# Second Midterm Project
# FYS-KJM4480

Jonas van den Brink

j.v.brink@fys.uio.no

December 6, 2014

## Exercise 1)

Show that $\hat{H}_0$ and $V$ commute with $\hat{S}_z$ and $\hat{S}^2$.

$$
\begin{aligned}
\hat{H}_0 &:= \xi \sum_{p\sigma} (p-1) a^\dagger_{p\sigma} a_{p\sigma}, \\
\hat{V} &:= -\frac{1}{2} g \sum_{pq} a^\dagger_{p+} a^\dagger_{p-} a_{q-} a_{q+}, \\
\hat{S}_z &:= \frac{1}{2} \sum_{p\sigma} \sigma a^\dagger_{p\sigma} a_{p\sigma}, \\
\hat{S}^2 &:= \hat{S}_z^2 + \frac{1}{2}\big(\hat{S}_+ \hat{S}_- + \hat{S}_- \hat{S}_+\big), \\
\hat{S}_\pm &:= \sum_p a^\dagger_{p\pm} a_{p\mp}.
\end{aligned}
$$

Anti-commutation relations

$$
\{\hat{a}^\dagger_\alpha, \hat{a}^\dagger_\beta\} = \{\hat{a}_\alpha, \hat{a}_\beta\} = 0, \qquad \{\hat{a}^\dagger_\alpha, \hat{a}_\beta\} = \delta_{\alpha\beta},
$$

### The commutator $[\hat{H}_0, \hat{S}_z]$

We start by inserting the operators in the definition

$$
\begin{aligned}
[\hat{H}_0, \hat{S}_z] &= \hat{H}_0 \hat{S}_z - \hat{S}_z \hat{H}_0 \\
&= \frac{\xi}{2} \sum_{pq\sigma\lambda} \lambda(p-1) \Big( a^\dagger_{p\sigma} a_{p\sigma} a^\dagger_{q\lambda} a_{q\lambda} - a^\dagger_{q\lambda} a_{q\lambda} a^\dagger_{p\sigma} a_{p\sigma} \Big).
\end{aligned}
$$

We now swap the two middle operators in the second term, this gives a delta-term

$$
\begin{aligned}
[\hat{H}_0, \hat{S}_z] &= \frac{\xi}{2} \sum_{pq\sigma\lambda} \lambda(p-1) \Big( a^\dagger_{p\sigma} a_{p\sigma} a^\dagger_{q\lambda} a_{q\lambda} - a^\dagger_{q\lambda} \big(\delta_{pq}\delta_{\sigma\lambda} - a^\dagger_{p\sigma} a_{q\lambda}\big) a_{p\sigma} \Big) \\
&= \frac{\xi}{2} \sum_{pq\sigma\lambda} \lambda(p-1) \Big( a^\dagger_{p\sigma} a_{p\sigma} a^\dagger_{q\lambda} a_{q\lambda} + a^\dagger_{q\lambda} a^\dagger_{p\sigma} a_{q\lambda} a_{p\sigma} - \delta_{pq}\delta_{\sigma\lambda} a^\dagger_{q\lambda} a_{p\sigma} \Big).
\end{aligned}
$$

We now swap the first and second, and third and fourth operator in the second term. We get no delta-terms, and we have no total change in sign

$$
[\hat{H}_0, \hat{S}_z] = \frac{\xi}{2} \sum_{pq\sigma\lambda} \lambda(p-1) \Big( a^\dagger_{p\sigma} a_{p\sigma} a^\dagger_{q\lambda} a_{q\lambda} + a^\dagger_{p\sigma} a^\dagger_{q\lambda} a_{p\sigma} a_{q\lambda} - \delta_{pq}\delta_{\sigma\lambda} a^\dagger_{q\lambda} a_{p\sigma} \Big).
$$

Again we swap the two middle operators, getting another delta term

$$
\begin{aligned}
[\hat{H}_0, \hat{S}_z] &= \frac{\xi}{2} \sum_{pq\sigma\lambda} \lambda(p-1) \Big( a^\dagger_{p\sigma} a_{p\sigma} a^\dagger_{q\lambda} a_{q\lambda} + a^\dagger_{p\sigma} \big(\delta_{pq}\delta_{\lambda\sigma} - a_{p\sigma} a^\dagger_{q\lambda}\big) a_{q\lambda} - \delta_{pq}\delta_{\sigma\lambda} a^\dagger_{q\lambda} a_{p\sigma} \Big) \\
&= \frac{\xi}{2} \sum_{pq\sigma\lambda} \lambda(p-1) \delta_{pq}\delta_{\lambda\sigma} \big( a^\dagger_{p\sigma} a_{q\lambda} - a^\dagger_{q\lambda} a_{p\sigma} \big).
\end{aligned}
$$

Due to the Kronecker-deltas the only surviving terms in the sums will have $p = q$ and $\sigma = \lambda$, meaning the two terms will cancel out, so we have

$$
[\hat{H}_0, \hat{S}_z] = 0,
$$

and we have confirmed that $\hat{H}_0$ and $\hat{S}_z$ commute.

**The commutator** $[\hat{V}, \hat{S}_z]$

Again, we start from the definition

$$\begin{aligned}[\hat{V}, \hat{S}_z] &= \hat{V}\hat{S}_z - \hat{S}_z\hat{V} \\ &= \frac{g}{4}\sum_{pqr\sigma}\sigma\bigg(a^\dagger_{r\sigma}a_{r\sigma}a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+} - a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}a^\dagger_{r\sigma}a_{r\sigma}\bigg).\end{aligned}$$

We now move the $a^\dagger_{r\sigma}$-operator in the second term to the front by succesively swapping it to the left

$$\begin{aligned}&a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}a^\dagger_{r\sigma}a_{r\sigma} \\ &\quad= a^\dagger_{p+}a^\dagger_{p-}a_{q-}\big(\delta_{qr}\delta_{\sigma+} - a^\dagger_{r\sigma}a_{q+}\big)a_{r\sigma} \\ &\quad= \delta_{qr}\delta_{\sigma+}a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{r\sigma} - a^\dagger_{p+}a^\dagger_{p-}\big(\delta_{qr}\delta_{\sigma-} - a^\dagger_{r\sigma}a_{q-}\big)a_{q+}a_{r\sigma} \\ &\quad= \delta_{qr}\delta_{\sigma+}a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{r\sigma} - \delta_{qr}\delta_{\sigma-}a^\dagger_{p+}a^\dagger_{p-}a_{q+}a_{r\sigma} + a^\dagger_{r\sigma}a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}a_{r\sigma}.\end{aligned}$$

In the final term here, we now move the $a_{r\sigma}$ by successive shifts

$$\begin{aligned}&a^\dagger_{r\sigma}a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}a_{r\sigma} \\ &\quad= a^\dagger_{r\sigma}a^\dagger_{p+}\big(\delta_{pr}\delta_{\sigma-} - a_{r\sigma}a^\dagger_{p-}\big)a_{q-}a_{q+} \\ &\quad= \delta_{pr}\delta_{\sigma-}a^\dagger_{r\sigma}a^\dagger_{p+}a_{q-}a_{q+} - a^\dagger_{r\sigma}\big(\delta_{pr}\delta_{\sigma+} - a_{r\sigma}a^\dagger_{p+}\big)a^\dagger_{p-}a_{q-}a_{q+} \\ &\quad= \delta_{pr}\delta_{\sigma-}a^\dagger_{r\sigma}a^\dagger_{p+}a_{q-}a_{q+} - \delta_{pr}\delta_{\sigma+}a^\dagger_{r\sigma}a^\dagger_{p-}a_{q-}a_{q+} + a^\dagger_{r\sigma}a_{r\sigma}a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}.\end{aligned}$$

