, but unlike those cases, the operators **do not have coordinate space representations**.

Instead, one can think of fermion creation/annihilation operators as a game of symbols that compactly reproduces what one would do, albeit clumsily, with full coordinate-space Slater determinants.

Reminder on the occupation representation (second quantization)

We start with a set of orthonormal single-particle states $\{\phi_i(x)\}$. (Note: this requirement, and others, can be relaxed, but leads to a more involved formalism.) **Any** orthonormal set will do.

To each single-particle state $\phi_i(x)$ we associate a creation operator \hat{a}_i^\dagger and an annihilation operator \hat{a}_i .

When acting on the vacuum state $|0\rangle$, the creation operator \hat{a}_i^\dagger causes a particle to occupy the single-particle state $\phi_i(x)$:

$$\phi_i(x) \rightarrow \hat{a}_i^\dagger |0\rangle$$

Quick repetition of the occupation representation

But with multiple creation operators we can occupy multiple states:

$$\phi_i(x)\phi_j(x')\phi_k(x'') \rightarrow \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k^\dagger |0\rangle.$$

Now we impose antisymmetry, by having the fermion operators satisfy **anti-commutation relations**:

$$\hat{a}_i^\dagger \hat{a}_j^\dagger + \hat{a}_j^\dagger \hat{a}_i^\dagger = [\hat{a}_i^\dagger, \hat{a}_j^\dagger]_+ = \{\hat{a}_i^\dagger, \hat{a}_j^\dagger\} = 0$$

so that

$$\hat{a}_i^\dagger \hat{a}_j^\dagger = -\hat{a}_j^\dagger \hat{a}_i^\dagger$$

Quick repetition of the occupation representation

Because of this property, automatically $\hat{a}_i^\dagger \hat{a}_i^\dagger = 0$, enforcing the Pauli exclusion principle. Thus when writing a Slater determinant using creation operators,

$$\hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k^\dagger \dots |0\rangle$$

each index i, j, k, \dots must be unique.

For some relevant exercises with solutions see chapter 8 of [Lecture Notes in Physics, volume 936](#).

Full Configuration Interaction Theory

We have defined the ansatz for the ground state as

$$|\Phi_0\rangle = \left(\prod_{i \leq F} \hat{a}_i^\dagger \right) |0\rangle,$$

where the index i defines different single-particle states up to the Fermi level. We have assumed that we have N fermions. A given one-particle-one-hole ($1p1h$) state can be written as

$$|\Phi_i^a\rangle = \hat{a}_a^\dagger \hat{a}_i |\Phi_0\rangle,$$

while a $2p2h$ state can be written as

$$|\Phi_{ij}^{ab}\rangle = \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i |\Phi_0\rangle,$$

and a general $NpNh$ state as

$$|\Phi_{ijk\dots}^{abc\dots}\rangle = \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_c^\dagger \dots \hat{a}_k \hat{a}_j \hat{a}_i |\Phi_0\rangle.$$

Full Configuration Interaction Theory

We can then expand our exact state function for the ground state as

$$|\Psi_0\rangle = C_0 |\Phi_0\rangle + \sum_{ai} C_i^a |\Phi_i^a\rangle + \sum_{abij} C_{ij}^{ab} |\Phi_{ij}^{ab}\rangle + \dots = (C_0 + \hat{C}) |\Phi_0\rangle,$$

where we have introduced the so-called correlation operator

$$\hat{C} = \sum_{ai} C_i^a \hat{a}_a^\dagger \hat{a}_i + \sum_{abij} C_{ij}^{ab} \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i + \dots$$

Since the normalization of Ψ_0 is at our disposal and since C_0 is by hypothesis non-zero, we may arbitrarily set $C_0 = 1$ with corresponding proportional changes in all other coefficients. Using this so-called intermediate normalization we have

$$\langle \Psi_0 | \Phi_0 \rangle = \langle \Phi_0 | \Phi_0 \rangle = 1,$$

resulting in

$$|\Psi_0\rangle = (1 + \hat{C}) |\Phi_0\rangle.$$

Full Configuration Interaction Theory

We rewrite

$$|\Psi_0\rangle = C_0|\Phi_0\rangle + \sum_{ai} C_i^a |\Phi_i^a\rangle + \sum_{abij} C_{ij}^{ab} |\Phi_{ij}^{ab}\rangle + \dots,$$

in a more compact form as

$$|\Psi_0\rangle = \sum_{PH} C_H^P \Phi_H^P = \left(\sum_{PH} C_H^P \hat{A}_H^P \right) |\Phi_0\rangle,$$

where H stands for $0, 1, \dots, n$ hole states and P for $0, 1, \dots, n$ particle states. Our requirement of unit normalization gives

$$\langle \Psi_0 | \Phi_0 \rangle = \sum_{PH} |C_H^P|^2 = 1,$$

and the energy can be written as

$$E = \langle \Psi_0 | \hat{H} | \Phi_0 \rangle = \sum_{PP'HH'} C_H^{*P} \langle \Phi_H^P | \hat{H} | \Phi_{H'}^{P'} \rangle C_{H'}^{P'}.$$

Full Configuration Interaction Theory

Normally

$$E = \langle \Psi_0 | \hat{H} | \Phi_0 \rangle = \sum_{PP'HH'} C_H^{*P} \langle \Phi_H^P | \hat{H} | \Phi_{H'}^{P'} \rangle C_{H'}^{P'},$$

is solved by diagonalization setting up the Hamiltonian matrix defined by the basis of all possible Slater determinants. A diagonalization is equivalent to finding the variational minimum of

$$\langle \Psi_0 | \hat{H} | \Phi_0 \rangle - \lambda \langle \Psi_0 | \Phi_0 \rangle,$$

where λ is a variational multiplier to be identified with the energy of the system. The minimization process results in

$$\delta \left[\langle \Psi_0 | \hat{H} | \Phi_0 \rangle - \lambda \langle \Psi_0 | \Phi_0 \rangle \right] = \sum_{P'H'} \left\{ \delta[C_H^{*P}] \langle \Phi_H^P | \hat{H} | \Phi_{H'}^{P'} \rangle C_{H'}^{P'} + C_H^{*P} \langle \Phi_H^P | \hat{H} | \Phi_{H'}^{P'} \rangle \delta[C_{H'}^{P'}] - \lambda (\delta[C_H^{*P}] C_{H'}^{P'} + C_H^{*P} \delta[C_{H'}^{P'}]) \right\} = 0.$$

Since the coefficients $\delta[C_H^{*P}]$ and $\delta[C_{H'}^{P'}]$ are complex conjugates it is necessary and sufficient to require the quantities that multiply with $\delta[C_H^{*P}]$ to vanish.

