The Potato and its dynamics

by

Øyvind Sigmundson Schøyen

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Abstract

This is an abstract text.

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Chapter 1

Introduction

Start your chapter by writing something smart. Then go get coffee.

Part I

Theory

Chapter 2

Quantum Mechanics

> YOLO
>
> P. A. M. Dirac

2.1 Density matrices

When working with many-body quantum mechanics, computing expectation values can at times prove easier when done using density matrices. A general density matrix of a *pure state* is on the form

$$\hat{\rho} = |\psi\rangle\langle\psi|, \tag{2.1}$$

that is, a pure state is a quantum state $|\psi\rangle$ containing the maximum amount of information about a given system. For a *mixed state*, i.e., a linear combination of pure states $|\psi_k\rangle$ with a classical probability p_k associated with the state, we get a density matrix on the form

$$\hat{\rho} = \sum_k p_k |\psi_k\rangle\langle\psi_k|. \tag{2.2}$$

Any density operator must satisfy the following properties [7]:

1. Hermiticity, that is

   $$p_k = p_k^* \implies \hat{\rho} = \hat{\rho}^\dagger. \tag{2.3}$$

   This translates to the probabilities being real, $p_k \in \mathbb{R}$.

2. Positivity,

   $$p_k \geqslant 0 \implies \langle\chi|\hat{\rho}|\chi\rangle \geqslant 0. \tag{2.4}$$

   In other words, density matrices are *positive semidefinite*.

3. Normalization of the probabilities,

$$\sum_k p_k = 1 \implies \mathrm{Tr}(\hat{\rho}), \tag{2.5}$$

   that is, the probabilities must sum up to one.

Furthermore, by squaring the density matrix and taking the trace we can infer if the system we are perusing is in a mixed state or a pure state [7].

$$\mathrm{Tr}(\hat{\rho}^2) = \sum_k p_k^2 \leqslant 1, \tag{2.6}$$

with equality if, and only if, the system is in a pure state, viz.

$$\hat{\rho} = |\psi\rangle\langle\psi| \implies \hat{\rho}^2 = \hat{\rho} \implies \mathrm{Tr}(\hat{\rho}^2) = 1. \tag{2.7}$$

Using density matrices, we can compute the expectation value of any operator $\hat{O}$, by [7]

$$\left\langle \hat{O} \right\rangle = \mathrm{Tr}(\hat{O}\hat{\rho}). \tag{2.8}$$

2.1.1 Many-body density matrices

In a seminal paper by Löwdin [8], the concept of a many-body density matrix in terms of the orbitals of a Slater determinant is discussed. These are dubbed N-body density matrices, where N depends on the N-body interaction, that is, the number of particles included in the interaction. Of the most useful for our work, we have the one- and two-body density matrices. As we will work almost exclusively in second quantization, we will follow the derivation of the one- and two-body density matrices done by Helgaker, Jørgensen, and Olsen. Löwdin's paper [8] did not employ second quantization, and all matrices are expressed in the coordinate representation. We will list these as they arrive.

Chapter 3

Formalism

Given a basis of L single particle functions $|p\rangle$ where

$$\{|p\rangle\}_{p=1}^{L} = \{|i\rangle\}_{i=1}^{N} \cup \{|a\rangle\}_{a=N+1}^{L} . \tag{3.1}$$

Here $i, j, k, \dots$ represents the N first occupied states of the reference Slater determinant whereas $a, b, c, \dots$ represent the remaining $M = L - N$ virtual states in the total basis $p, q, r, \dots$[1].

---

[1] Occupied and virtual states are also known as hole and particle states if we treat the reference Slater determinant as the *Fermi level*

Chapter 4

Hartree-Fock theory

One can not tackle the subject of many-body theory without meeting the Hartree-Fock approximation. It serves as an excellent initial approximation, and in many cases the *only* approximation, to the many-body wavefunction for a given system. It is a rather inexpensive approximation, in terms of computational intensity, and explains much of the underlying physics of a given system of many particles.

4.1 Deriving the Hartree-Fock equations

The main goal of the Hartree-Fock approximation is to solve the time-independent Schrödinger equation,

$$\hat{H}|\Psi\rangle = E|\Psi\rangle, \tag{4.1}$$

for a given Hamiltonian, $\hat{H}$. The goal of Hartree-Fock is to find the "best" wavefunction, $|\Psi\rangle$, under the constraints that it consists of a single Slater determinant,

$$|\Psi\rangle = |\Phi\rangle = |\phi_1 \dots \phi_N\rangle \tag{4.2}$$

where $\{\phi_i\}_{i=1}^{L}$ is the basis of unknown *molecular orbitals*, and N is the number of occupied orbitals.

Chapter 5

Configuration interaction

A popular post Hartree-Fock method is *configuration interaction*. It consists of expressing the wavefunction as a linear combination of excited Slater determinants in a truncated single-particle and Slater determinant basis.

$$|\Psi_{CI}\rangle = A_0|\Phi\rangle + \sum_{ai} A_i^a|\Phi_i^a\rangle + \frac{1}{4}\sum_{abij} A_{ij}^{ab}|\Phi_{ij}^{ab}\rangle + \dots, \tag{5.1}$$

where we have divided by a factor 4 in the double sum to avoid over counting as both the coefficients and the excited determinants are antisymmetric. By generating all the possible Slater determinants from the L single-particle functions we employ the *full configuration interaction* method. This will give the most accurate value of the energy for the system, but quickly becomes computationally impossible as the FCI space grows in dimensions as $\binom{L}{N}$. [6]

5.1 Time-independent configuration interaction theory

We start with the time-independent Schrödinger equation

$$\hat{H}|\Psi_J\rangle = E_J|\Psi_J\rangle, \tag{5.2}$$

where $(E_J, |\Psi_J\rangle)$ is an eigenpair for $\hat{H}$. Expanding the CI wavefunction in a Slater determinant basis.