Putting this result back into the original expression gives

$$\begin{aligned}[\hat{V}, \hat{S}_z] = \frac{g}{4}\sum_{pqr\sigma}\sigma\big(&\delta_{pr}\delta_{\sigma+}a^\dagger_{r\sigma}a^\dagger_{p-}a_{q-}a_{q+} + \delta_{qr}\delta_{\sigma-}a^\dagger_{p+}a^\dagger_{p-}a_{q+}a_{r\sigma} \\ &- \delta_{qr}\delta_{\sigma+}a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{r\sigma} - \delta_{pr}\delta_{\sigma-}a^\dagger_{r\sigma}a^\dagger_{p+}a_{q-}a_{q+}\big).\end{aligned}$$

We now perform the sum over $\sigma$, giving

$$\begin{aligned}[\hat{V}, \hat{S}_z] = \frac{g}{4}\sum_{pqr}\delta_{pr}\big(&a^\dagger_{r+}a^\dagger_{p-}a_{q-}a_{q+} + a^\dagger_{r-}a^\dagger_{p+}a_{q-}a_{q+}\big) \\ &- \delta_{qr}\big(a^\dagger_{p+}a^\dagger_{p-}a_{q+}a_{r-} + a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{r+}\big).\end{aligned}$$

We now perform the sum over $p$ and $q$, we see the only surviving terms are those were $p = r$ or $q = r$, giving

$$[\hat{V}, \hat{S}_z] = \frac{g}{4}\sum_{r}\big(a^\dagger_{r+}a^\dagger_{r-}a_{r-}a_{r+} + a^\dagger_{r-}a^\dagger_{r+}a_{r-}a_{r+} - a^\dagger_{r+}a^\dagger_{r-}a_{r+}a_{r-} - a^\dagger_{r+}a^\dagger_{r-}a_{r-}a_{r+}\big).$$

We see that the terms cancel each other out, leaving

$$[\hat{V}, \hat{S}_z] = 0,$$

and we have confirmed that $\hat{V}$ and $\hat{S}_z$ commute.

**The commutator** $[\hat{H}_0, \hat{S}_\pm]$

From the definition, we have

$$\begin{aligned}[\hat{H}_0, \hat{S}_\pm] &= \hat{H}_0\hat{S}_\pm - \hat{S}_\pm\hat{H}_0 \\ &= \xi \sum_{pq\sigma}(p-1)\big(a^\dagger_{p\sigma}a_{p\sigma}a^\dagger_{q\pm}a_{q\mp} - a^\dagger_{q\pm}a_{q\mp}a^\dagger_{p\sigma}a_{p\sigma}\big).\end{aligned}$$

Again, we shift the operators around in the second term around, so that it cancels with the first term, we get the following result

$$[\hat{H}_0, \hat{S}_\pm] = \xi \sum_{pq\sigma}(p-1)\delta_{pq}(\delta_{\sigma\pm} - \delta_{\sigma\mp}).$$

We can now take the sum over $\sigma$, which makes the entire commutator vanish, as the two Kronecker-delta's with $\sigma$ cancel each other out, so we have

$$[\hat{H}_0, \hat{S}_\pm] = 0.$$

And $\hat{H}_0$ commutes with $\hat{S}_\pm$.

**The commutator** $[\hat{V}, \hat{S}_\pm]$

From the definition, we have

$$\begin{aligned}[\hat{V}, \hat{S}_\pm] &= \hat{V}\hat{S}_\pm - \hat{S}_\pm\hat{V} \\ &= -\frac{g}{2}\sum_{pqr} a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}a^\dagger_{r\pm}a_{r\mp} - a^\dagger_{r\pm}a_{r\mp}a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}.\end{aligned}$$

Shifting the operators around in the second term makes it cancel with the first, but shifting the operators generates some terms, we have

$$\begin{aligned}[\hat{V}, \hat{S}_\pm] &= \hat{V}\hat{S}_\pm - \hat{S}_\pm\hat{V} \\ &= \frac{g}{2}\sum_{pqr}\big(\delta_{pr}\delta_{\mp+}a^\dagger_{r\pm}a^\dagger_{p-}a_{q-}a_{q+} - \delta_{pr}\delta_{\mp-}a^\dagger_{r\pm}a^\dagger_{p+}a_{q-}a_{q+} \\ &\qquad + \delta_{qr}\delta_{\pm-}a^\dagger_{p+}a^\dagger_{p-}a_{q+}a_{r\mp} - \delta_{qr}\delta_{\pm+}a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{r\mp}\big).\end{aligned}$$

Summing over $p$ and $q$ gives

$$\begin{aligned}[\hat{V}, \hat{S}_\pm] &= \hat{V}\hat{S}_\pm - \hat{S}_\pm\hat{V} \\ &= \frac{g}{2}\sum_{r}\big(\delta_{\mp+}a^\dagger_{r\pm}a^\dagger_{r-}a_{r-}a_{r+} - \delta_{\mp-}a^\dagger_{r\pm}a^\dagger_{r+}a_{r-}a_{r+} \\ &\qquad + \delta_{\pm-}a^\dagger_{r+}a^\dagger_{r-}a_{r+}a_{r\mp} - \delta_{\pm+}a^\dagger_{r+}a^\dagger_{r-}a_{r-}a_{r\mp}\big).\end{aligned}$$

We can now look at the case for $\hat{S}_+$

$$-\frac{g}{2}\sum_{r}\big(a^\dagger_{r+}a^\dagger_{r+}a_{r-}a_{r+} + a^\dagger_{r+}a^\dagger_{r-}a_{r-}a_{r-}\big).$$

For top

$$\begin{aligned}-a^\dagger_{r+}a^\dagger_{r+}a_{r-}a_{r+} - a^\dagger_{r+}a^\dagger_{r-}a_{r-}a_{r-}. \\ a^\dagger_{r-}a^\dagger_{r-}a_{r-}a_{r+} + a^\dagger_{r+}a^\dagger_{r-}a_{r+}a_{r+}\end{aligned}$$

# 1 THIS MUST BE FIXED

**The commutator $[\hat{H}_0, \hat{S}^2]$**

To compute the commutator between $\hat{H}_0$ and $\hat{S}^2$ we express the total spin by the operators $\hat{S}_z$ and $\hat{S}_\pm$, so we get

$$\begin{aligned}[\hat{H}_0, \hat{S}^2] &= [\hat{H}_0, \hat{S}_z^2 + \frac{1}{2}(\hat{S}_+\hat{S}_- + \hat{S}_-\hat{S}_+)] \\ &= [\hat{H}_0, \hat{S}_z^2] + \frac{1}{2}[\hat{H}_0, \hat{S}_+\hat{S}_-] + \frac{1}{2}[\hat{H}_0, \hat{S}_-\hat{S}_+].\end{aligned}$$

We now use that fact that for any operators $\hat{A}$, $\hat{B}$ and $\hat{C}$

$$[\hat{A}, \hat{B}\hat{C}] = \hat{A}\hat{B}\hat{C} - \hat{B}\hat{C}\hat{A} = \hat{A}\hat{B}\hat{C} - \hat{B}\hat{A}\hat{C} + \hat{B}\hat{A}\hat{C} - \hat{B}\hat{C}\hat{A} = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}].$$

So we get

$$\begin{aligned}[\hat{H}_0, \hat{S}_z^2] &= [\hat{H}_0, \hat{S}_z]\hat{S}_z + \hat{S}_z[\hat{H}_0, \hat{S}_z] = 0, \\ [\hat{H}_0, \hat{S}_+\hat{S}_-] &= [\hat{H}_0, \hat{S}_+]\hat{S}_- + \hat{S}_+[\hat{H}_0, \hat{S}_-] = 0, \\ [\hat{H}_0, \hat{S}_-\hat{S}_+] &= [\hat{H}_0, \hat{S}_-]\hat{S}_+ + \hat{S}_-[\hat{H}_0, \hat{S}_+] = 0.\end{aligned}$$