Full Configuration Interaction Theory

This leads to

$$\sum_{P'H'} \langle \Phi_H^P | \hat{H} | \Phi_{H'}^{P'} \rangle C_{H'}^{P'} - \lambda C_H^P = 0,$$

for all sets of P and H .

If we then multiply by the corresponding C_H^{*P} and sum over PH we obtain

$$\sum_{PP'HH'} C_H^{*P} \langle \Phi_H^P | \hat{H} | \Phi_{H'}^{P'} \rangle C_{H'}^{P'} - \lambda \sum_{PH} |C_H^P|^2 = 0,$$

leading to the identification $\lambda = E$. This means that we have for all PH sets

$$\sum_{P'H'} \langle \Phi_H^P | \hat{H} - E | \Phi_{H'}^{P'} \rangle = 0. \quad (1)$$

Full Configuration Interaction Theory

An alternative way to derive the last equation is to start from

$$(\hat{H} - E) |\Psi_0\rangle = (\hat{H} - E) \sum_{P'H'} C_{H'}^{P'} |\Phi_{H'}^{P'}\rangle = 0,$$

and if this equation is successively projected against all Φ_H^P in the expansion of Ψ , then the last equation on the previous slide results. As stated previously, one solves this equation normally by diagonalization. If we are able to solve this equation exactly (that is numerically exactly) in a large Hilbert space (it will be truncated in terms of the number of single-particle states included in the definition of Slater determinants), it can then serve as a benchmark for other many-body methods which approximate the correlation operator \hat{C} .

Shell-model jargon

If we do not make any truncations in the possible sets of Slater determinants (many-body states) we can make all possible configurations by distributing A nucleons among n single-particle states, we call such a calculation for **Full configuration interaction theory**

If we make truncations, we have different possibilities

- The standard nuclear shell-model. Here we define an effective Hilbert space with respect to a given core. The calculations are normally then performed for all many-body states that can be constructed from the effective Hilbert spaces. This approach requires a properly defined effective Hamiltonian
- We can truncate in the number of excitations. For example, we can limit the possible Slater determinants to only $1p - 1h$ and $2p - 2h$ excitations. This is called a configuration interaction calculation at the level of singles and doubles excitations, or just CISD.

- We can limit the number of excitations in terms of the excitation energies. If we do not define a core, this defines normally what is called the no-core shell-model approach.

FCI and the exponential growth

Full configuration interaction theory calculations provide in principle, if we can diagonalize numerically, all states of interest. The dimensionality of the problem explodes however quickly.

The total number of Slater determinants which can be built with say N neutrons distributed among n single particle states is

$$\binom{n}{N} = \frac{n!}{(n-N)!N!}.$$

For a model space which comprises the first for major shells only $0s$, $0p$, $1s0d$ and $1p0f$ we have 40 single particle states for neutrons and protons. For the eight neutrons of oxygen-16 we would then have

$$\binom{40}{8} = \frac{40!}{(32)!8!} \sim 10^9,$$

and multiplying this with the number of proton Slater determinants we end up with approximately with a dimensionality d of $d \sim 10^{18}$.

Exponential wall

This number can be reduced if we look at specific symmetries only. However, the dimensionality explodes quickly!

- For Hamiltonian matrices of dimensionalities which are smaller than $d \sim 10^5$, we would use so-called direct methods for diagonalizing the Hamiltonian matrix
- For larger dimensionalities iterative eigenvalue solvers like Lanczos' method are used. The most efficient codes at present can handle matrices of $d \sim 10^{10}$.

A non-practical way of solving the eigenvalue problem

To see this, we look at the contributions arising from

$$\langle \Phi_H^P | = \langle \Phi_0 |$$

in Eq. (1), that is we multiply with $\langle \Phi_0 |$ from the left in

$$(\hat{H} - E) \sum_{P'H'} C_{H'}^{P'} |\Phi_{H'}^{P'}\rangle = 0.$$

If we assume that we have a two-body operator at most, Slater's rule gives then an equation for the correlation energy in terms of C_i^a and C_{ij}^{ab} only. We get then

$$\langle \Phi_0 | \hat{H} - E | \Phi_0 \rangle + \sum_{ai} \langle \Phi_0 | \hat{H} - E | \Phi_i^a \rangle C_i^a + \sum_{abij} \langle \Phi_0 | \hat{H} - E | \Phi_{ij}^{ab} \rangle C_{ij}^{ab} = 0,$$

or

$$E - E_0 = \Delta E = \sum_{ai} \langle \Phi_0 | \hat{H} | \Phi_i^a \rangle C_i^a + \sum_{abij} \langle \Phi_0 | \hat{H} | \Phi_{ij}^{ab} \rangle C_{ij}^{ab},$$

where the energy E_0 is the reference energy and ΔE defines the so-called correlation energy. The single-particle basis functions could be the results of a Hartree-Fock calculation or just the eigenstates of the non-interacting part of the Hamiltonian.

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Rewriting the FCI equation

In our notes on Hartree-Fock calculations, we have already computed the matrix $\langle \Phi_0 | \hat{H} | \Phi_i^a \rangle$ and $\langle \Phi_0 | \hat{H} | \Phi_{ij}^{ab} \rangle$. If we are using a Hartree-Fock basis, then the matrix elements $\langle \Phi_0 | \hat{H} | \Phi_i^a \rangle = 0$ and we are left with a *correlation energy* given by

$$E - E_0 = \Delta E^{HF} = \sum_{abij} \langle \Phi_0 | \hat{H} | \Phi_{ij}^{ab} \rangle C_{ij}^{ab}.$$

Rewriting the FCI equation

Inserting the various matrix elements we can rewrite the previous equation as

$$\Delta E = \sum_{ai} \langle i | \hat{f} | a \rangle C_i^a + \sum_{abij} \langle ij | \hat{v} | ab \rangle C_{ij}^{ab}.$$

This equation determines the correlation energy but not the coefficients C .