$$|\Psi_J\rangle = \sum_K A_{KJ}|\Phi_K\rangle, \tag{5.3}$$

where A_{KJ} are the amplitudes for a certain excitation K for a specific energy level J. Inserting Equation 5.3 into Equation 5.2 and left projecting on a state

$|\Phi_I\rangle$ we get

$$\sum_K \langle \Phi_I|\hat{H}|\Phi_K\rangle A_{KJ} = E_J \sum_K \langle \Phi_I|\Phi_K\rangle A_{KJ}. \tag{5.4}$$

We now define the Hamiltonian matrix $H_{IK} = \langle \Phi_I|\hat{H}|\Phi_K\rangle$ and the overlap matrix $S_{IK} = \langle \Phi_I|\Phi_K\rangle$. We can thus formulate the generalized eigenvalue equation

$$\sum_K H_{IK} A_{KJ} = E_J \sum_K S_{IK} A_{KJ} \tag{5.5}$$

$$\implies HA = ESA, \tag{5.6}$$

where $S_{IK} = 1 \iff \langle \Phi_I|\Phi_K\rangle = \delta_{IK}$. We will in this text only care about systems where the Slater determinants are orthonormal. Thus the eigenvalue equation we will solve will be

$$HA = EA, \tag{5.7}$$

which means our job is to construct H_{IJ} and diagonalize the matrix[4]. The elements H_{IJ} are computed by

$$\langle \Phi_I|\hat{H}|\Phi_J\rangle = \sum_{pq} \langle p|\hat{h}|q\rangle \langle \Phi_I|\hat{p}^\dagger \hat{q}|\Phi_J\rangle + \frac{1}{4}\sum_{pqrs} \langle pq||rs\rangle \langle \Phi_I|\hat{p}^\dagger \hat{q}^\dagger \hat{s}\hat{r}|\Phi_J\rangle. \tag{5.8}$$

Chapter 6

Coupled cluster theory

In coupled cluster theory one seeks to approximate the “true” many-body wavefunction using an *exponential ansatz*.

$$|\Psi_{CC}\rangle \equiv e^{\hat{T}}|\Phi\rangle = \sum_{n=0}^{\infty} \frac{1}{n!}\hat{T}^n|\Phi\rangle, \tag{6.1}$$

where the *cluster operator* $\hat{T}$ is given by a sum of excitation operators $\hat{T}_p$.

$$\hat{T} = \sum_{p=1}^{n} \hat{T}_p = \tau_i^a \hat{a}^\dagger \hat{i} + \left(\frac{1}{2!}\right)^2 \tau_{ij}^{ab} \hat{a}^\dagger \hat{b}^\dagger \hat{i}\hat{j} + \left(\frac{1}{3!}\right)^2 \tau_{ijk}^{abc} \hat{a}^\dagger \hat{b}^\dagger \hat{c}^\dagger \hat{i}\hat{j}\hat{k} + \dots. \tag{6.2}$$

Here the *coupled cluster amplitudes* $\tau_{ij\dots}^{ab\dots}$ are the unknowns. As the method only uses a single reference Slater determinant in Equation 6.1 the approximation is called single-reference coupled cluster theory.

Part II

Appendices

Appendix A

Hartree-Fock

Hartree-Fock appendix.

Appendix B

Coupled cluster equations

In this appendix we will show the explicit equations used for ground state calculations in coupled cluster for different truncation levels.

B.1 Coupled cluster doubles

The energy for the doubles truncation is given by

$$E_{CCD} = E_0 + \langle \Phi | e^{-\hat{T}_2} H_N e^{\hat{T}_2} | \Phi \rangle = E_0 + \frac{1}{4} t^{cd}_{kl} u^{kl}_{cd}. \tag{B.1}$$

The doubles amplitude equations is given by[10]

$$\begin{aligned} 0 = g(f, u, t) &\equiv \langle \Phi^{ab}_{ij} | e^{-\hat{T}_2} H_N e^{\hat{T}_2} | \Phi \rangle \qquad \text{(B.2)} \\ &= u^{ab}_{ij} + f^b_c t^{ac}_{ij} P(ab) - f^k_j t^{ab}_{ik} P(ij) + \frac{1}{2} t^{cd}_{ij} u^{ab}_{cd} + \frac{1}{2} t^{ab}_{kl} u^{kl}_{ij} \\ &\quad + t^{ac}_{ik} u^{bk}_{jc} P(ab) P(ij) + \frac{1}{4} t^{cd}_{ij} t^{ab}_{kl} u^{kl}_{cd} + t^{ac}_{ik} t^{bd}_{jl} u^{kl}_{cd} P(ij) \\ &\quad - \frac{1}{2} t^{ab}_{lj} t^{dc}_{ik} u^{kl}_{cd} P(ij) - \frac{1}{2} t^{ac}_{lk} t^{db}_{ij} u^{kl}_{cd} P(ab). \qquad \text{(B.3)} \end{aligned}$$

In order to reduce the number of FLOPS when contracting the tensors, we introduce so-called *intermediates*[3]. In practice, this consists of precomputing some of the terms by choosing which tensors to contract first. In the doubles approximation there are four sensible intermediates we can define[1].

$$g(f,u,t) \leftarrow \frac{1}{4}t_{ij}^{cd}t_{kl}^{ab}u_{cd}^{kl} + \frac{1}{2}t_{ij}^{cd}u_{cd}^{ab} = t_{ij}^{cd}\left(\frac{1}{4}t_{kl}^{ab}u_{cd}^{kl} + \frac{1}{2}u_{cd}^{ab}\right) = t_{ij}^{cd}W_{cd}^{ab}, \tag{B.4}$$

$$g(f,u,t) \leftarrow \frac{1}{2}t_{jk}^{cd}t_{il}^{ab}u_{cd}^{kl}P(ij) = t_{il}^{ab}\left(\frac{1}{2}t_{jk}^{cd}u_{cd}^{kl}\right)P(ij) = t_{il}^{ab}W_{j}^{l}P(ij), \tag{B.5}$$

$$g(f,u,t) \leftarrow \frac{1}{2}t_{ij}^{ac}t_{kl}^{bd}u_{cd}^{kl}P(ab) = t_{ij}^{ac}\left(\frac{1}{2}t_{kl}^{bd}u_{cd}^{kl}\right)P(ab) = t_{ij}^{ac}W_{c}^{b}P(ab). \tag{B.6}$$