So we see that

$$[\hat{H}_0, \hat{S}^2] = 0.$$

**The commutator $[\hat{V}, \hat{S}^2]$**

We immediately see that $\hat{V}$ and $\hat{S}^2$ commutes from the same argument as for $\hat{H}_0$.

$$[\hat{V}, \hat{S}^2] = 0.$$

## Rewriting the Hamiltonian

We now introduce the pair creation and annihilation operators

$$\hat{P}_p^+ = a_{p+}^\dagger a_{p-}^\dagger \qquad \hat{P}_p^- = a_{p-} a_{p+},$$

which lets us write $\hat{V}$ as

$$\hat{V} = -\frac{1}{2} g \sum_{pq} \hat{P}_p^+ \hat{P}_q^-.$$

If we also set $\xi = 1$, we can write the full Hamiltonian as

$$\hat{H} = \hat{H}_0 + \hat{V} = \sum_{p\sigma} (p-1) a_{p\sigma}^\dagger a_{p\sigma} - \frac{1}{2} g \sum_{pq} \hat{P}_p^+ \hat{P}_q^-.$$

**The commutator $[\hat{H}, \hat{P}_p^+ \hat{P}_q^-]$**

We now want to show that the Hamiltonian commutes with the product of the pair creation and annihilation operators. We start of by showing how the pair operators commute internally.

$$\hat{P}_p^+ \hat{P}_q^- = a_{p+}^\dagger a_{p-}^\dagger a_{q-} a_{q+}.$$

First, we swap the two middle operators

$$\begin{aligned}\hat{P}_p^+\hat{P}_q^- &= a_{p+}^\dagger(\delta_{pq} - a_{q-}a_{p-}^\dagger)a_{q+} \\ &= \delta_{pq}a_{p+}^\dagger a_{q+} - a_{p+}^\dagger a_{q-}a_{p-}^\dagger a_{q+}.\end{aligned}$$

For the last term, we swap the first two operators and the last two operators, as they have different $\sigma$-values, we only get two changes in sign that cancel each other out, so we have

$$\hat{P}_p^+\hat{P}_q = \delta_{pq}a_{p+}^\dagger a_{q+} - a_{q-}a_{p+}^\dagger a_{q+}a_{p-}^\dagger.$$

We again swap the two middle operators to get

$$\begin{aligned}\hat{P}_p^+\hat{P}_q^- &= \delta_{pq}a_{p+}^\dagger a_{q+} - a_{q-}(\delta_{pq} - a_{q+}a_{p+}^\dagger)a_{p-}^\dagger \\ &= \delta_{pq}(a_{p+}^\dagger a_{q+} - a_{q-}a_{p-}^\dagger) + a_{q-}a_{q+}a_{p+}^\dagger a_{p-}^\dagger \\ &= \hat{P}_q^-\hat{P}_p^+ + \delta_{pq}(a_{p+}^\dagger a_{p+} - a_{p-}a_{p-}^\dagger).\end{aligned}$$

So we see that we have

$$[\hat{P}_p^+, \hat{P}_q^-] = \delta_{pq}$$

And for $[\hat{P}_p^\pm, \hat{P}_q^\pm]$ we easily see that four swaps will change the operators with no total change in sign, meaning we have

$$[\hat{P}_p^\pm, \hat{P}_q^\pm] = 0.$$

If we then look at the commutator

$$\begin{aligned}[\hat{V}, \hat{P}_r^+\hat{P}_r^-] &= -\frac{g}{2}\sum_{pq}[\hat{P}_p^+\hat{P}_q^-, \hat{P}_r^+\hat{P}_r^-] \\ &= -\frac{g}{2}\sum_{pq}[\hat{P}_p^+, \hat{P}_r^+]\hat{P}_q^-\hat{P}_r^- + \hat{P}_p^+[\hat{P}_q^-, \hat{P}_r^+]\hat{P}_r^- \\ &\qquad + \hat{P}_r^+\hat{P}_p^+[\hat{P}_q^-, \hat{P}_r^-] + \hat{P}_r^+[\hat{P}_p^+, \hat{P}_r^-]\hat{P}_q^- \\ &= -\frac{g}{2}\sum_{pq}\delta_{qr}\hat{P}_p^+\hat{P}_r^- + \delta_{pr}\hat{P}_r^+\hat{P}_q^- \\ &= -\frac{g}{2}\sum_{p}\hat{P}_p^+\hat{P}_r^- + \hat{P}_r^+\hat{P}_p^- \\ &= -\frac{g}{2}\sum_{p}\end{aligned}$$

## Exercise 2)

We now look at a system with four particles. We limit our system to have no broken pairs and always have a total spin of $S = 0$. We also limit our system to only inhabit the four lowest levels $p = 1, 2, 3, 4$. This gives rise to six different Slater determinants

$$|\Phi^0\rangle = \hat{P}_1^+\hat{P}_2^+|0\rangle, \qquad |\Phi_2^3\rangle = \hat{P}_1^+\hat{P}_3^+|0\rangle, \qquad |\Phi_2^4\rangle = \hat{P}_1^+\hat{P}_4^+|0\rangle,$$
$$|\Phi_1^3\rangle = \hat{P}_2^+\hat{P}_3^+|0\rangle, \qquad |\Phi_1^4\rangle = \hat{P}_2^+\hat{P}_4^+|0\rangle, \qquad |\Phi_{12}^{34}\rangle = \hat{P}_3^+\hat{P}_4^+|0\rangle.$$

Where we have denoted the first state as our Fermi-vacuum, the four other Slater determinants are then four 2-particle 2-hole states, and the final SD is a 4-particle 4-hole state. The Slater determinants are illustrated in figure 1.

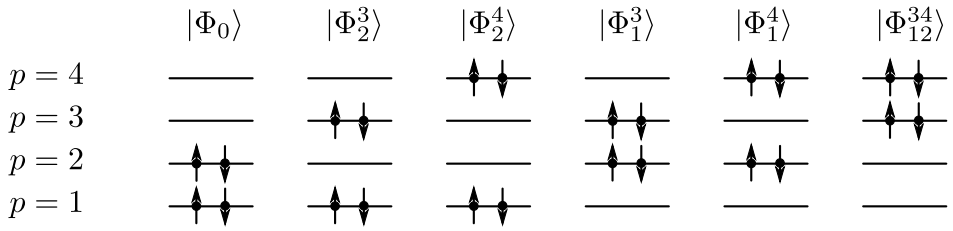



**Figure 1.** Sketch of the six possible Slater determinants.

These six Slater determinants are orthonormal and span a six-dimensional Hilbert space. We want to compute the matrix representation of the Hamiltonian in this space, which is given by

$$H_{ij} = \langle\Phi_i|\hat{H}|\Phi_j\rangle,$$

where $\{\Phi_i\}_{i=1}^6$ is the set of the six Slater determinants. To calculate the different matrix elements, it's easiest to split up the Hamiltonian, so we have

$$H_{ij} = \langle\Phi_i|\hat{H}_0|\Phi_j\rangle + \langle\Phi_i|\hat{V}|\Phi_j\rangle.$$

The one-body operator is

$$\hat{H}_0 = \sum_{p\sigma}(p-1)a_{p\sigma}^\dagger a_{p\sigma},$$

so we see that the for the off-diagonal terms, the one-body contribution vanishes. For the diagonal terms we find

$$\langle\Phi_0|\hat{H}_0|\Phi_0\rangle = 2, \qquad \langle\Phi_2^3|\hat{H}_0|\Phi_2^3\rangle = 4, \qquad \langle\Phi_2^4|\hat{H}_0|\Phi_2^4\rangle = 6,$$
$$\langle\Phi_1^3|\hat{H}_0|\Phi_1^3\rangle = 6, \qquad \langle\Phi_2^4|\hat{H}_0|\Phi_2^4\rangle = 8, \qquad \langle\Phi_{12}^{34}|\hat{H}_0|\Phi_{12}^{34}\rangle = 10.$$

For the two-body operator we have

$$\hat{V} = -\frac{g}{2}\sum_{pq}P_p^+P_q^-.$$

When calculating the matrix elements, we see that we can either have no non-coincidences, two non-coincidences or four non-coincidences. Another way to state this is to say that there can a mismatch of zero, one or two pairs.