Rewriting the FCI equation, does not stop here

We need more equations. Our next step is to set up

$$\langle \Phi_i^a | \hat{H} - E | \Phi_0 \rangle + \sum_{bj} \langle \Phi_i^a | \hat{H} - E | \Phi_j^b \rangle C_j^b + \sum_{bcjk} \langle \Phi_i^a | \hat{H} - E | \Phi_{jk}^{bc} \rangle C_{jk}^{bc} + \sum_{bcdjkl} \langle \Phi_i^a | \hat{H} - E | \Phi_{jkl}^{bcd} \rangle C_{jkl}^{bcd} = 0,$$

as this equation will allow us to find an expression for the coefficients C_i^a since we can rewrite this equation as

$$\langle i | \hat{f} | a \rangle + \langle \Phi_i^a | \hat{H} | \Phi_i^a \rangle C_i^a + \sum_{bj \neq ai} \langle \Phi_i^a | \hat{H} | \Phi_j^b \rangle C_j^b + \sum_{bcjk} \langle \Phi_i^a | \hat{H} | \Phi_{jk}^{bc} \rangle C_{jk}^{bc} + \sum_{bcdjkl} \langle \Phi_i^a | \hat{H} | \Phi_{jkl}^{bcd} \rangle C_{jkl}^{bcd} = E C_i^a.$$

Rewriting the FCI equation, please stop here

We see that on the right-hand side we have the energy E . This leads to a non-linear equation in the unknown coefficients. These equations are normally solved iteratively (that is we can start with a guess for the coefficients C_i^a). A common choice is to use perturbation theory for the first guess, setting thereby

$$C_i^a = \frac{\langle i | \hat{f} | a \rangle}{\epsilon_i - \epsilon_a}.$$

Rewriting the FCI equation, more to add

The observant reader will however see that we need an equation for C_{jk}^{bc} and C_{jkl}^{bcd} as well. To find equations for these coefficients we need then to continue our multiplications from the left with the various Φ_H^P terms.

For C_{jk}^{bc} we need then

$$\begin{aligned} & \langle \Phi_{ij}^{ab} | \hat{H} - E | \Phi_0 \rangle + \sum_{kc} \langle \Phi_{ij}^{ab} | \hat{H} - E | \Phi_k^c \rangle C_k^c + \\ & \sum_{cdkl} \langle \Phi_{ij}^{ab} | \hat{H} - E | \Phi_{kl}^{cd} \rangle C_{kl}^{cd} + \sum_{cdeklm} \langle \Phi_{ij}^{ab} | \hat{H} - E | \Phi_{klm}^{cde} \rangle C_{klm}^{cde} + \sum_{cdefklmn} \langle \Phi_{ij}^{ab} | \hat{H} - E | \Phi_{klmn}^{cdef} \rangle C_{klmn}^{cdef} = 0, \end{aligned}$$

and we can isolate the coefficients C_{kl}^{cd} in a similar way as we did for the coefficients C_i^a .

Rewriting the FCI equation, more to add

A standard choice for the first iteration is to set

$$C_{ij}^{ab} = \frac{\langle ij|\hat{v}|ab\rangle}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}.$$

At the end we can rewrite our solution of the Schroedinger equation in terms of n coupled equations for the coefficients C_H^P . This is a very cumbersome way of solving the equation. However, by using this iterative scheme we can illustrate how we can compute the various terms in the wave operator or correlation operator \hat{C} . We will later identify the calculation of the various terms C_H^P as parts of different many-body approximations to full CI. In particular, we can relate this non-linear scheme with Coupled Cluster theory and many-body perturbation theory.

Summarizing FCI and bringing in approximative methods

If we can diagonalize large matrices, FCI is the method of choice since:

- It gives all eigenvalues, ground state and excited states
- The eigenvectors are obtained directly from the coefficients C_H^P which result from the diagonalization
- We can compute easily expectation values of other operators, as well as transition probabilities
- Correlations are easy to understand in terms of contributions to a given operator beyond the Hartree-Fock contribution. This is the standard approach in many-body theory.

Definition of the correlation energy

The correlation energy is defined as, with a two-body Hamiltonian,

$$\Delta E = \sum_{ai} \langle i|\hat{f}|a\rangle C_i^a + \sum_{abij} \langle ij|\hat{v}|ab\rangle C_{ij}^{ab}.$$

The coefficients C result from the solution of the eigenvalue problem. The energy of say the ground state is then

$$E = E_{ref} + \Delta E,$$

where the so-called reference energy is the energy we obtain from a Hartree-Fock calculation, that is

$$E_{ref} = \langle \Phi_0|\hat{H}|\Phi_0\rangle.$$

FCI equation and the coefficients

However, as we have seen, even for a small case like the four first major shells and a nucleus like oxygen-16, the dimensionality becomes quickly intractable. If we wish to include single-particle states that reflect weakly bound systems, we need a much larger single-particle basis. We need thus approximative methods that sum specific correlations to infinite order.

Popular methods are

- Many-body perturbation theory (in essence a Taylor expansion)
- Coupled cluster theory (coupled non-linear equations)
- Green's function approaches (matrix inversion)
- Similarity group transformation methods (coupled ordinary differential equations)

All these methods start normally with a Hartree-Fock basis as the calculational basis.

Example case: pairing Hamiltonian

Now we take the following Hamiltonian

$$\hat{H} = \sum_n n\delta\hat{N}_n - G\hat{P}^\dagger\hat{P}$$

where

$$\hat{N}_n = \hat{a}_{n,m=+1/2}^\dagger \hat{a}_{n,m=+1/2} + \hat{a}_{n,m=-1/2}^\dagger \hat{a}_{n,m=-1/2}$$

and

$$\hat{P}^\dagger = \sum_n \hat{a}_{n,m=+1/2}^\dagger \hat{a}_{n,m=-1/2}^\dagger$$

We can write down the 6×6 Hamiltonian in the basis from the prior slide:

$$H = \begin{pmatrix} 2\delta - 2G & -G & -G & -G & -G & 0 \\ -G & 4\delta - 2G & -G & -G & -0 & -G \\ -G & -G & 6\delta - 2G & 0 & -G & -G \\ -G & -G & 0 & 6\delta - 2G & -G & -G \\ -G & 0 & -G & -G & 8\delta - 2G & -G \\ 0 & -G & -G & -G & -G & 10\delta - 2G \end{pmatrix}$$

(You should check by hand that this is correct.)