The last intermediate requires a little work, as we have to insert an extra exchange operator, $P(ij)$, in one of the terms in order to group two terms into a single intermediate.

$$g(f,u,t) \leftarrow t_{ik}^{ac}t_{jl}^{bd}u_{cd}^{kl}P(ab) + t_{ik}^{ac}u_{jc}^{bk}P(ab)P(ij) \tag{B.7}$$

$$= t_{ik}^{ac}\left(\frac{1}{2}t_{jl}^{bd}u_{cd}^{kl} + u_{jc}^{bk}\right)P(ab)P(ij) \tag{B.8}$$

$$= t_{ik}^{ac}W_{jc}^{bk}P(ab)P(ij). \tag{B.9}$$

We summarize the expression for the intermediates in Table B.1, along with their computational complexity. The total right-hand side of the t-amplitudes in the doubles approximation using the intermediate calculations is thus

$$\begin{aligned} g(f,u,t) = {}& f_{c}^{b}t_{ij}^{ac}P(ab) - f_{j}^{k}t_{ik}^{ab}P(ij) + t_{ij}^{cd}W_{cd}^{ab} + t_{il}^{ab}W_{j}^{l}P(ij) \\ & + t_{ik}^{ac}W_{jc}^{bk}P(ab)P(ij) - t_{ij}^{ac}W_{c}^{b}P(ab) + \frac{1}{2}t_{kl}^{ab}u_{ij}^{kl} + u_{ij}^{ab}. \end{aligned} \tag{B.10}$$

The most time-consuming contraction is now the term $t_{ij}^{cd}W_{cd}^{ab}$. This term uses $\mathcal{O}(m^4n^2)$ FLOPS, which is a reduction from $\mathcal{O}(m^4n^4)$ when computing $t_{ij}^{cd}t_{kl}^{ab}u_{cd}^{kl}$ directly.

B.2 Coupled cluster singles doubles

The energy for the singles-doubles truncation is given by

$$E_{CCSD} = E_0 + \langle\Phi|e^{-\hat{T}_1-\hat{T}_2}H_N e^{\hat{T}_1+\hat{T}_2}|\Phi\rangle \tag{B.11}$$

$$= E_0 + f_{c}^{k}t_{k}^{c} - \frac{1}{2}t_{l}^{c}t_{k}^{d}u_{cd}^{kl} + \frac{1}{4}t_{kl}^{cd}u_{cd}^{kl}. \tag{B.12}$$

---

[1] Note that we use the notation "←" to signify part of the expression, i.e., some of the terms contained in the function.

Table B.1: In this table we summarize the intermediates used in the t-amplitudes of the coupled cluster doubles approximation. We also list the computational complexity in FLOPS needed to construct the intermediate. Recall that n is the number of holes and m the number of particles.

Intermediate	Complexity [FLOPS]
$W^{ab}_{cd} = \frac{1}{4} t^{ab}_{kl} u^{kl}_{cd} + \frac{1}{2} u^{ab}_{cd}$	$\mathcal{O}(m^4 n^2)$
$W^{l}_{j} = \frac{1}{2} t^{cd}_{jk} u^{kl}_{cd}$	$\mathcal{O}(m^2 n^3)$
$W^{b}_{c} = \frac{1}{2} t^{bd}_{kl} u^{kl}_{cd}$	$\mathcal{O}(m^3 n^2)$
$W^{bk}_{jc} = \frac{1}{2} t^{bd}_{jl} u^{kl}_{cd} + u^{bk}_{jc}$	$\mathcal{O}(m^3 n^3)$

The singles amplitude equations becomes

$$
\begin{aligned}
0 &= \langle \Phi^{a}_{i} | e^{-\hat{T}_1 - \hat{T}_2} H_N e^{\hat{T}_1 + \hat{T}_2} | \Phi \rangle \qquad \text{(B.13)} \\
&= f^{a}_{i} - f^{k}_{c} t^{c}_{i} t^{a}_{k} + f^{k}_{c} t^{ac}_{ik} - f^{k}_{i} t^{a}_{k} + f^{a}_{c} t^{c}_{i} - t^{c}_{k} t^{d}_{i} t^{a}_{l} u^{kl}_{cd} - t^{c}_{k} t^{d}_{i} u^{ak}_{cd} \\
&\quad + t^{c}_{k} t^{a}_{l} u^{kl}_{ic} + t^{c}_{k} t^{ad}_{il} u^{kl}_{cd} + t^{c}_{k} u^{ak}_{ic} - \frac{1}{2} t^{c}_{i} t^{ad}_{kl} u^{kl}_{cd} \\
&\quad + \frac{1}{2} t^{a}_{l} t^{cd}_{ik} u^{kl}_{cd} + \frac{1}{2} t^{cd}_{ik} u^{ak}_{cd} - \frac{1}{2} t^{ac}_{kl} u^{kl}_{ic}. \qquad \text{(B.14)}
\end{aligned}
$$