If there is a mismatch of two paris, the matrix element clearly vanishes.

$$\langle\Phi_0|\hat{V}|\Phi_{12}^{34}\rangle = 0,$$
$$\langle\Phi_2^3|\hat{V}|\Phi_1^4\rangle = 0,$$
$$\langle\Phi_2^4|\hat{V}|\Phi_1^3\rangle = 0.$$

Next, if there is a mismatch of one pair, the two-body operator has to remove it, meaning there is only one term in the sum over $p$ and $q$ that will contribute to the matrix elements, so we have

$$\begin{aligned}\langle\Phi_0|\hat{V}|\Phi_i^a\rangle &= -g/2,\\ \langle\Phi_i^a|\hat{V}|\Phi_i^b\rangle &= -g/2,\\ \langle\Phi_i^a|\hat{V}|\Phi_j^a\rangle &= -g/2,\\ \langle\Phi_i^a|\hat{V}|\Phi_{12}^{34}\rangle &= -g/2.\end{aligned}$$

Note that we do not have to worry about a change in sign for the terms, as the pair creation and annihilation operators have "opposite" commutation relations from the normal creation and annihilation operators, so there is no change in sign.

When there is no mismatches between the pairs, i.e., we are looking at the diagonal terms. We see that there are two terms in the sum that contribute to the matrix elements, so we have

$$\langle\Phi_i|\hat{V}|\Phi_i\rangle = -g.$$

We summarize our results by setting up the Hamiltonian matrix

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

Numerically, we find the eigenvalues and eigenvectors of this matrix. The lowest eigenvalue then corresponds to the ground state energy. Numerically, we can generate the Hamiltonian matrix and find the eigenvalue for any value of $g$, effectively giving us the ground state energy as a function of the strength of the interaction. We will for the rest of this project refer to that energy as the "exact" energy of the system. The exact energy function is shown as the blue line in figure 2 on the next page.

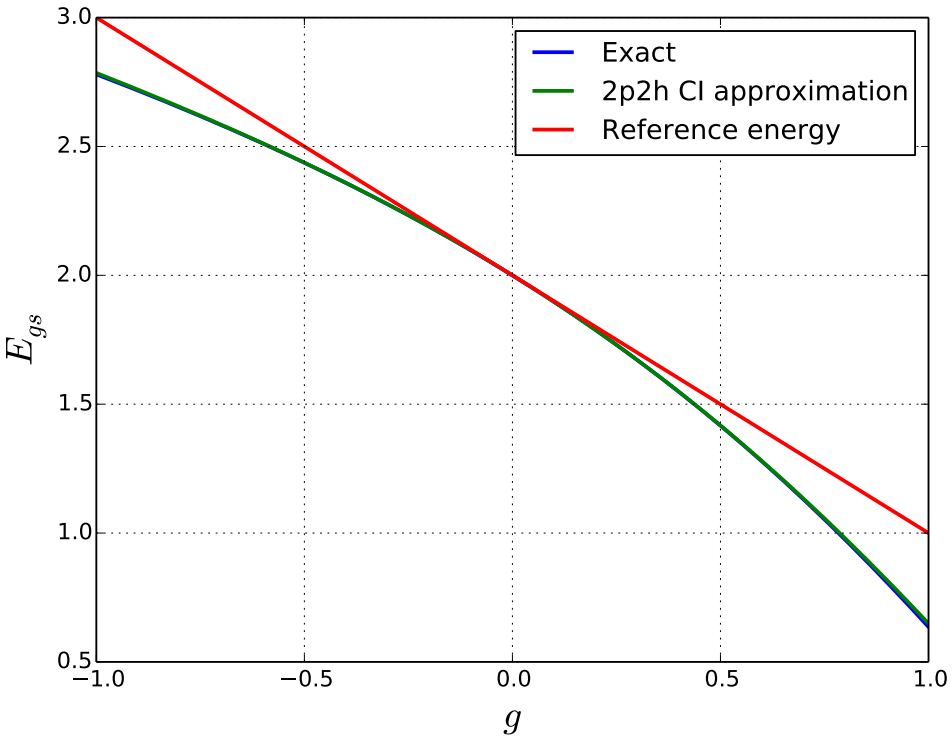



**Figure 2.** Ground state energy as a function of the interaction-parameter $g$.

## Exercise 3)

We now limit our system to at most two-particle-two-hole excitations, meaning only a single pair of particles can be excited. This means we have to discard $|\Phi_{12}^{34}\rangle$, and only look at a five-dimensional system.

The Hamiltonian matrix is unchanged except for the fact that it is reduced to a five-by-five matrix by stripping the rows and columns that corresponded to the removed Slater determinant. The Hamiltonian matrix is

$$\hat{H} = \begin{pmatrix} 2-g & -g/2 & -g/2 & -g/2 & -g/2 \\ -g/2 & 4-g & -g/2 & -g/2 & 0 \\ -g/2 & -g/2 & 6-g & 0 & -g/2 \\ -g/2 & -g/2 & 0 & 6-g & -g/2 \\ -g/2 & 0 & -g/2 & -g/2 & 8-g \end{pmatrix}$$

Again we calculate the ground state energy as a function of the interaction strength $g$. The results are also shown in figure 2 as the green line. Note that we refer to this result as the "approximate" result, as it is only an approximation to the exact result.

## Exercise 4)

We now turn to Hartree-Fock theory. First we will partition our Hamiltonian and define our Fock operator. This will illuminate the difference between a cannonical and a non-cannonical Hartree-Fock case. For each of these cases, as well as a general (i.e., a non Hartree-Fock) case, we will set up the normal-ordered Hamiltonian in both diagramatic and algebraic form.

### Partitioning the Hamiltonian

If we limit ourselves to at most two-body interactions, the Hamiltonian can be generally written as a sum of one-body and two-body operators, which in second quantization looks like

$$\hat{H} = \hat{H}_1 + \hat{H}_2 = \sum_{\mu} \hat{h}_\mu + \sum_{\mu\nu} \hat{v}_{\mu\nu}.$$

For our system we have a single one-body and a single two-body interaction, labeling them $\hat{h}_0$ and $\hat{v}$, we get

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

where we use Shavitt and Bartlet's shorthand of $\langle \alpha\beta || \gamma\delta \rangle = \langle \alpha\beta | \hat{v} | \gamma\delta \rangle_{\mathrm{AS}}$.

