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

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

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

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

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

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

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 $\hat{S}^2$.

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

$$|\Phi^{12}\rangle = \hat{P}_1^+ \hat{P}_2^+ |0\rangle, \qquad |\Phi^{13}\rangle = \hat{P}_1^+ \hat{P}_3^+ |0\rangle, \qquad |\Phi^{14}\rangle = \hat{P}_1^+ \hat{P}_4^+ |0\rangle,$$
$$|\Phi^{23}\rangle = \hat{P}_2^+ \hat{P}_3^+ |0\rangle, \qquad |\Phi^{24}\rangle = \hat{P}_2^+ \hat{P}_4^+ |0\rangle, \qquad |\Phi^{34}\rangle = \hat{P}_3^+ \hat{P}_4^+ |0\rangle.$$

These Slater determinants are illustrated in figure 1.

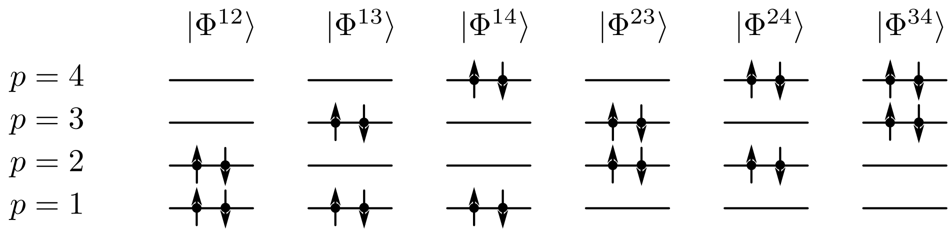

Figure 1. Sketch of the six possible Slater determinants.

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

$$\sum_{p\sigma} (p-1) a_{p\sigma}^\dagger a_{p\sigma},$$

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

$$\langle \Phi^{12} | \hat{H}_0 | \Phi^{12} \rangle = 2, \qquad \langle \Phi^{12} | \hat{H}_0 | \Phi^{12} \rangle = 4, \qquad \langle \Phi^{12} | \hat{H}_0 | \Phi^{12} \rangle = 6,$$
$$\langle \Phi^{12} | \hat{H}_0 | \Phi^{12} \rangle = 6, \qquad \langle \Phi^{12} | \hat{H}_0 | \Phi^{12} \rangle = 8, \qquad \langle \Phi^{12} | \hat{H}_0 | \Phi^{12} \rangle = 10.$$

For the two-body operator we have

$$\langle \Phi^{ij} | \hat{V} | \Phi^{kl} \rangle = -\frac{g}{2} \sum_{pq} \langle 0 | \hat{P}_i \hat{P}_j \hat{P}_p^+ \hat{P}_q \hat{P}_k^+ \hat{P}_l^+ | 0 \rangle.$$

There can be two, one or no non-coincidences between the Slater determinants. If there are two non-coincidences, we see that the matrix element vanishes as we can only remove one non-coincidence. If there is one non-coincidence we have

$$\langle \Phi^{ij} | \hat{V} | \Phi^{ik} \rangle = -\frac{g}{2} \sum_{pq} \langle 0 | \hat{P}_i \hat{P}_j \hat{P}_p^+ \hat{P}_q \hat{P}_i^+ \hat{P}_k^+ | 0 \rangle.$$

When we sum over p and q, the only term that survives is the term were $p = j$ and $q = k$, all other terms vanish due to the orthogonality of the the Slater determinants, so we

If there are no non-coincidences, we have

$$\langle\Phi^{ij}|\hat{V}|\Phi^{ij}\rangle = -\frac{g}{2}\sum_{pq}\langle 0|\hat{P}_i\hat{P}_j\hat{P}_p^+\hat{P}_q\hat{P}_i^+\hat{P}_j^+|0\rangle$$

The only terms that survive in the sums are now the terms were $p = q = i$ or $p = q = j$, so we get two terms contributing to the final result.

We can then set 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

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

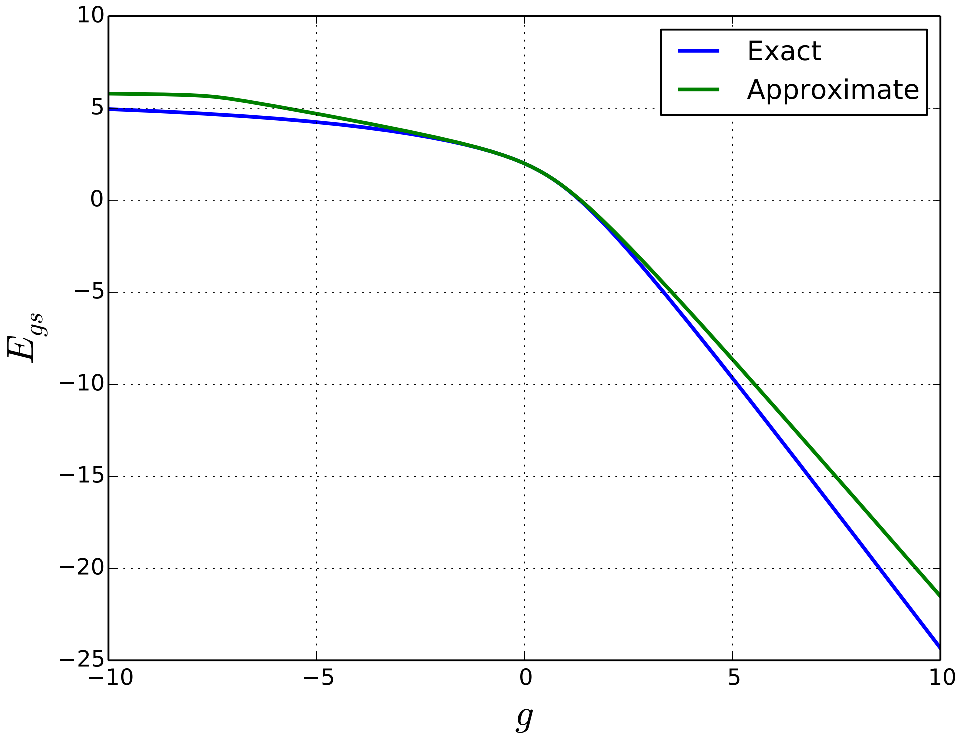

Figure 2. Ground state energy as a function of the interaction-parameter g.

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

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

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 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.

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

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

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

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

If we are looking at canonical HF

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

If we are looking at non-canonical HF

Exercise 5)

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