The doubles amplitude equations are

$$
\begin{aligned}
0 &= \langle \Phi^{ab}_{ij} | e^{-\hat{T}_1 - \hat{T}_2} H_N e^{\hat{T}_1 + \hat{T}_2} | \Phi \rangle \qquad \text{(B.15)} \\
&= f^{k}_{c} t^{c}_{i} t^{ab}_{jk} P(ij) + f^{k}_{c} t^{a}_{k} t^{bc}_{ij} P(ab) + f^{k}_{i} t^{ab}_{jk} P(ij) - f^{a}_{c} t^{bc}_{ij} P(ab) \\
&\quad + t^{c}_{k} t^{d}_{i} t^{ab}_{jl} u^{kl}_{cd} P(ij) + t^{c}_{k} t^{a}_{l} t^{bd}_{ij} u^{kl}_{cd} P(ab) - t^{c}_{k} t^{ad}_{ij} u^{bk}_{cd} P(ab) \\
&\quad + t^{c}_{k} t^{ab}_{il} u^{kl}_{jc} P(ij) + t^{c}_{i} t^{d}_{j} t^{a}_{k} t^{b}_{l} u^{kl}_{cd} + t^{c}_{i} t^{d}_{j} t^{a}_{k} u^{bk}_{cd} P(ab) + \frac{1}{2} t^{c}_{i} t^{d}_{j} t^{ab}_{kl} u^{kl}_{cd} 1 \\
&\quad + t^{c}_{i} t^{d}_{j} u^{ab}_{cd} - t^{c}_{i} t^{a}_{k} t^{b}_{l} u^{kl}_{jc} P(ij) - t^{c}_{i} t^{a}_{k} t^{bd}_{jl} u^{kl}_{cd} P(ab) P(ij) \\
&\quad - t^{c}_{i} t^{a}_{k} u^{bk}_{jc} P(ab) P(ij) - t^{c}_{i} t^{ad}_{jk} u^{bk}_{cd} P(ab) P(ij) - \frac{1}{2} t^{c}_{i} t^{ab}_{kl} u^{kl}_{jc} P(ij) \\
&\quad - t^{c}_{i} u^{ab}_{jc} P(ij) + \frac{1}{2} t^{a}_{k} t^{b}_{l} t^{cd}_{ij} u^{kl}_{cd} + t^{a}_{k} t^{b}_{l} u^{kl}_{ij} + \frac{1}{2} t^{a}_{k} t^{cd}_{ij} u^{bk}_{cd} 1 P(ab) \\
&\quad + t^{a}_{k} t^{bc}_{il} u^{kl}_{jc} P(ab) P(ij) + t^{a}_{k} u^{bk}_{ij} P(ab) + \frac{1}{4} t^{cd}_{ij} t^{ab}_{kl} u^{kl}_{cd} 1 + \frac{1}{2} t^{cd}_{ij} u^{ab}_{cd} \\
&\quad + \frac{1}{2} t^{cd}_{jk} t^{ab}_{il} u^{kl}_{cd} P(ij) + t^{ac}_{ik} t^{bd}_{jl} u^{kl}_{cd} P(ab) + t^{ac}_{ik} u^{bk}_{jc} P(ab) P(ij) \\
&\quad - \frac{1}{2} t^{ac}_{ij} t^{bd}_{kl} u^{kl}_{cd} P(ab) + \frac{1}{2} t^{ab}_{kl} u^{kl}_{ij} 1 + u^{ab}_{ij}. \qquad \text{(B.16)}
\end{aligned}
$$

B.3 Coupled cluster doubles triples

The energy of the doubles-triples truncation is given by

$$\begin{aligned} E_{CCDT} &= E_0 + \langle \Phi | e^{-\hat{T}_2 - \hat{T}_3} H_N e^{\hat{T}_2 + \hat{T}_3} | \Phi \rangle && \text{(B.17)} \\ &= E_0 + \frac{1}{4} t_{lm}^{de} u_{de}^{lm}. && \text{(B.18)} \end{aligned}$$

The doubles amplitude equations are

$$\begin{aligned} 0 &= \langle \Phi_{ij}^{ab} | e^{-\hat{T}_2 - \hat{T}_3} H_N e^{\hat{T}_2 + \hat{T}_3} | \Phi \rangle && \text{(B.19)} \\ &= f_d^l t_{ijl}^{abd} + f_i^l t_{jl}^{ab} P(ij) - f_d^a t_{ij}^{bd} P(ab) + \frac{1}{4} t_{ij}^{de} t_{lm}^{ab} u_{de}^{lm} \\ &\quad + \frac{1}{2} t_{ij}^{de} u_{de}^{ab} + \frac{1}{2} t_{jl}^{de} t_{im}^{ab} u_{de}^{lm} P(ij) + t_{il}^{ad} t_{jm}^{be} u_{de}^{lm} P(ab) \\ &\quad + t_{il}^{ad} u_{jd}^{bl} P(ab) P(ij) - \frac{1}{2} t_{ij}^{ad} t_{lm}^{be} u_{de}^{lm} P(ab) + \frac{1}{2} t_{lm}^{ab} u_{ij}^{lm} \\ &\quad + \frac{1}{2} t_{ijl}^{ade} u_{de}^{bl} P(ab) - \frac{1}{2} t_{ilm}^{abd} u_{jd}^{lm} P(ij) + u_{ij}^{ab}. && \text{(B.20)} \end{aligned}$$

Now to the beast...

The triples amplitude equations are

$$0 = \langle \Phi_{ijk}^{abc} | e^{-\hat{T}_2 - \hat{T}_3} H_N e^{\hat{T}_2 + \hat{T}_3} | \Phi \rangle \tag{B.21}$$