For $\delta = 0$ we have the closed form solution of the g.s. energy given by $-6G$.

Coupled cluster theory

The coupled cluster method is an efficient tool to compute atomic nuclei with an effort that grows polynomial with system size. While this might still be expensive, it is now possible to compute nuclei with mass numbers about $A > 200$ with this method. Recall that full configuration interaction (FCI) such as the no-core shell model exhibits an exponential cost and is therefore limited to light nuclei.

The normal-ordered Hamiltonian

We start from the reference state

$$|\Phi_0\rangle = \prod_{i=1}^A a_i^\dagger |0\rangle \quad (2)$$

for the description of a nucleus with mass number A . Usually, this reference is the Hartree-Fock state, but that is not necessary. In the shell-model picture, it could also be a product state where the lowest A harmonic oscillator states are occupied. Here and in what follows, the indices i, j, k, \dots run over hole states, i.e. orbitals occupied in the reference state (2), while a, b, c, \dots 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 A is of course the number of occupied states. We consider the Hamiltonian

$$H = \sum_{pq} \varepsilon_q^p a_p^\dagger a_q + \frac{1}{4} \sum_{pqrs} \langle pq|V|rs\rangle a_p^\dagger a_q^\dagger a_s a_r \quad (3)$$

The reference state (2) 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

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

Here,

$$f_q^p = \varepsilon_q^p + \sum_i \langle pi|V|qi\rangle \quad (5)$$

is the Fock matrix. We note that the Fock matrix is diagonal in the Hartree-Fock basis. The brackets $\{\dots\}$ in Eq. (4) denote normal ordering, i.e. all operators that annihilate the nontrivial vacuum (2) are to the right of those operators that create with respect to that vacuum. Normal ordering implies that $\langle \Phi_0|H_N|\Phi_0\rangle = 0$.

*

Exercise 1: Practice in normal ordering

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

Hint.

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

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

$$\sum_{pq} \varepsilon_q^p a_p^\dagger a_q = \sum_{ab} \varepsilon_b^a a_a^\dagger a_b + \sum_{ai} \varepsilon_i^a a_a^\dagger a_i + \sum_{ai} \varepsilon_a^i a_i^\dagger a_a + \sum_{ij} \varepsilon_j^i a_i^\dagger a_j \quad (7)$$

$$= \sum_{ab} \varepsilon_b^a a_a^\dagger a_b + \sum_{ai} \varepsilon_i^a a_a^\dagger a_i + \sum_{ai} \varepsilon_a^i a_i^\dagger a_a + \sum_{ij} \varepsilon_j^i (-a_j a_i^\dagger + \delta_i^j) \quad (8)$$

$$= \sum_{ab} \varepsilon_b^a a_a^\dagger a_b + \sum_{ai} \varepsilon_i^a a_a^\dagger a_i + \sum_{ai} \varepsilon_a^i a_i^\dagger a_a - \sum_{ij} \varepsilon_j^i a_j a_i^\dagger + \sum_i \varepsilon_i^i \quad (9)$$

$$= \sum_{pq} \varepsilon_q^p \{a_p^\dagger a_q\} + \sum_i \varepsilon_i^i \quad (10)$$

=====

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

$$E_{HF} \equiv \langle \Phi_0 | H | \Phi_0 \rangle = \sum_i \varepsilon_i^i + \frac{1}{2} \sum_{ij} \langle ij | V | ij \rangle \quad (11)$$

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.

*

Exercise 2: 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 (5) 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 A orbitals are filled.

=====

If symmetry-restricted Hartree-Fock is used, one is limited to compute nuclei with closed subshells for neutrons and for protons. On a first view, this might seem as a severe limitation. But is it?

*

Exercise 3: 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 $N, Z = 2, 6, 8, 14, 16, 20, 28, 32, 34, 40, 50, \dots$

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

$$|\Psi\rangle = e^T |\Phi_0\rangle, \quad (12)$$

Here, T is an operator that induces correlations. We can now demand that the correlated state (12) becomes an 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 Schrödinger equation with e^{-T} and find

$$\overline{H_N} |\Phi_0\rangle = E_c |\Phi_0\rangle. \quad (13)$$

Here, E_c is the correlation energy, and the total energy is $E = E_c + E_{HF}$. The similarity-transformed Hamiltonian is defined as

$$\overline{H_N} \equiv e^{-T} H_N e^T. \quad (14)$$

A more productive view on coupled-cluster theory thus emerges: This method seeks a similarity transformation such that the uncorrelated reference state (2) becomes an exact eigenstate of the similarity-transformed Hamiltonian (14).

*

Exercise 4: 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, coupled cluster theory employs a non-Hermitian Hamiltonian.

*

Exercise 5: 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

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

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.

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

$$\overline{H_N} = \sum_{\alpha} |R_\alpha\rangle E_\alpha \langle L_\alpha| \quad (15)$$

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

=====

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

$$T \equiv \sum_{ia} t_i^a a_a^\dagger a_i + \frac{1}{4} \sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i + \dots + \frac{1}{(A!)^2} \sum_{i_1 \dots i_A a_1 \dots a_A} t_{i_1 \dots i_A}^{a_1 \dots a_A} a_{a_1}^\dagger \dots a_{a_A}^\dagger a_{i_A} \dots a_{i_1}. \quad (16)$$

Thus, the operator (16) 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 amplitudes t_i^a , t_{ij}^{ab} , ..., $t_{i_1, \dots, i_A}^{a_1, \dots, a_A}$.