Using Wick's theorem, we can write these out as

$$\hat{H}_1 = \sum_{pq} \langle p | \hat{h}_0 | q \rangle \{ \hat{p}^\dagger \hat{q} \} + \sum_{i} \langle i | \hat{h}_0 | i \rangle,$$
$$\hat{H}_2 = \frac{1}{4} \sum_{pqrs} \langle pq || rs \rangle \{ \hat{p}^\dagger \hat{q}^\dagger \hat{s} \hat{r} \} + \sum_{pqi} \langle pi || qi \rangle \{ \hat{p}^\dagger \hat{q} \} + \frac{1}{2} \sum_{ij} \langle ij || ij \rangle.$$

We now define the *reference energy* as

$$E_{\mathrm{ref}} = \sum_{i} \langle i | \hat{h}_0 | i \rangle + \frac{1}{2} \sum_{ij} \langle ij || ij \rangle.$$

Which enables us to split the Hamiltonian into its normal-ordered part and the reference energy

$$\hat{H} = \hat{H}_{\mathrm{N}} + E_{\mathrm{ref}}.$$

The normal-ordered Hamiltonian is then

$$\hat{H}_{\mathrm{N}} = \sum_{pq} \langle p | \hat{h}_0 | q \rangle \{ \hat{p}^\dagger \hat{q} \} + \sum_{pqi} \langle pi || qi \rangle \{ \hat{p}^\dagger \hat{q} \} + \frac{1}{4} \sum_{pqrs} \langle pq || rs \rangle \{ \hat{p}^\dagger \hat{q}^\dagger \hat{s} \hat{r} \}.$$

We now relabel the first two terms into the normal-ordered *Fock-operator*, giving us

$$\hat{H}_{\mathrm{N}} = \hat{F}_{\mathrm{N}} + \frac{1}{4} \sum_{pqrs} \langle pq || rs \rangle \{ \hat{p}^\dagger \hat{q}^\dagger \hat{s} \hat{r} \}.$$

We can now think of the normal-ordered Hamiltonian as the sum of a one-body part and the perturbation

$$\hat{W}_{\mathrm{N}} = \frac{1}{4} \sum_{pqrs} \langle pq || rs \rangle \{ \hat{p}^\dagger \hat{q}^\dagger \hat{s} \hat{r} \},$$

we will get back to this when we turn to many-body perturbation theory.

For now, we will look closer at the normal-ordered Fock-operator

$$\hat{F}_{\mathrm{N}} = \sum_{pq} \langle p|\hat{h}_0|q\rangle \{\hat{p}^\dagger \hat{q}\} + \sum_{pqi} \langle pi||qi\rangle \{\hat{p}^\dagger \hat{q}\} = \sum_{pq} f_{pq} \{\hat{p}^\dagger \hat{q}\},$$

where

$$f_{pq} = \langle p|\hat{h}_0|q\rangle + \sum_{pqi} \langle pi||qi\rangle = h_{pq} + u_{pq}.$$

We see that the exact form of the Fock-matrix is then the result of the form of the one-body and two-body operators $\hat{h}_0$ and $\hat{v}$ and also of our choice of single-particle basis.

The form of the Fock-matrix is quite important for our further discussion of how to solve the problem, and so we will label three different cases:

1. First we have the possibility of the Fock-matrix being purely diagonal

   $$f_{pq} = \epsilon_p \delta_{pq},$$

   this case is known as the *cannonical Hartree-Fock* case.

2. Next, we have the case where the Fock-matrix is not entirely diagonal, but it is *block-diagonal*, meaning the blocks of the Fock-matrix corresponding to the matrix elements between hole and particle states vanish. So we have

   $$f_{ai} = 0,$$

   this is the *non-cannonical* Hartree-Fock case. Note that some people do not distinguish between the cannonical and non-cannonical HF cases.

3. All cases not covered by the two HF cases are collectively reffered to as *general* cases.

As the normal-ordered Fock-operator can be non-diagonal, it is often conveniant to split it into its diagonal and off-diagonal contributions

$$\hat{F}_{\mathrm{N}} = \sum_{p} f_{pp} \{\hat{p}^\dagger \hat{p}\} + \sum_{p \neq q} f_{pq} \{\hat{p}^\dagger \hat{q}\} = \hat{F}_{\mathrm{N}}^{\mathrm{D}} + \hat{F}_{\mathrm{N}}^{\mathrm{O}}.$$

In the cases where $\hat{F}_{\mathrm{N}}^{\mathrm{O}} \neq 0$, it is common to include this part of the Fock-operator in the perturbation.

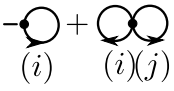
The total normal-product Hamiltonian is then

$$\hat{H}_{\mathrm{N}} = \hat{F}_{\mathrm{N}} + \hat{W}_{\mathrm{N}} = \hat{F}_{\mathrm{N}}^{\mathrm{d}} + \hat{F}_{\mathrm{N}}^{\mathrm{o}} + \hat{W}_{\mathrm{N}} = \hat{F}_{\mathrm{N}}^{\mathrm{d}} + \tilde{W}_{\mathrm{N}}.$$

### The Hamiltonian in diagrams

We will now draw the diagrams representing the Hamiltonian for all three cases. First of, let us draw the the reference energy, which is what separates the complete Hamiltonian from the normal-ordered Hamiltonian.

$$E_{\mathrm{ref}} = \sum_{i} \langle i|\hat{h}_0|i\rangle + \sum_{ij} \langle ij||ij\rangle =$$

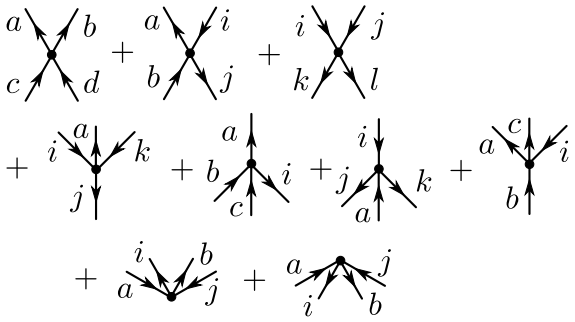


Let us now move on to the normal-ordered Hamiltonian, which is given by

$$\hat{H}_{\mathrm{N}} = \hat{F}_{\mathrm{N}} + \hat{W}_{\mathrm{N}}.$$

For all three cases the $\hat{W}_{\mathrm{N}}$ term is the same, so let us show that term first

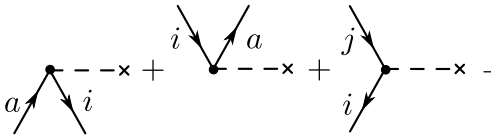
$$\hat{W}_{\mathrm{N}} = \frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} =$$




That leaves the contributions from the Fock-operator, and that is where the three cases will differ. The final term is given by

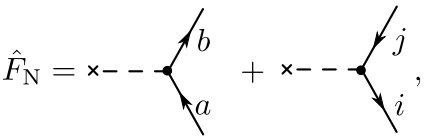
$$\hat{F}_{\mathrm{N}} = \sum_{pq} f_{pq}\{\hat{p}^\dagger\hat{q}\}.$$

For the general case, no terms vanish, so we have

$\hat{F}_{\mathrm{N}} =$ 

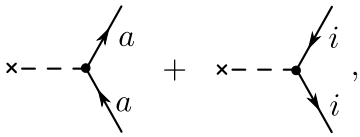
, (general case).

If we have a non-canonical Hartree-Fock case, the first two terms are guaranteed to vanish, as they are contained in the off-diagonal blocks of the Fock-matrix. So we are left with

$\hat{F}_{\mathrm{N}} =$ 

, (non-cannonical HF).

For the cannonical Hartree-Fock case, only the diagonal terms $f_{aa}$ and $f_{ii}$ survive, so we have

$\hat{F}_{\mathrm{N}} =$ 

, (cannonical HF).