$$\begin{aligned}
&= f_d^l t_{ij}^{ad} t_{kl}^{bc} P(ab)P(ik) + f_d^l t_{il}^{ab} t_{jk}^{cd} P(ij) + f_d^l t_{kl}^{ab} t_{ij}^{cd} + f_d^l t_{jl}^{ac} t_{ik}^{bd} P(ab) \\
&\quad - f_i^l t_{jkl}^{abc} P(ij) - f_k^l t_{ijl}^{abc} + f_d^a t_{ijk}^{bcd} P(ab) + f_d^c t_{ijk}^{abd} \\
&\quad + \frac{1}{2} t_{il}^{de} t_{jkm}^{abc} u_{de}^{lm} P(ij) + \frac{1}{2} t_{ij}^{de} t_{kl}^{ab} u_{de}^{cl} - \frac{1}{2} t_{ij}^{de} t_{kl}^{ac} u_{de}^{bl} P(ab) \\
&\quad + \frac{1}{4} t_{ij}^{de} t_{klm}^{abc} u_{de}^{lm} - \frac{1}{4} t_{ik}^{de} t_{jlm}^{abc} u_{de}^{lm} P(ij) + \frac{1}{2} t_{jk}^{de} t_{il}^{ab} u_{de}^{cl} P(ij) \\
&\quad - \frac{1}{2} t_{jk}^{de} t_{il}^{ac} u_{de}^{bl} P(ab)P(ij) + \frac{1}{2} t_{kl}^{de} t_{ijm}^{abc} u_{de}^{lm} + \frac{1}{2} t_{lm}^{ad} t_{ijk}^{bce} u_{de}^{lm} P(ab) \\
&\quad + t_{il}^{ad} t_{jm}^{bc} u_{kd}^{lm} P(ab) + t_{il}^{ad} t_{jk}^{ce} u_{de}^{bl} P(ab)P(ij) + t_{il}^{ad} t_{jkm}^{bce} u_{de}^{lm} P(ab)P(ij) \\
&\quad - t_{ij}^{ad} t_{kl}^{be} u_{de}^{cl} P(ab) + t_{ij}^{ad} t_{kl}^{ce} u_{de}^{bl} P(ab) + \frac{1}{2} t_{ij}^{ad} t_{klm}^{bce} u_{de}^{lm} P(ab) \\
&\quad - t_{ij}^{ad} u_{kd}^{bc} P(ab) + t_{ik}^{ad} t_{jl}^{be} u_{de}^{cl} P(ab)P(ij) + \frac{1}{2} t_{ik}^{ad} t_{lm}^{bc} u_{jd}^{lm} P(ab)P(ij) \\
&\quad - t_{ik}^{ad} t_{jl}^{ce} u_{de}^{bl} P(ab)P(ij) - \frac{1}{2} t_{ik}^{ad} t_{jlm}^{bce} u_{de}^{lm} P(ab)P(ij) + t_{ik}^{ad} u_{jd}^{bc} P(ab)P(ij) \\
&\quad + t_{kl}^{ad} t_{ij}^{ce} u_{de}^{bl} P(ab) + t_{kl}^{ad} t_{ijm}^{bce} u_{de}^{lm} P(ab) - \frac{1}{2} t_{lm}^{ab} t_{ij}^{cd} u_{kd}^{lm} \\
&\quad + \frac{1}{2} t_{lm}^{ab} t_{ik}^{cd} u_{jd}^{lm} P(ij) + \frac{1}{4} t_{lm}^{ab} t_{ijk}^{cde} u_{de}^{lm} + t_{il}^{ab} t_{jm}^{cd} u_{kd}^{lm} P(ij) \\
&\quad - t_{il}^{ab} t_{km}^{cd} u_{jd}^{lm} P(ij) + \frac{1}{2} t_{il}^{ab} t_{jkm}^{cde} u_{de}^{lm} P(ij) + t_{il}^{ab} u_{jk}^{cl} P(ij) \\
&\quad + t_{kl}^{ab} t_{im}^{cd} u_{jd}^{lm} P(ij) + \frac{1}{2} t_{kl}^{ab} t_{ijm}^{cde} u_{de}^{lm} + t_{kl}^{ab} u_{ij}^{cl} \\
&\quad + \frac{1}{2} t_{lm}^{ac} t_{ij}^{bd} u_{kd}^{lm} P(ab) - \frac{1}{4} t_{lm}^{ac} t_{ijk}^{bde} u_{de}^{lm} P(ab) - t_{il}^{ac} t_{jm}^{bd} u_{kd}^{lm} P(ab) \\
&\quad + t_{il}^{ac} t_{km}^{bd} u_{jd}^{lm} P(ab)P(ij) - \frac{1}{2} t_{il}^{ac} t_{jkm}^{bde} u_{de}^{lm} P(ab)P(ij) - t_{il}^{ac} u_{jk}^{bl} P(ab)P(ij) \\
&\quad - t_{kl}^{ac} t_{im}^{bd} u_{jd}^{lm} P(ab)P(ij) - \frac{1}{2} t_{kl}^{ac} t_{ijm}^{bde} u_{de}^{lm} P(ab) - t_{kl}^{ac} u_{ij}^{bl} P(ab) \\
&\quad - t_{ij}^{cd} u_{kd}^{ab} + t_{ik}^{cd} u_{jd}^{ab} P(ij) - \frac{1}{2} t_{lm}^{ce} t_{ijk}^{abd} u_{de}^{lm} \\
&\quad + t_{im}^{ce} t_{jkl}^{abd} u_{de}^{lm} P(ij) - \frac{1}{2} t_{ij}^{ce} t_{klm}^{abd} u_{de}^{lm} + \frac{1}{2} t_{ik}^{ce} t_{jlm}^{abd} u_{de}^{lm} P(ij) \\
&\quad + t_{km}^{ce} t_{ijl}^{abd} u_{de}^{lm} + \frac{1}{2} t_{ijk}^{ade} u_{de}^{bc} P(ab) + t_{ijl}^{abd} u_{kd}^{cl} \\
&\quad - t_{ikl}^{abd} u_{jd}^{cl} P(ij) + \frac{1}{2} t_{ilm}^{abc} u_{jk}^{lm} P(ij) + \frac{1}{2} t_{klm}^{abc} u_{ij}^{lm} \\
&\quad - t_{ijl}^{acd} u_{kd}^{bl} P(ab) + t_{ikl}^{acd} u_{jd}^{bl} P(ab)P(ij) + \frac{1}{2} t_{ijk}^{cde} u_{de}^{ab}.
\end{aligned} \tag{B.22}$$

Appendix C

Reformulating the amplitude equations as matrix products

We will in this appendix show how to formulate the tensor contractions occuring in the coupled cluster equations as matrix products. The reason we wish to do this is to be able to perform these contractions as dot products (or matrix products) as there exists highly optimized code performing these operations, e.g., BLAS[1].