*

Exercise 6: 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

$$\sum_{n=0}^A \binom{n_u}{n} \binom{A}{A-n} = \binom{A+n_u}{A}. \quad (17)$$

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

=====

Thus, the coupled-cluster method with the full cluster operator (16) 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

$$T \equiv \sum_{ia} t_i^a a_a^\dagger a_i + \frac{1}{4} \sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i. \quad (18)$$

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

$$|\Phi_i^a\rangle = a_a^\dagger a_i |\Phi_0\rangle, \quad (19)$$

$$|\Phi_{ij}^{ab}\rangle = a_a^\dagger a_b^\dagger a_j a_i |\Phi_0\rangle \quad (20)$$

be 1p-1h and 2p-2h excitations of the reference. Computing matrix elements of the Schroedinger Equation (13) yields

$$\langle \Phi_0 | \overline{H}_N | \Phi_0 \rangle = E_c, \quad (21)$$

$$\langle \Phi_i^a | \overline{H}_N | \Phi_0 \rangle = 0, \quad (22)$$

$$\langle \Phi_{ij}^{ab} | \overline{H}_N | \Phi_0 \rangle = 0. \quad (23)$$

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. (21).

We note that in the CCSD approximation the reference state is not an exact eigenstate. Rather, it is decoupled from simple states but \overline{H} still connects this state to 3p-3h, and 4p-4h states etc.

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 correlation 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.

*

Exercise 7: Why is CCD not exact?

Above we argued that a similarity transformation preserves all eigenvalues. Nevertheless, the CCD correlation energy is not the exact correlation energy. Explain!

Answer. 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. (21), and the computation of the correlation energy requires us to compute matrix elements of the similarity-transformed Hamiltonian (14). This can be done with the Baker-Campbell-Hausdorff expansion

$$\overline{H_N} = e^{-T} H_N e^T \quad (24)$$

$$= H_N + [H_N, T] + \frac{1}{2!} [[H_N, T], T] + \frac{1}{3!} [[[H_N, T], T], T] + \dots \quad (25)$$

We now come to a key element of coupled-cluster theory: the cluster operator (16) 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 (24) can only be non-zero because each T must connect to H_N (but no T with another T). Thus, the expansion is finite.

*

Exercise 8: 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 $\overline{H_N}$?

Answer. 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 .

=====

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.

We write the similarity-transformed Hamiltonian as

$$\overline{H_N} = \sum_{pq} \overline{H}_q^p a_q^\dagger a_p + \frac{1}{4} \sum_{pqrs} \overline{H}_{rs}^{pq} a_p^\dagger a_q^\dagger a_s a_r + \dots \quad (26)$$

with

$$\overline{H}_q^p \equiv \langle p | \overline{H}_N | q \rangle, \quad (27)$$

$$\overline{H}_{rs}^{pq} \equiv \langle pq | \overline{H}_N | rs \rangle. \quad (28)$$

Thus, the CCSD Eqs. (21) for the amplitudes can be written as $\overline{H}_i^a = 0$ and $\overline{H}_{ij}^{ab} = 0$.

*

Exercise 9: Compute the matrix element $\overline{H}_{ab}^{ij} \equiv \langle ij | \overline{H}_N | ab \rangle$

Answer. This is a simple task. This matrix element is part of the operator $\overline{H}_{ab}^{ij} a_i^\dagger a_j^\dagger a_b a_a$, 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 $\overline{H}_{ab}^{ij} = \langle ij | V | ab \rangle$.

=====

We need to work out the similarity-transformed Hamiltonian of Eq. (24). 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

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

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.

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

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

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

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 diagrams come in handy.

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Diagrams. The pictures in this Subsection are taken from Crawford and Schaefer.

By convention, hole lines (labels i, j, k, \dots) are pointing down.

By convention, particle lines (labels a, b, c, \dots) are pointing up.

Let us look at the one-body operator of the normal-ordered Hamiltonian, i.e. Fock matrix. Its diagrams are as follows.

We now turn to the two-body interaction. It is denoted as a horizontal dashed line with incoming and outgoing lines attached to it. We start by noting that the following diagrams of the interaction are all related by permutation symmetry.

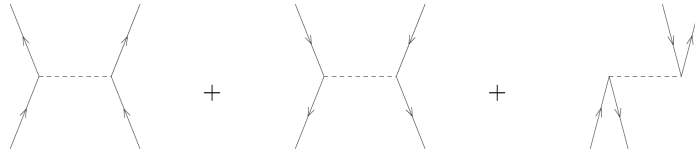
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Exercise 10: Assign the correct matrix element $\langle pq|V|rs\rangle$ to each of the following diagrams of the interaction

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

paragraphparagraph>paragraph>-0.5em

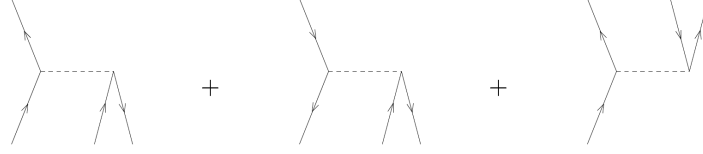
a)



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

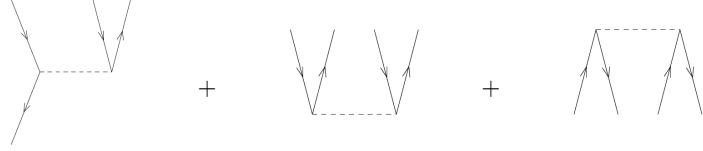
paragraphparagraph>paragraph>-0.5em

b)



Answer. $\langle ai|V|bc\rangle + \langle ij|V|ka\rangle + \langle ab|V|ci\rangle$
 paragraphparagraph>paragraph>-0.5em

c)



Answer. $\langle ia|V|jk\rangle + \langle ab|V|ij\rangle + \langle ij|V|ab\rangle$
 =====

Finally, we have the following diagrams for the T_1 and T_2 amplitudes.

We are now in the position to construct the diagrams of the similarity-transformed Hamiltonian, keeping in mind that these diagrams correspond to matrix elements of \overline{H}_N . The rules are as follows.

1. Write down all *topologically different* diagrams corresponding to the desired matrix element. Topologically different diagrams differ in the number and type of lines (particle or hole) that connect the Fock matrix F or the interaction V to the cluster amplitudes T , but not whether these connections are left or right (as those are related by antisymmetry). As an example, all diagrams in Fig. 7 are topologically identical, because they consist of incoming particle and hole lines and of outgoing particle and hole lines.
2. Write down the matrix elements that enter the diagram, and sum over all internal lines.
3. The overall sign is (-1) to the power of [(number of hole lines) – (number of loops)].