## Exercise 5)

$$\hat{H} = \hat{H}_0 + \hat{V} = \sum_{p\sigma}(p-1)a^\dagger_{p\sigma}a_{p\sigma} - \frac{1}{2}g\sum_{pq} a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}.$$

### Canonical and non-canonical Hartree-Fock

For canonical Hartree-Fock, we now that the Fock-operator is diagonal, meaning

$$f_{pq} = \epsilon_p\delta_{pq}, \qquad \epsilon_p = h_{pp} + \sum_i \langle pi||pi\rangle.$$

For the non-canonical Hartree-Fock, the Fock-operator is a block-diagonal matrix, this means that $f_{ai}$ is zero, but $f_{ab}$ and $f_{ij}$ are generally not zero. For the completely general case, there is no guarantee that any element of the Fock matrix is zero.

$$\hat{H} = \sum_{pq} p^\dagger q + \frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle p^\dagger q^\dagger sr.$$

$$\hat{H}_0 = \sum_{pq}\langle p|\hat{h}_0|q\rangle\{\hat{p}^\dagger\hat{q}\} + \sum_i\langle i|\hat{h}_0|i\rangle,$$
$$\hat{H}_1 = \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle_{\mathrm{AS}}\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} + \sum_{pqi}\langle pi|\hat{v}|qi\rangle_{\mathrm{AS}}\{\hat{p}^\dagger\hat{q}\} + \frac{1}{2}\sum_{ij}\langle ij|\hat{v}|ij\rangle_{\mathrm{AS}}.$$

We can then see that we have the Fock-operator

$$\hat{F} = \sum_{pq}\langle p|\hat{h}_0|q\rangle\{\hat{p}^\dagger\hat{q}\} + \sum_{pqi}\langle p||q\rangle\{\hat{p}^\dagger\hat{q}\}.$$

So that the matrix elements of the Fock-matrix are given by

$$f_{pq} = h_{pq} + \sum_i\langle pi||qi\rangle.$$

We then have

$$\hat{H} = \hat{F} + \hat{E}_{ref} + \frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle,$$

where

$$E_{ref} = \sum_i\langle i|\hat{h}_0|i\rangle + \frac{1}{2}\sum_{ij}\langle ij||ij\rangle.$$

So we have

$$\hat{H}_{\mathrm{N}} = \hat{F} + \frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle.$$

If we are looking at canonical HF

$$f_{pq} = \epsilon_p\delta_{pq}.$$

If we are looking at non-canonical HF

## Exercise 5)

We will now set up the Hartree-Fock equations. While we will describe briefly how these are found, we won't show the derivation in detail, as this was done in the previous midterm project. For a detailed explanation of the Hartree-Fock equations and their origin, look to exercise 1e in midterm project 1.

### Setting up the equations

The first step to finding the Hartree-Fock equations is setting up the reference energy of a general Slater determinant

$$E_{\text{ref}} = \langle \Phi | \hat{H} | \Phi \rangle = \sum_{p=1}^{N} \langle p | \hat{h}_0 | p \rangle + \frac{1}{2} \sum_{p=1}^{N} \sum_{q=1}^{N} \langle pq || pq \rangle.$$

We then expand the states $p$ into another general basis

$$E = \sum_{p=1}^{N} \sum_{\alpha\beta} C_{p\alpha}^{*} C_{p\beta} \langle \alpha | \hat{h}_0 | \beta \rangle + \frac{1}{2} \sum_{p=1}^{N} \sum_{q=1}^{N} \sum_{\alpha\beta\gamma\delta} C_{p\alpha}^{*} C_{q\beta}^{*} C_{p\gamma} C_{q\delta} \langle \alpha\beta || \gamma\delta \rangle.$$

We can now minimize the reference energy with respect to the coefficients $C$. This is a mathematical minimization problem with constraints resulting from limitations in the wavefunctions. Introducing the Lagrangian multipliers $\epsilon_k$, we get $k$ equations

$$h^{\text{HF}} \mathbf{C}_k = \epsilon_k \mathbf{C}_k.$$

Here $h^{\text{HF}}$ is a matrix with elements given by

$$h_{\alpha\gamma}^{\text{HF}} = \langle \alpha | \hat{h}_0 | \gamma \rangle + \sum_{p=1}^{N} \sum_{\beta\delta} C_{p\beta}^{*} C_{p\delta} \langle \alpha\beta || \gamma\delta \rangle.$$

### Solving the equations

When solving the Hartree-Fock equations, we usually do it as an iterative process, but as we will see, we don't really have to do any iterations—it turns out we are already in the correct basis! We will now show this. For the first iteration, we start of by claiming $C_{pq} = \delta_{pq}$, this is simply due to the fact that we start in our original basis. The elements of $h^{\text{HF}}$ then become

$$h_{\alpha\gamma}^{\text{HF}} = \langle \alpha | \hat{h}_0 | \gamma \rangle + \sum_{p=1}^{N} \sum_{\beta\delta} \delta_{p\beta} \delta_{p\delta} \langle \alpha\beta || \gamma\delta \rangle.$$

Performing the sums over $\beta$ and $\delta$ simplifies this to

$$h_{\alpha\gamma}^{\text{HF}} = \langle \alpha | \hat{h}_0 | \gamma \rangle + \sum_{p=1}^{N} \langle \alpha p | \gamma p \rangle.$$

Here, the sum over $p$ is actually a sum over the particles in our system, thus the sum actually corresponds to a sum over all the hole states of the system. We then recognize that the elements are equal to the Fock-elements we found in the previous exercise

$$h_{pq}^{\text{HF}} = f_{pq} = \langle p | \hat{h}_0 | q \rangle + \sum_{i} \langle pi || qi \rangle.$$

Let us explicitly calculate these elements. For our system, the one-body operator is given by

$$\hat{h}_0 = \sum_{p\sigma}(p-1)\hat{a}^\dagger_{p\sigma}\hat{a}_{p\sigma}, \quad h_{pq} = \delta_{pq}(p-1),$$

so we immediatly see that the one-body operator is diagonal in the sense $h_{pq} = \delta_{pq}k_p$.

For the two-body operator we have

$$\hat{v} = -\frac{g}{2}\sum_{pq}\hat{P}^+_p\hat{P}^-_q.$$

So we have

$$u_{pq} = -\frac{g}{2}\sum_i \langle pi||qi\rangle = \sum_i\sum_{rs}\langle pi|\hat{P}^+_r\hat{P}^-_s|qi\rangle_{AS},$$

note that in this sums over $p, q$ and $i$ sum over both of the quantum numbers $p$ and $\sigma$, but the sums over $r$ and $s$ only sum over the first quantum number.

If we let a bar denote the same state, but with opposite spin we see that for $\hat{P}^-_s|qi\rangle$ to not vanish, we must have $i = \bar{q}$. An d for $\langle pi|\hat{P}^+_r$ to not vanish, we need $i = \bar{p}$. Meaning we only get a contribution to $u_{pq}$ if and only if $p$ and $q$ are the same hole state. We can summarize this result as

$$\begin{aligned} u_{ap} &= u_{pa} = 0, \\ u_{ij} &= -\delta_{ij}g/2. \end{aligned}$$

We define our model space to consist of the single-particle levels $p = 1, 2$ and the excluded space is then $p = 3, 4$. This means we define our reference state to be

$$|\Phi_0\rangle = \hat{P}^+_1\hat{P}^+_2|0\rangle,$$

We can then set up our Hartree-Fock matrix

$$h^{\mathrm{HF}} = \begin{pmatrix} -g/2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -g/2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1-g/2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1-g/2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 \end{pmatrix}$$

And we now see that the matrix is *already diagonal*, so there really isn't anything to solve here. The eigenvalues of the matrix are equal to the diagonal elements, and the eigenvectors are simply the unit vectors: $C_k = \hat{e}_k$. This means we were already in the correct basis, and our Hartree-Fock iteration didn't change our basis.