To be able to treat tensors of rank > 2 as matrices we have to create *compound indices* by stacking the dimensions after one another. For instance, by looking at the tensor $g \in \mathbb{C}^{I\times J\times K\times L}$, where we denote a single element by g_{ijkl}. Here g is a tensor of rank 4. By creating compound indices $\tilde{I} = IJ$ and $\tilde{K} = KL$ we can create a new tensor $\tilde{g} = \mathbb{C}^{\tilde{I}\times\tilde{K}}$ of rank 2 (represented as a matrix). Using the indices $\tilde{i} = iJ + j$ and $\tilde{k} = kL + l$ we now construct $\tilde{g}$ in such a way that $\tilde{g}_{\tilde{i}\tilde{k}} = g_{ijkl}$.

It is also possible to create compound indices of more than two indices. For instance; choosing $\tilde{J} = JKL$ and setting $\tilde{j} = jKL + kL + l$ we can construct $\bar{g} = \mathbb{C}^{I\times\tilde{J}}$ where $\bar{g}_{i\tilde{j}} = g_{ijkl}$.

For the sake of brevity and clarity we will in the following avoid renaming the compound indices and their sizes, but we will instead indicate with a comma where we construct new indices.

C.1 Reformulating the CCD equations

C.2 Reformulating the CCSD equations

We use the expressions for the CCSD equations derived by Gauss et al.[1]. We start with the *effective double excitation amplitudes* found at the bottom of table 3 in their article. Note that we rename $\tilde{\tau} \to \xi$, thus reserving the twiddle for intermediate calculations.

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[1] BLAS can be found here: http://www.netlib.org/blas/

$$\tau_{ij}^{ab} = t_{ij}^{ab} + \frac{1}{2}P(ij)P(ab)t_i^a t_j^b \tag{C.1}$$

$$\implies \tau_{ab,ij} = t_{ab,ij} + \frac{1}{2}P(ij)P(ab)\left(t_{a,i}t_{b,j}\right)_{ab,ij}, \tag{C.2}$$

$$\xi_{ij}^{ab} = t_{ij}^{ab} + \frac{1}{4}P(ij)P(ab)t_i^a t_j^b \tag{C.3}$$

$$\implies \xi_{ab,ij} = t_{ab,ij} + \frac{1}{4}P(ij)P(ab)\left(t_{a,i}t_{b,j}\right)_{ab,ij}. \tag{C.4}$$

Next we look at the one-body intermediates found at the top of table 3 in the article by Gauss et al.[1]. We use the notation

$$u_{ef}^{am} \equiv \langle am||ef\rangle, \tag{C.5}$$

that is, we treat the matrix elements u as the antisymmetric matrix elements of the two-body operator.

$$F_e^a = f_e^a - \frac{1}{2}f_e^m t_m^a + t_m^f u_{ef}^{am} - \frac{1}{2}\xi_{mn}^{af} u_{ef}^{mn} \tag{C.6}$$

$$\implies F_{a,e} = f_{a,e} - \frac{1}{2}t_{a,m}f_{m,e} + \left(t_{fm}\tilde{u}_{fm,ae}\right)_{a,e} - \frac{1}{2}\xi_{a,fmn}\tilde{u}_{fmn,e}, \tag{C.7}$$

$$F_i^m = f_i^m + \frac{1}{2}f_e^m t_i^e + t_n^e u_{ie}^{mn} + \frac{1}{2}\xi_{in}^{ef} u_{ef}^{mn} \tag{C.8}$$

$$\implies F_{m,i} = f_{m,i} + \frac{1}{2}f_{m,e}t_{e,i} + \left(t_{en}\tilde{u}_{en,mi}\right)_{m,i} + \frac{1}{2}\tilde{u}_{m,nef}\tilde{\xi}_{nef,i}, \tag{C.9}$$

$$F_e^m = f_e^m + t_n^f u_{ef}^{mn} \tag{C.10}$$

$$\implies F_{m,e} = f_{m,e} + \left(t_{fn}\tilde{u}_{fn,me}\right)_{m,e}. \tag{C.11}$$

We now move on to the two-body intermediates found just below the one-body intermediates in table 3 in the article by Gauss et al.[1]. To avoid storing two matrices with M^4 elements we will not create the intermediate W_{ef}^{ab} but rather compute the products in place in the amplitude equations by splitting up the products and do them one-by-one (this will shown in due time). We will therefore still preserve the asymptotical scaling $\mathcal{O}(M^4N^2)$ but add a constant term at the price of saving memory.

Appendix D

Computing one-body density matrices

From Kvaal[5] we have an expression for the one-body density matrices ρ^q_p[1] as a function of the coupled cluster amplitudes t and λ.

$$\rho^q_p = \langle \tilde{\Psi} | \hat{p}^\dagger \hat{q} | \Psi \rangle = \langle \tilde{\Phi} | (1 + \Lambda) e^{-T} \hat{p}^\dagger \hat{q} e^T | \Phi \rangle. \tag{D.1}$$

We wish to find an expression for ρ^q_p in terms of the amplitudes t and λ which we can contract. We start by splitting up the expression to

$$\rho^q_p = \langle \tilde{\Phi} | e^{-T} \hat{p}^\dagger \hat{q} e^T | \Phi \rangle + \langle \tilde{\Phi} | \Lambda e^{-T} \hat{p}^\dagger \hat{q} e^T | \Phi \rangle. \tag{D.2}$$

Next we expand the exponentials and use the Baker-Campbell-Hausdorff formula. This lets us write

$$e^{-T} \hat{p}^\dagger \hat{q} e^T = \hat{p}^\dagger \hat{q} + \left[\hat{p}^\dagger \hat{q}, T \right] + \frac{1}{2!} \left[\left[\hat{p}^\dagger \hat{q}, T \right], T \right] + \dots. \tag{D.3}$$