4. Symmetry factor: For each pair of equivalent lines (i.e. lines that connect the same two operators) multiply with a factor $1/2$. For n identical vertices, multiply the algebraic expression by the symmetry factor $1/n!$ to account properly for the number of ways the diagram can be constructed.
5. Antisymmetrize the outgoing and incoming lines as necessary.

Please note that this really works. You could derive these rules for yourself from the commutations and factors that enter the Baker-Campbell-Hausdorff expansion. The sign comes obviously from the arrangement of creation and annihilation operators, while the symmetry factor stems from all the different ways, one can contract the cluster operator with the normal-ordered Hamiltonian.

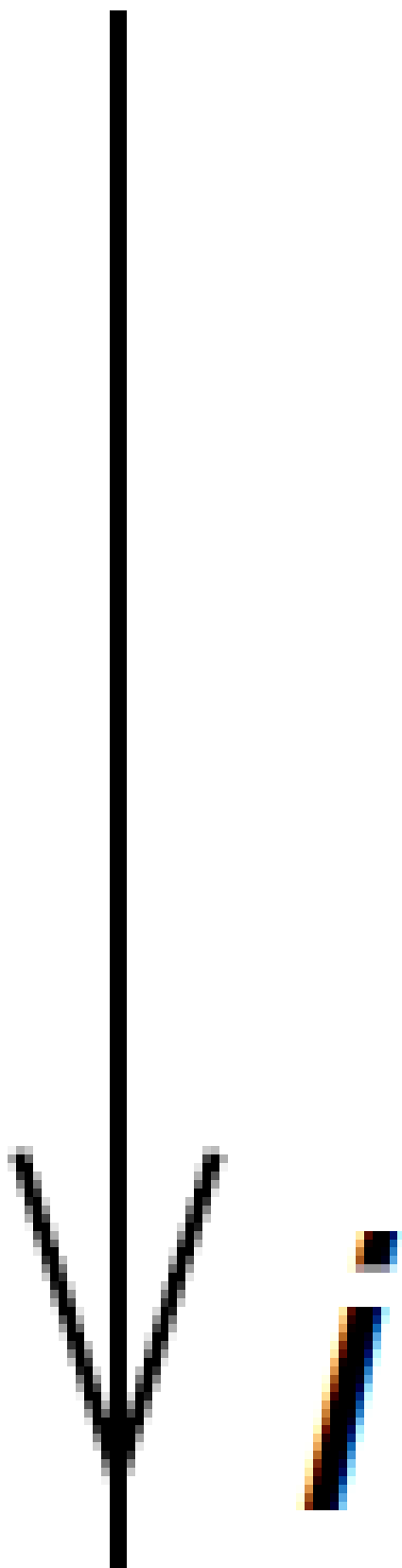
Example: CCSD correlation energy

The CCSD correlation energy, $E_c = \langle \Phi_0 | \overline{H_N} | \Phi_0 \rangle$, is the first of the CCSD equations (21). It is a vacuum expectation value and thus consists of all diagrams with no external legs. There are three such diagrams:

The corresponding algebraic expression is $E_c = \sum_{ia} f_a^i t_i^a + \frac{1}{4} \sum_{ijab} \langle ij | V | ab \rangle t_{ij}^{ab} + \frac{1}{2} \sum_{ijab} \langle ij | V | ab \rangle t_i^a t_j^b$.

The first algebraic expression is clear. We have one hole line and one loop, giving it a positive sign. There are no equivalent lines or vertices, giving it no symmetry factor. The second diagram has two loops and two hole lines, again leading to a positive sign. We have a pair of equivalent hole lines and a pair of equivalent particle lines, each giving a symmetry factor of $1/2$. The third diagram has two loops and two hole lines, again leading to a positive sign. We have two identical vertices (each connecting to a T_1 in the same way) and thus a symmetry factor $1/2$.

=====



1

a

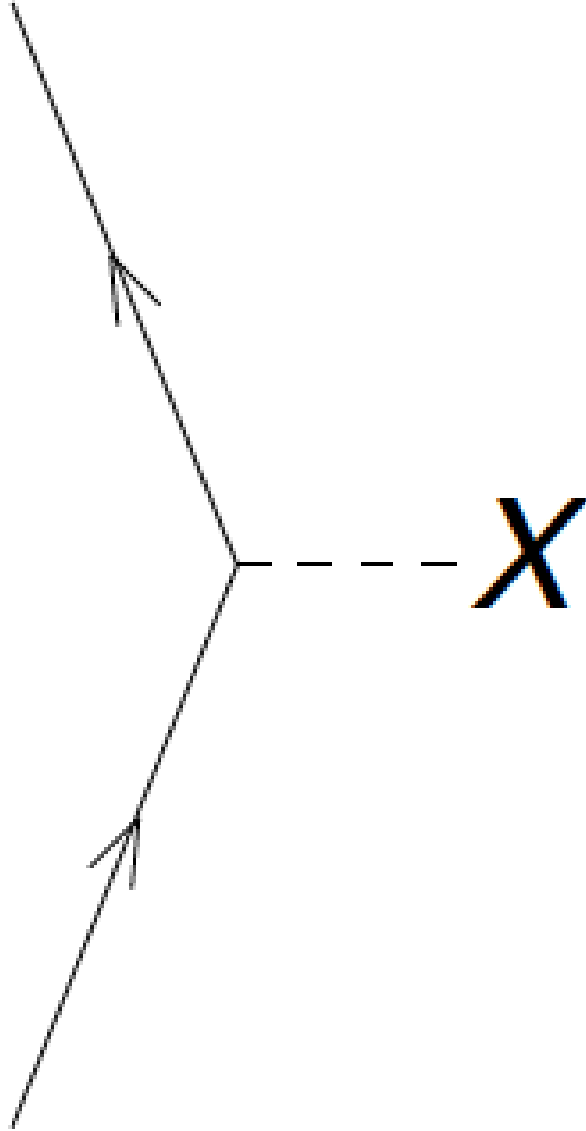


Figure 3: The diagrams corresponding to f_a^b . The dashed line with the 'X' denotes the interaction F between the incoming and outgoing lines. The labels a and b are not denoted, but you should label the outgoing and incoming lines accordingly.