### Finding the reference energy

We have now shown that our original basis already gave a minimum for the reference energy, so let us calculate this reference energy. As our basis did not change, we can find it from the expression

$$E_{\text{ref}} = \langle\Phi|\hat{H}|\Phi\rangle = \sum_{p=1}^{N}\langle p|\hat{h}_0|p\rangle + \frac{1}{2}\sum_{p=1}^{N}\sum_{q=1}^{N}\langle pq||pq\rangle.$$

Again, the sums over $N$ comes from the particles in our system, and so for the ground state, they actually correspond to the hole states, so we have

$$E_{\text{ref}} = \langle\Phi_0|\hat{H}|\Phi_0\rangle = \sum_{i}\langle i|\hat{h}_0|i\rangle + \frac{1}{2}\sum_{ij}\langle ij||ij\rangle.$$

The hole states are now $i \in \{1_\uparrow, 1_\downarrow, 2_\uparrow, 2_\downarrow\}$, a quick calculation then gives us the reference energy. For the one-body operator we have

$$\langle i|\hat{h}_0|i\rangle = (p-1) \quad \Rightarrow \quad \sum_{i}\langle i|\hat{h}_0|i\rangle = 2.$$

And for the two-body operator, we see that any matrix elements with broken pairs will vanish, leaving us with

$$E_{\text{ref}} = \frac{1}{2}\big(\langle 1_\uparrow 1_\downarrow||1_\uparrow 1_\downarrow\rangle + \langle 1_\downarrow 1_\uparrow||1_\downarrow 1_\uparrow\rangle + \langle 2_\uparrow 2_\downarrow||2_\uparrow 2_\downarrow\rangle + \langle 2_\downarrow 2_\uparrow||2_\downarrow 2_\uparrow\rangle\big).$$

Here, all terms contribute $-g/2$, so we get the final result

$$E_{\text{ref}} = 2 - g.$$

### Finding the correlation energy

Let us take a quick recap of what we have done so far. In exercise 2 we defined an ansatz ground state and then found the possible 2p2h and 4p4h excitations from this ansatz ground state. This gave us a complete orthogonal basis for our system. With a complete basis, we could represent the Hamiltonian as a matrix and diagonalize it to find the lowest eigenvalue of the Hamiltonian, which by definition is the ground state energy. As we had a complete basis, we knew our result was actually the exact solution for our system.

In exercise 3 we tried truncating the 4p4h excitation, meaning we no longer had a complete basis. By diagonalizing the Hamiltonian in this incomplete basis, we found a ground state energy, but this time it was an approximate result. Due to the variational principle we expected this aprroximation to lie above the exact result, which it did for $g = 0$.

Now, in this exercise, we have looked at the Hartree-Fock method. It is important to remember that the Hartree-Fock method simply finds the single Slater determinant with the lowest energy of the system. There is no guarantee that the ground state energy is actually given by a single Slater determinant, instead it must usually be expressed as a linear combination of different SDs, such as we did in exercise 2 and 3. The Hartree-Fock method therefore doesn't find the exact energy, and it doesn't really aim to do that at all—it simply finds the reference energy.

Now, this means that we have the exact solution, which is given by a combination of different SDs, and we have the reference energy, the best single SD energy. The difference between these two energies is known as the correleation energy, so we have

$$E_{\text{exact}} = E_{\text{correlation}} + E_{\text{ref}}.$$

As we know the exact energy from exercise 2, and found the reference energy in this exercise, we can easily compute the correlation energy as a function of $g$. The results of these calculations is shown in figure 3.

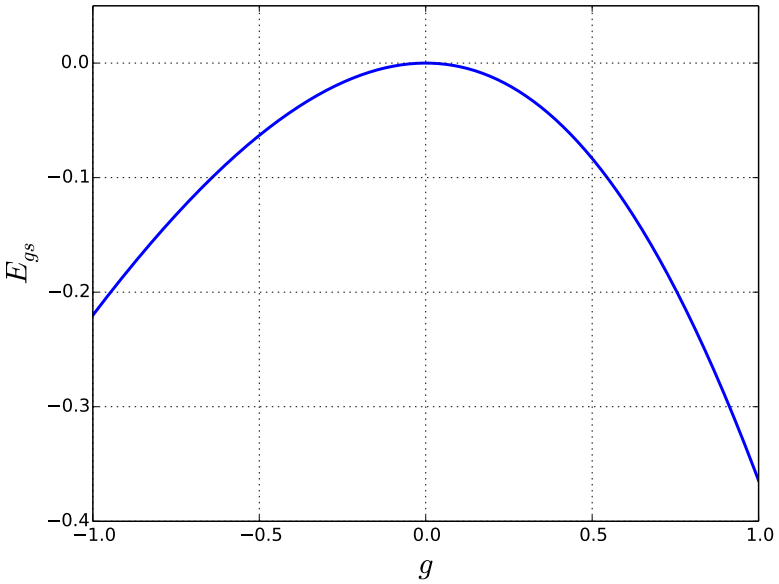



**Figure 3.** The correlation energy of the system as a function of the interaction strength.

Note that the correlation energy is only 0 for $g = 0$. This means that only the case where there is no interaction has a ground state that can be described by a single Slater determinant.

## Perturbation theory

We just saw how the Hartree-Fock method gave us the reference energy. Now we want to find some approximate method that can give us the *correlation energy*. To do that, we turn to many-body perturbation theory. The basis for this method is quite elaborate, so we won't go into details now, but they can be found in for example Shavitt and Bartlett.

We first look at perturbation to the third order. The zero and first order combined simply gives us the reference energy, and as we are interested in the correlation energy, we look at the second and third orders only. All possible second and third order contributions are shown in figure 2. We will now discuss which of these diagrams are important in our case. Let us start by looking in detail and 1 and 2, simply to see the system of the diagrams, and then we will go through the rest of the diagrams a bit faster.

Diagrams 1 and 2 are the only two diagrams that form the second order contribution. All the diagrams are drawn as anti-symmetric Goldstone diagrams, and we must remember to include a Resolvent line between any vertical set of operators, even

tough they are not drawn in. Looking at diagram 1, we can interpret this diagram as

$$(\text{diag. } 1) = \frac{1}{4}\sum_{abij}\frac{\langle ab||ij\rangle\langle ij||ab\rangle}{\epsilon_{ij}^{ab}}.$$

Here, the matrix elements in the denominator are found from the two-body operator at the top and bottom, as we are looking at the product, the order is unimportant. The numerator is given by the resolvant line, and is given by what hole lines and particle lines cross the resolvant line. The term $\epsilon_{ij}^{ab}$ should be interpred as

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

The sums over $a, b, i$ and $j$ are implicit as we have two hole and two particle lines. Finally, the 1/4 weight-factor is added because the two particle and two hole lines are both equivalent, so each pair adds a factor of 1/2.

Similarily for figure 2, remembering the resolvant line, we get

$$(\text{diag. } 2) = \sum_{ai}\frac{\langle a|\hat{f}|i\rangle\langle i|\hat{f}|a\rangle}{\epsilon_i^a}.$$

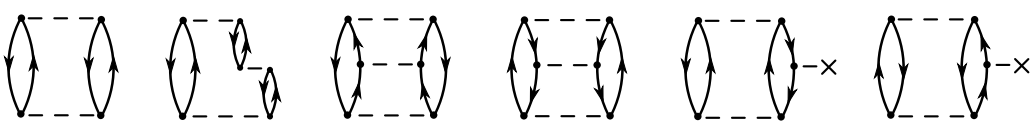
This time we only get a sum over $a$ and $i$ as we have a single particle and single hole line. No equivalent lines means to extra weight factors. The resolvent in the denominator becomes $\epsilon_i^a = \epsilon_i - \epsilon_a$ as it is only crossed by two lines. The denominator is given by the two one-body matrix elements, the order is unimportant. This figures shows and important result, as figure 2 has both $f_{ai}$ and $f_{ia}$ in the denominator, it vanishes for a Hartree-Fock basis—figure 2 only has to be included in the general case.