To determine how many terms to include we have to look at the number of excitations that will be performed by the excitation operators T and relaxation operators Λ. We know that T will *at least* excite the reference by 1. The combined operator $\hat{p}^\dagger \hat{q}$ is able to excite and relax the reference with at most 1 or leave it unchanged. The relaxation operator Λ will *at least* relax the reference by 1. As $\langle \tilde{\Phi}_X | \Phi_Y \rangle = \delta_{XY}$, where X and Y are arbitrary excitations, the only non-zero contributions to ρ^q_p will be the operator combinations that leave the reference unchanged after applying the total operator chain. For the term without Λ in ρ^q_p this leaves us with

$$\langle \tilde{\Phi} | e^{-T} \hat{p}^\dagger \hat{q} e^T | \Phi \rangle = \langle \tilde{\Phi} | \hat{p}^\dagger \hat{q} | \Phi \rangle + \langle \tilde{\Phi} | \left[\hat{p}^\dagger \hat{q}, T \right] | \Phi \rangle, \tag{D.4}$$

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[1] Note the ordering of the indices. We use the same convention as Kvaal in his article.

where the last term of the commutator will not contribute as leaving a T on the left hand side of $\hat{p}^\dagger\hat{q}$ will leave the reference excited.

$$\langle\tilde{\Phi}|\Lambda e^{-T}\hat{p}^\dagger\hat{q}e^{T}|\Phi\rangle = \langle\tilde{\Phi}|\Lambda\hat{p}^\dagger\hat{q}|\Phi\rangle + \langle\tilde{\Phi}|\Lambda\left[\hat{p}^\dagger\hat{q}, T\right]|\Phi\rangle + \frac{1}{2!}\langle\tilde{\Phi}|\Lambda\left[\left[\hat{p}^\dagger\hat{q}, T\right], T\right]|\Phi\rangle + \dots. \tag{D.5}$$

Depending on the truncation level of the coupled cluster equations, e.g., singles, doubles etc, this will provide a natural truncation for Equation D.5.

D.1 The one-body density matrix for doubles excitation

In the doubles truncation, the only contribution to Equation D.5 will be

$$\langle\tilde{\Phi}|\Lambda e^{-T}\hat{p}^\dagger\hat{q}e^{T}|\Phi\rangle = \langle\tilde{\Phi}|\Lambda\left[\hat{p}^\dagger\hat{q}, T\right]|\Phi\rangle. \tag{D.6}$$

This happens as the first term in Equation D.5 will at best leave the reference relaxed by 1 as $\hat{p}^\dagger\hat{q}$ can only excite a single particle. The next commutator will suffer the same effect, but in reverse. Two T operators will leave the reference in a +4 state, $\hat{p}^\dagger\hat{q}$ will at best relax this to a +3 state. Then, Λ, will only be able to relax the total down to a +1, thus annihilating the overlap. The one-body density matrix for coupled cluster doubles is then

$$\rho^q_p = \langle\tilde{\Phi}|\hat{p}^\dagger\hat{q}|\Phi\rangle + \langle\tilde{\Phi}|\left[\hat{p}^\dagger\hat{q}, T\right]|\Phi\rangle + \langle\tilde{\Phi}|\Lambda\left[\hat{p}^\dagger\hat{q}, T\right]|\Phi\rangle \tag{D.7}$$

$$= \delta^q_j\delta^i_p\left(\delta^j_i + \frac{1}{2}l^{ik}_{ab}t^{ab}_{kj}\right) - \frac{1}{2}\delta^q_b\delta^a_p l^{ij}_{ac}t^{cb}_{ij}. \tag{D.8}$$

We note that there are no contribution to the terms with an occupied and a virtual index, that is, $\rho^i_a = \rho^a_i = 0$. This is a direct consequence of the lack of single excitations. The density operators $\hat{a}^\dagger\hat{\imath}$ and $\hat{\imath}^\dagger\hat{a}$ will excite and relax a single particle respectively. But, Λ and T only works on pairs therefore leaving the reference oddly excited or relaxed thus annihilating the overlap.

D.2 The one-body density matrix for singles and doubles excitations

For coupled cluster singles-and-doubles Equation D.5 will truncate at the double commutator as written. Employing SymPy[9] we can compute an expression for the one-body density matrices.

$$
\begin{aligned}
\rho_p^q &= \langle\tilde{\Phi}|\hat{p}^\dagger\hat{q}|\Phi\rangle + \langle\tilde{\Phi}|\left[\hat{p}^\dagger\hat{q}, T\right]|\Phi\rangle + \langle\tilde{\Phi}|\Lambda\hat{p}^\dagger\hat{q}|\Phi\rangle \\
&\quad + \langle\tilde{\Phi}|\Lambda\left[\hat{p}^\dagger\hat{q}, T\right]|\Phi\rangle + \frac{1}{2!}\langle\tilde{\Phi}|\Lambda\left[\left[\hat{p}^\dagger\hat{q}, T\right], T\right]|\Phi\rangle \qquad \text{(D.9)} \\
&= \delta_p^a\delta_b^q\left(l_a^i t_i^b + \frac{1}{2}l_{ac}^{ij}t_{ij}^{bc}\right) + \delta_p^a\delta_i^q l_a^i + \delta_j^q\delta_p^i\left(\delta_i^j - l_a^j t_i^a + \frac{1}{2}l_{ab}^{jk}t_{ki}^{ab}\right) \\
&\quad + \delta_a^q\delta_p^i\left(t_i^a + l_b^j\left[t_{ij}^{ab} - t_i^b t_j^a\right] + \frac{1}{2}t_i^b l_{cb}^{kj}t_{kj}^{ac} - \frac{1}{2}t_j^a l_{cb}^{kj}t_{ki}^{cb}\right). \qquad \text{(D.10)}
\end{aligned}
$$

In this expression we have only kept the fully contracted terms. SymPy sets the indices arbitrarily so the expression shown in Equation D.10 has been factorized and had a relabeling of the indices for improved readability.