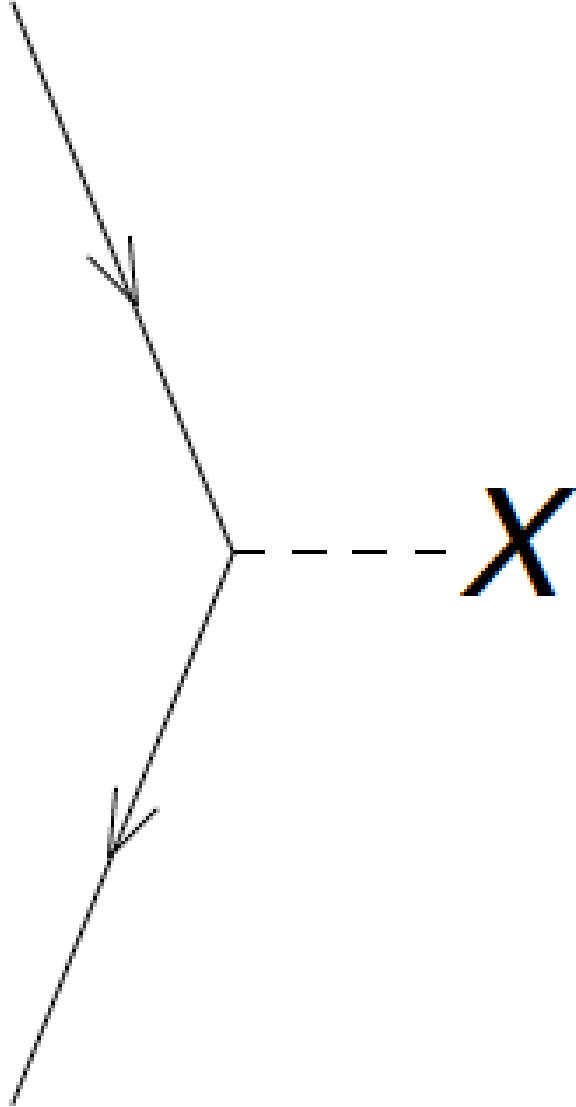


Figure 4: The diagrams corresponding to f_i^j . The dashed line with the 'X' denotes the interaction F between the incoming and outgoing lines.

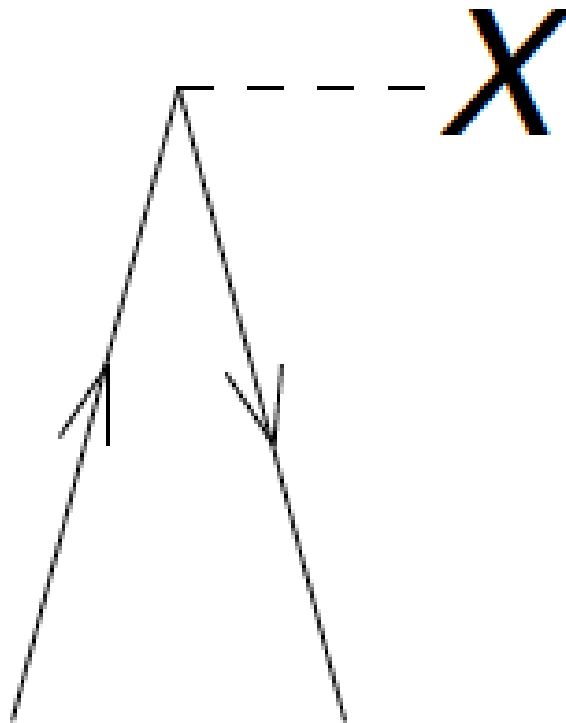


Figure 5: The diagrams corresponding to f_a^i . The dashed line with the 'X' denotes the interaction F between the incoming and outgoing lines.

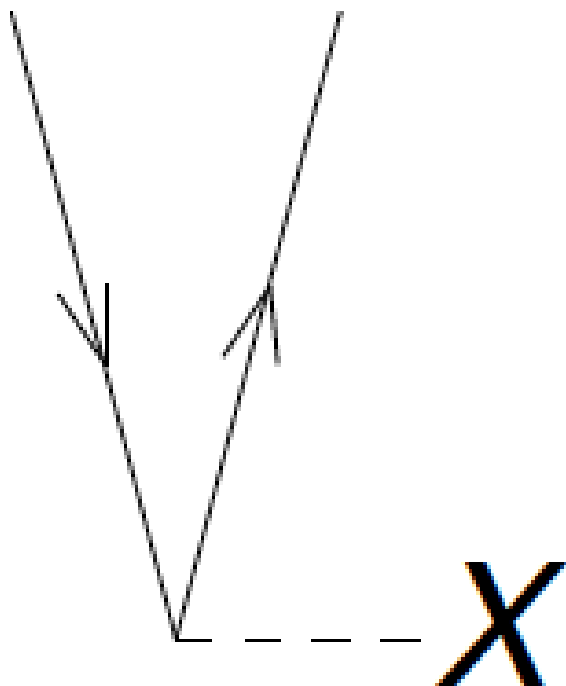


Figure 6: The diagrams corresponding to f_i^a . The dashed line with the 'X' denotes the interaction F between the incoming and outgoing lines.

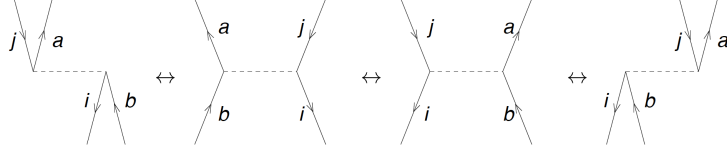


Figure 7: The diagrams corresponding to $\langle ai|V|jb\rangle = -\langle ai|V|bj\rangle = -\langle ia|V|jb\rangle = \langle ia|V|bj\rangle$.

$$\hat{T}_1 = \sum_{ia} t_i^a \{a_a^\dagger a_i\} = \text{diagram with two lines meeting at a vertex, one incoming from the left and one outgoing to the right, with a horizontal full line below them}$$

$$\hat{T}_2 = \frac{1}{4} \sum_{ijab} t_{ij}^{ab} \{a_a^\dagger a_b^\dagger a_j a_i\} = \text{diagram with two vertices connected by a horizontal full line, each vertex having two lines meeting at it, one incoming from the left and one outgoing to the right}$$

Figure 8: The horizontal full line is the cluster amplitude with incoming hole lines and outgoing particle lines as indicated.