The interpretations of the third order figures is completely analogous. The main difference is that since there's three operatos working, the denominator will in each case consist of the product of three matrix elements and the numerator will be the product of two resolvant contributions. Let us look at diagram 4 as an example, it becomes

$$(\text{diag. } 4) = \frac{1}{8}\sum_{abcdij}\frac{\langle ab||ij\rangle\langle ab||cd\rangle\langle cd||ij\rangle}{\epsilon_{ij}^{ab}\epsilon_{ij}^{cd}}.$$

Now that we have looked at some examples, we noted that figure 2 vanishes for the Hartree-Fock case. Looking at the third-order diagrams, we recognize that diagrams 6, 7, 10, 11, 12, 13, 14, 15 and 16 all vanish in the HF case as they are multiplied with at least one $f_{ai}$ matrix element. Note that diagrams 8 and 9 do *not* necessarily vanish in the HF-case, as they only have $f_{ab}$ and $f_{ij}$ elements, which can be non-zero in both the cannonical and non-cannonical cases. In fact, the only *general* difference between the cannonical and non-cannonical cases is that diagrams 8 and 9 will contribute only a single term for the canonnical HF-case (the diagonal term), while they will contribute the complete sum for the non-cannonical term.

The diagrams that generally contribute in the HF-case are then




Now, the discussion of the diagrams so far has not used any information about our specific interaction, and the results so far is true for any interaction. Now however, we will use our knowledge of our interaction to simplify things even further.

If we write out diagram three, we see that it has the form

$$(\text{diag. } 3) = \sum_{abcijk} \frac{\langle ij||ab\rangle\langle ac||jk\rangle\langle bk||ci\rangle}{\epsilon_{ij}^{ab}\epsilon_{kj}^{ac}}.$$

The one-body contribution is given by $\langle\alpha|\hat{h}_0|\gamma\rangle = \delta_{\alpha\gamma}(p-1)$. The two-body contribution becomes a sum over the four hole states, we have

A general Slater determinant

Diagram 3 vanishes due to the nature of the interaction.

Diagram 2 is only in non-can, diagram 6, 7, 6, 10, 11, 12, 13, 14, 15 and 16 all vanish.

We define the reference vacuum, which is our ansatz for the ground state $|\Phi_0\rangle$. We can define 1p-1h and 2p-2h excitations as $\hat{T}_1|\Phi_0\rangle$ and $\hat{T}_2|\Phi_0\rangle$.

We usually use the non-interacting part of the Hamiltonian as our single-particle wave functions.

We can then expand our exact ground state as

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

Where we have introduced the correlation operators

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

We now set $C_0 = 1$, giving

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

$$|\Psi_0\rangle = \sum_{PH} C_H^P \Phi_H^P.$$

For all PH sets we get

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

In Perturbation theory we assume that the exact ground state wave function is dominated by $|\Phi_0\rangle$ and can be written in intermediate normalization as

$$|\Psi_0\rangle = |\Phi_0\rangle + \sum_{m=1}^{\infty} C_m |\Phi_m\rangle.$$

From the Schrödinger equation, we have

$$\langle \Phi_0 | \hat{H} | \Psi_0 \rangle = E,$$

And

$$\langle \Psi_0 | \hat{H}_0 | \Phi_0 \rangle = W_0,$$

so we can define

$$\Delta E = E - W_0 = \langle \Phi_0 | \hat{H}_I | \Psi_0 \rangle.$$

This quantity is called the correlation energy.

$$\hat{P} = |\Phi_0\rangle\langle\Phi_0|,$$

$$\hat{Q} = \sum_{m=1}^{\infty} |\Phi_m\rangle\langle\Phi_m|.$$

$$|\Psi_0\rangle = (\hat{P} + \hat{Q})|\Psi_0\rangle = |\Phi_0\rangle + \hat{Q}|\Psi_0\rangle.$$

$$\chi_n = |\Psi_n\rangle - |\Phi_n\rangle.$$

$$\langle \Phi_n | \Phi_n \rangle = 1, \quad \langle \Psi_n | \Phi_n \rangle = 1, \quad \langle \chi_n | \Phi_n \rangle = 0, \quad \langle \Psi_n | \Psi_n \rangle = 1 + \langle \chi_n | \chi_n \rangle.$$

Idempotenence

$$\hat{P}^2 = \hat{P}, \quad \hat{Q}^2 = \hat{Q}$$

$$\hat{P}\hat{Q} = 0.$$

The operator $\hat{P}$ projects the component of $\Psi$ that is parallel to $\Phi_0$, which can be seen from

$$\hat{P}\Psi = \sum_{a_i} |\Phi_0\rangle\langle\Phi_0||\Phi_i\rangle = a_0|\Phi_0\rangle.$$

While $\hat{Q}$ annihilates the $\Phi_0$ component, leaving everything else intact. This also means that

$$\Psi = (\hat{P} + \hat{Q})\Psi.$$

## Exercise 6)

# Exercise 7)

### Linked and unlinked diagrams

A diagram is called unlinked if and only if it has a disconnected part that is closed, meaning it has no open lines. Goldstones linked-diagram theorem states that all unliked diagrams will cancel agains the renormalization terms in RSPT, meaning we can express the energy and wave function in each order as a sum of linked diagrams only [1].

[1] See Shavitt and Bartlet section 5.8.

In general, we have

$$\left(E^{(0)-\hat{H}}\right)\Psi^{(m)} = (E^{(1)} - \hat{V})\Psi^{(m-1)} - \sum_{l=0}^{m-1} E^{m-l}\Psi^{(l)}.$$

We can apply $\langle\Phi|$ to the equation and find

$$E^{(m)} = \langle\Phi|\hat{V}|\Psi^{(m-1)}\rangle.$$

As $\xi$ is only a scalar that is multiplied with $H_0$, and we already the scaling $g$, we can se the parameter $\xi$ equal to 1, without a loss of generality.

Decompose the solution into

$$\Psi = (\hat{P} + \hat{Q})\Psi = \hat{P}\Psi + \hat{Q}\Psi = \Phi + \chi.$$

$$\Psi = \sum_{m=0}^{\infty} \left[\hat{R}_0(\hat{V} - \hat{E})\right]^m \Phi,$$

$$\Delta E = \sum_{m=0}^{\infty} \langle\Phi|\hat{V}\left[\hat{R}_0(\hat{V} - \hat{E})\right]^m|\Phi\rangle$$

Cannonical HF

$$f_{pq} = \epsilon_p \delta_{pq}$$

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

Non-cannonical HF

$$f_{ia} = 0.$$

Fock-operator

$$\hat{F} = \sum_{pq} f_{pq}\hat{p}^\dagger\hat{q}.$$

$$\hat{U} = \sum_{pq} u_{pq}\hat{p}^\dagger\hat{q}.$$

$$\hat{F} = \hat{H}_0 + \hat{U} = \sum_{pq}(h_{pq} + u_{pq})\hat{p}^\dagger\hat{q}.$$

$$\hat{u} = \sum_i (\hat{J}_i - \hat{K}_i).$$

The normal-product Schrodinger equation is

$$\hat{H}_{\mathrm{N}}\Psi = \Delta E\Psi,$$

where $\Delta E$ is the correlation energy in the Hartree-Fock case, the normal-product Hamiltonian is

$$\hat{H}_{\mathrm{N}} = \hat{F}_{\mathrm{N}} + \hat{W} = \hat{F}^d_{\mathrm{N}} + \hat{F}^o + \hat{W} = \hat{F}^d + \hat{V}_{\mathrm{N}}.$$

The projection operator $\hat{P}$ projects onto the model space, which is spanned by the reference function, so $\hat{P} = |\Phi_0\rangle\langle\Phi_0|$.

Quote from page 132 of Shavitt and Bartlett "The absence of single excitations from the second-order energy expression in the HF case is a reflection of the Brillouin theorem, Sec. 15 which states that for Hartree.Fock reference functions"