Second Midterm Project FYS-KJM4480

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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

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

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

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

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

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

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

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

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

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

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

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

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

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

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 σ, 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 σ, which makes the entire commutator vanish, as the two Kronecker-delta's with σcancel 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

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

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

Summary of commutators

We have shown that $\hat{H}_0$ and $\hat{V}$ both commute with $\hat{S}_z$, $\hat{S}_\pm$ and $\hat{S}^2$.

Pair operators commutation relations

For the creation and annihilation operators we have the anti-commutation relations

$$\{a^\dagger_p, a_q\} = \delta_{pq}, \qquad \{a_p, a_q\} = \{a^\dagger_p, a^\dagger_q\} = 0.$$

If we then look at the pair creation and annihilation operators, we have

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

First, we swap the two middle operators

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

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

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

We again swap the two middle operators to get

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

So we see that we have

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

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

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

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

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

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.

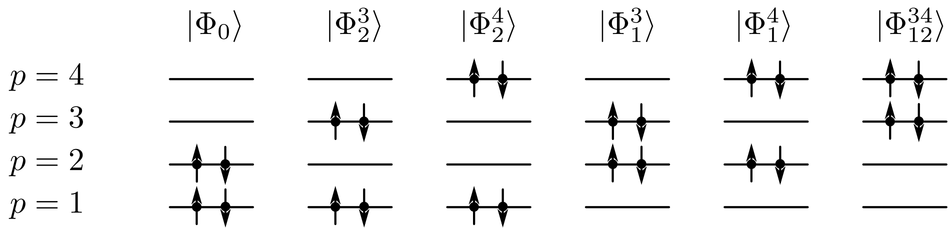

Figure 1. Sketch of the six possible Slater determinants.

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

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

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.

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

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

$$\lambda = \begin{pmatrix} 0.780 \\ 9.364 \\ 7.065 \\ 5.000 \\ 2.791 \\ 5.000 \end{pmatrix}, \quad V = \begin{pmatrix}
0.972 & -0.041 & -0.104 & -0.154 & -0.136 & 0.004 \\
-0.185 & -0.101 & -0.014 & -0.309 & -0.927 & 0.008 \\
-0.089 & -0.154 & -0.170 & -0.617 & 0.242 & -0.691 \\
-0.089 & -0.154 & -0.170 & -0.617 & 0.242 & 0.723 \\
-0.066 & -0.271 & -0.908 & 0.309 & -0.046 & -0.008 \\
0.026 & -0.931 & 0.326 & 0.154 & 0.039 & -0.004
\end{pmatrix}.$$

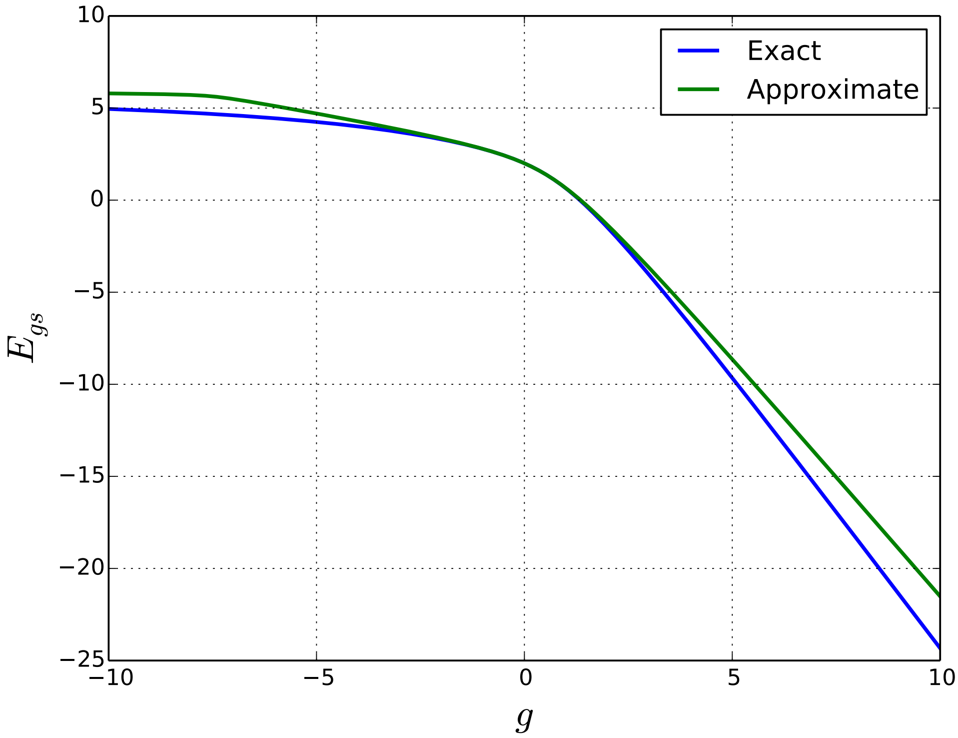

Figure 2. Ground state energy as a function of the interaction-parameter g.

Exercise 3)

We now limit our system to at most two-particle-two-hole excitations. This means we discard $|\Phi^{34}\rangle$, and only look at a five-dimensional system.

The Hamiltonian matrix is then the five-by-five matrix

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

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

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

Calculating the Fock-matrix

The Fock-operator is given by a h_{pq} term and a u_{pq} term

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

For our system, the one-body operator is given by

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

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 σ, 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 Fock-matrix as

$$F = \begin{pmatrix} -g/2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -g/2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1-g/2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1-g/2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 \end{pmatrix}$$

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

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.

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

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

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

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

If we are looking at canonical HF

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

If we are looking at non-canonical HF

Exercise 5)

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 Ψ that is parallel to Φ_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 Φ_0 component, leaving everything else intact. This also means that

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

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]. This means we have

[1]See Shavitt and Bartlet section 5.8.

In general, we have

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

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

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

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

Decompose the solution into

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

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

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

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 ΔE 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 $\hat{P} = |\Phi_0\rangle\langle\Phi_0|$.