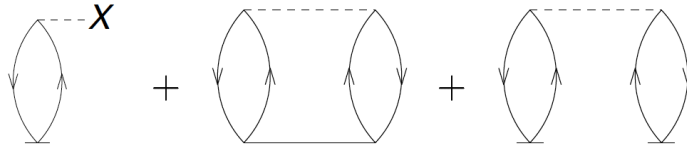


Figure 9: Three diagrams enter for the CCSD correlation energy, i.e. all diagrams that leave no external legs.

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 $\bar{H}_i^a = 0$. 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).

*

Exercise 11: Derive the CCD equations!

Let us consider the matrix element \bar{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.

Hint. Start systematically! Consider all combinations of F and V diagrams with 0, 1, and 2 cluster amplitudes T_2 .

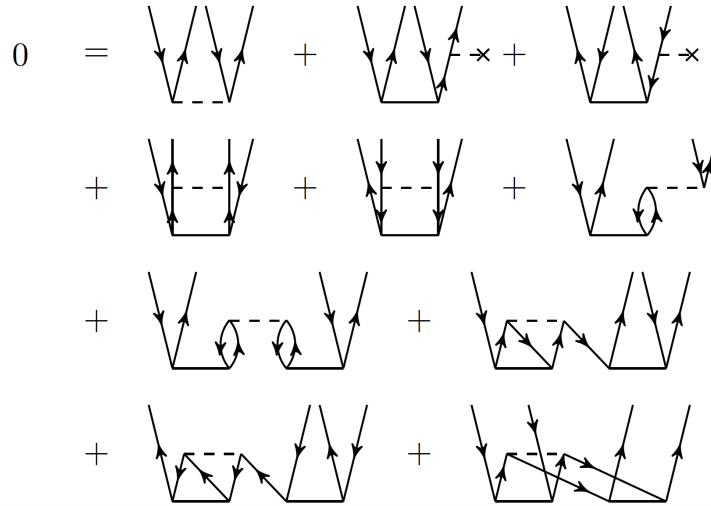


Figure 10: The diagrams for the T_2 equation, i.e. the matrix elements of \bar{H}_{ij}^{ab} . Taken from Baardsen et al (2013).

Answer. The corresponding algebraic expression is

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

=====

Let us now turn to the computational cost of a CCD computation.

*

Exercise 12: Computational scaling of CCD

For each of the diagrams in Fig. 10 write down the computational cost in terms of the number of occupied A and the number of unoccupied n_u orbitals.

Answer. 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.

=====

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 Fig. 10. We break up the computation into two steps, computing first the intermediate

$$\chi_{ij}^{kl} \equiv \frac{1}{2} \sum_{cd} \langle kl|V|cd\rangle t_{ij}^{cd} \quad (29)$$

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

$$\frac{1}{2} \sum_{kl} \chi_{ij}^{kl} t_{kl}^{ab} \quad (30)$$

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.”

*

Exercise 13: Factorize the remaining diagrams of the CCD equation
Diagrams 7, 8, and 9 of Fig. 10 also need to be factorized.

Answer. For diagram number 7, we compute

$$\chi_{id}^{al} \equiv \sum_{kc} \langle kl|V|cd \rangle t_{ik}^{ac} \quad (31)$$

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

$$\frac{1}{2} P(ij) P(ab) \sum_{ld} \chi_{id}^{al} t_{lj}^{db} \quad (32)$$

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

For diagram number 8, we compute

$$\chi_i^l \equiv -\frac{1}{2} \sum_{kcd} \langle kl|V|cd \rangle t_{ik}^{cd} \quad (33)$$

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

$$-P(ij) \sum_l \chi_i^l t_{lj}^{ab} \quad (34)$$

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

For diagram number 9, we compute

$$\chi_d^a \equiv \frac{1}{2} \sum_{kcl} \langle kl|V|cd \rangle t_{kl}^{ac} \quad (35)$$

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

$$P(ab) \sum_d \chi_d^a t_{ij}^{db} \quad (36)$$

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

=====

We are now ready, to derive the full CCSD equations, i.e. the matrix elements of \overline{H}_i^a and \overline{H}_{ij}^{ab} .

*

Project 14: (Optional) Derive the CCSD equations!

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a) Let us consider the matrix element \overline{H}_i^a first. Clearly, it consists of all diagrams (i.e. all combinations of T_1 , T_2 , and a single F or V that have an incoming hole line and an outgoing particle line. Write down all these diagrams.

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

Figure 11: The diagrams for the T_1 equation, i.e. the matrix elements of \overline{H}_i^a . Taken from Crawford and Schaefer. Here $\langle pq || rs \rangle \equiv \langle pq | V | rs \rangle$ and $f_{pq} \equiv f_q^p$.

Answer.

paragraphparagraph>paragraph>-0.5em

b) Let us now consider the matrix element \overline{H}_{ij}^{ab} . Clearly, it consists of all diagrams (i.e. all combinations of T_1 , T_2 , and a single F or V that have two incoming hole lines and two outgoing particle lines. Write down all these diagrams and corresponding algebraic expressions.

=====

We can now turn to the solution of the coupled-cluster equations.

Solving the CCD equations

The CCD equations, depicted in Fig. 10, 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

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

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

$$t_{ij}^{ab} = t_{ij}^{ab} + \frac{\overline{H}_{ij}^{ab}}{f_i^i + f_j^j - f_a^a - f_b^b} \quad (37)$$

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

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

Figure 12: The diagrams for the T_2 equation, i.e. the matrix elements of \overline{H}_{ij}^{ab} . Taken from Crawford and Schaefer. Here $\langle pq||rs\rangle \equiv \langle pq|V|rs\rangle$, $f_{pq} \equiv f_q^p$, and $P(ab) = 1 - (a \leftrightarrow b)$ antisymmetrizes.

to a solution. We take the perturbative result

$$(t_{ij}^{ab})_0 = \frac{\langle ab|V|ij\rangle}{f_i^i + f_j^j - f_a^a - f_b^b} \quad (38)$$

as a starting point, compute \overline{H}_{ij}^{ab} , and find a new t_{ij}^{ab} from the right-hand side of Eq. (37). 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. We can then 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. (38), and solve Eq. (37) 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.