Appendix E

Overlap between time-evolved coupled cluster wavefunctions

We compute the overlap of any wavefunction from an initial state at time t_0 to a later time t by

$$P(t_0 \to t) \equiv |\langle \psi(t)|\psi(t_0)\rangle|^2. \tag{E.1}$$

That is, we compute the squared overlap between the initial state $|\psi(t_0)\rangle$ and the final state $|\psi(t)\rangle$. In the case of coupled cluster and the use of the bivariational principle some care must be taken as to how the squared overlap should be computed. We get

$$P(t_0 \to t) \equiv |\langle \tilde{\Psi}(t)|\Psi(t_0)\rangle|^2 = \langle \tilde{\Psi}(t)|\Psi(t_0)\rangle\langle \tilde{\Psi}(t_0)|\Psi(t)\rangle. \tag{E.2}$$

This is a consequence of treating the two different Hilbert spaces indepedently. Choosing $t_0 = 0$ as the ground state we can compute the overlap of the ground state to all later states t. For time-independent spin-orbitals we only evolve the amplitudes in time. We thus have to find an expression for the two inner-products below.

$$\langle \tilde{\Psi}(t)|\Psi(0)\rangle = \langle \tilde{\Phi}| \left[1 + \hat{\Lambda}(t)\right] e^{-\hat{T}(t)} e^{\hat{T}} |\Phi\rangle, \tag{E.3}$$

$$\langle \tilde{\Psi}(0)|\Psi(t)\rangle = \langle \tilde{\Phi}| \left[1 + \hat{\Lambda}\right] e^{-\hat{T}} e^{\hat{T}(t)} |\Phi\rangle. \tag{E.4}$$

Note that $\hat{T}(t) \neq \hat{T}$ and $\hat{\Lambda}(t) \neq \hat{\Lambda}$. We split up the equations on $\hat{\Lambda}$ and expand the exponentials. As $\hat{T}$ provides a net excitation of at least 1 and $\hat{\Lambda}$ a net relaxation of at least 1[1], only terms with a combination of $\hat{\Lambda}$ and $\hat{T}$ will survive. This yields

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[1] Note that this applies to the time-dependent versions of these operators as well. It is only the amplitudes that are time-dependent and not the creation nor the annihilation operators.

$$\begin{aligned}\langle\tilde{\Psi}(t)|\Psi(0)\rangle &= \langle\tilde{\Phi}|e^{-\hat{T}(t)}e^{\hat{T}}|\Phi\rangle + \langle\tilde{\Phi}|\hat{\Lambda}(t)e^{-\hat{T}(t)}e^{\hat{T}}|\Phi\rangle && \text{(E.5)}\\ &= 1 + \sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\frac{1}{n!m!}\langle\tilde{\Phi}|\hat{\Lambda}(t)[-\hat{T}(t)]^n\hat{T}^m|\Phi\rangle. && \text{(E.6)}\end{aligned}$$

The conjugate of this equation is then

$$\langle\tilde{\Psi}(0)|\Psi(t)\rangle = 1 + \sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\frac{1}{n!m!}\langle\tilde{\Phi}|\hat{\Lambda}\left[-\hat{T}^n\right]\hat{T}(t)^m|\Phi\rangle. \tag{E.7}$$

E.1 Time-dependent overlap for the coupled cluster doubles wavefunction

E.2 Time-dependent overlap for the coupled cluster singles-and-doubles wavefuntion

Restricting ourselves to the singles and doubles approximation we will get that the $\hat{T}$ operator can yield a net excitation of 1 and 2, whereas $\hat{\Lambda}$ yields a net relaxation of 1 and 2. This truncates the infinite sums to $n, m \in \{0, 1, 2\}$. We get

$$\langle\tilde{\Psi}(t)|\Psi(0)\rangle = 1 + \langle\tilde{\Phi}|\hat{\Lambda}(t)\left[1 - \hat{T}(t) + \hat{T} - \hat{T}(t)\hat{T} + \frac{1}{2}\hat{T}(t)^2 + \frac{1}{2}\hat{T}^2\right]|\Phi\rangle, \tag{E.8}$$

$$\langle\tilde{\Psi}(0)|\Psi(t)\rangle = 1 + \langle\tilde{\Phi}|\hat{\Lambda}\left[1 - \hat{T} + \hat{T}(t) - \hat{T}\hat{T}(t) + \frac{1}{2}\hat{T}^2 + \frac{1}{2}\hat{T}(t)^2\right]|\Phi\rangle. \tag{E.9}$$

We again utilize SymPy [9] to get explicit tensor contractions. This yields

$$\begin{aligned}\langle\tilde{\Psi}(t)|\Psi(0)\rangle = 1 &+ \lambda(t)^{i}_{a}\left[\tau^{a}_{i} - \tau(t)^{a}_{i}\right]\\ &+ \lambda(t)^{ij}_{ab}\left[\frac{1}{4}\tau^{ab}_{ij} - \frac{1}{2}\tau^{a}_{j}\tau^{b}_{i} - \tau(t)^{a}_{i}\tau^{b}_{j} - \frac{1}{2}\tau(t)^{a}_{j}\tau(t)^{b}_{i} - \frac{1}{4}\tau(t)^{ab}_{ij}\right],\end{aligned} \tag{E.10}$$

$$\begin{aligned}\langle\tilde{\Psi}(0)|\Psi(t)\rangle = 1 &+ \lambda^{i}_{a}\left[\tau(t)^{a}_{i} - \tau^{a}_{i}\right]\\ &+ \lambda^{ij}_{ab}\left[\frac{1}{4}\tau(t)^{ab}_{ij} - \frac{1}{2}\tau^{a}_{j}\tau^{b}_{i} - \tau(t)^{a}_{i}\tau^{b}_{j} - \frac{1}{2}\tau(t)^{a}_{j}\tau(t)^{b}_{i} - \frac{1}{4}\tau^{ab}_{ij}\right].\end{aligned} \tag{E.11}$$

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