Midterm 2

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1 Quantum mechanics for many-particle systems

a)

For this exercise, we will use the commutation relations:

$$[A, BC] = [A, B]C + B[A, C]$$

and

$$[AB, CD] = A[B, C]D + AC[B, D] + [A, C]DB + C[A, D]B$$

We want to show that $\hat{H}_0$ and $\hat{V}$ commutes with $\hat{S}_z$ and $\hat{S}^2$.
The operators are defined as:

$$\hat{H}_0 = \xi \sum_{p\sigma} (p-1) a^\dagger_{p\sigma} a_{p\sigma}$$

$$\hat{V} = \sum_{pq} a^\dagger_{p-} a^\dagger_{p+} a_{p-} a_{p+}$$

$$\hat{S}_z = \sum_{p\sigma} \sigma a^\dagger_{p\sigma} a_{p\sigma}$$

$$\hat{S}^2 = \hat{S}_z^2 + \frac{1}{2}(\hat{S}_+ \hat{S}_- + \hat{S}_- \hat{S}_+)$$

Where $\hat{S}_\pm = \sum_p a^\dagger_{p\pm} a_\mp$, $\sigma = \pm 1$ for spin and $p = 1, 2, ...$ is the index for the single-particle states.
We start by showing that $\hat{H}_0$ commutes with $\hat{S}_z$:

$$[\hat{H}_0, \hat{S}_z] = \xi \sum_{p\sigma} (p-1) [a^\dagger_{p\sigma} a_{p\sigma}, \sum_\tau \tau a^\dagger_{q\tau} a_{q\tau}]$$

Lets take the operators to the side and look at those first:

$$[a_{p\sigma^\dagger a_{p\sigma}}, a^\dagger_{q\tau} a_{q\tau}]$$

$$= a^\dagger_{p\sigma}[a_{p\sigma}, a^\dagger_{q\tau}]a_{q\tau} + a^\dagger_{p\sigma} a^\dagger_{q\tau}[a_{p\sigma}, a_{q\tau}] + [a^\dagger_{p\sigma}, a^\dagger_{q\tau}]a_{p\sigma} a_{q\tau} + a^\dagger_{q\tau}[a^\dagger_{p\sigma}, a_{q\tau}]a_{p\sigma}$$

Two creation operators commute and two annihilation operators commute, so two of them er directly zero, while the other two leaves croenecker deltas

$$= a^\dagger_{p\sigma}\delta_{pq}\delta_{\sigma\tau}a_{q\tau} - a^\dagger_{q\tau}\delta_{pq}\delta_{\sigma\tau}a_{p\sigma}$$

$$[\hat{H}_0, \hat{S}_z] = \xi\sum_{p\sigma}(p-1)[a^\dagger_{p\sigma}a_{p\sigma}, \sum_\tau \tau a^\dagger_{q\tau}a_{q\tau}]$$

$$= \xi\sum_{p\sigma}(p-1)\sum_\tau \tau(a^\dagger_{p\sigma}\delta_{pq}\delta_{\sigma\tau}a_{q\tau} - a^\dagger_{q\tau}\delta_{pq}\delta_{\sigma\tau}a_{p\sigma}) = 0$$

Now we want to show that $\hat{H}_0$ commutes with $\hat{S}^2$.

$$[\hat{H}_0, \hat{S}^2] = [H_0, S_z^2] + \frac{1}{2}([H_0, S_+S_-] + [H_0, S_-S_+])$$

We know that $[H_0, S_z] = 0$ and therefor the first term is zero.
Lets look at the second term:

$$[H_0, S_+S_-] = \xi\sum_{pq\sigma}(p-1)[a^\dagger_{p\sigma}a_{p\sigma}, a^\dagger_{q+}a_{q-}a^\dagger_{q-}a_{q+}]$$

$$= \xi\sum_{pq\sigma}(p-1)\left([a^\dagger_{p\sigma}a_{p\sigma}, a^\dagger_{q+}a_{q-}]a^\dagger_{q-}a_{q+} + a^\dagger_{q-}a_{q+}[a^\dagger_{p\sigma}a_{p\sigma}, a^\dagger_{q+}a_{q-}]\right)$$

$$= \xi\sum_{pq\sigma}(p-1)\Big(\left(a^\dagger_{p\sigma}[a_{p\sigma}, a^\dagger_{q+}]a_{q-} + a^\dagger_{p\sigma}a_{q-}[a_{p\sigma}, a^\dagger_{q+}]\right)a^\dagger_{q-}a_{q+}$$

$$+a^\dagger_{q+}a_{q-}\left(a^\dagger_{p\sigma}[a_{p\sigma}, a^\dagger_{q-}]a_{q+} + a^\dagger_{p\sigma}a_{q+}[a_{p\sigma}, a^\dagger_{q-}]\right)\Big)$$

$$= \xi\sum_{p\sigma}(p-1)\Big(\left(a^\dagger_{p+}a_{p-} - a^\dagger_{p+}a_{p-}\right)a^\dagger_{p-}a_{p+} + a^\dagger_{p+}a_{p-}\left(a^\dagger_{p-}a_{p+} - a^\dagger_{p-}a_{p+}\right)\Big) = 0$$

The same goes for the last term, and therefor $[H_0, S^2] = 0$
Now we can move over to check if $\hat{V}$ commutes with $\hat{S}_z$ and $\hat{S}^2$. First we check if $\hat{V}$ commutes with $\hat{S}_z$:

$$[\hat{V}, \hat{S}_z] = \frac{1}{4}g[\sum_{pq} a^\dagger_{p-}a^\dagger_{p+}a_{q-}a_{q+}, \sum_{r\sigma}\sigma a^\dagger_{r\sigma}a_{r\sigma}]$$

$$= \frac{1}{4}g\sum_{pqr}\sigma\Big(a^\dagger_{p+}a^\dagger_{p-}[a_{q-}a_{q+}, a^\dagger_{r\sigma}a_{r\sigma}] + [a^\dagger_{p+}a^\dagger_{p-}, a^\dagger_{r\sigma}a_{r\sigma}]a_{q-}a_{q+}\Big)$$

The first term:

$$[a_{q-}a_{q+}, a^\dagger_{r\sigma}a_{r\sigma}] = a_{q-}[a_q+, a^\dagger_{r\sigma}]a_{r\sigma} + a_{q-}a^\dagger_{r\sigma}[a_{q+}, a_{r\sigma}]$$

$$+[a_{q-}, a^\dagger_{r\sigma}]a_{r\sigma}a_{q+} + a^\dagger_{r\sigma}[a_{q-}, a_{r\sigma}]a_{q+}$$

Where the only surviving therm, the ones with one creation and one annihilation operator, are:

$$= a_{q-}\delta_{qr}\delta_{\sigma+}a_{r\sigma} + a_{q+}\delta_{qr}\delta_{\sigma-}a_{r\sigma}$$

$$= a_{q-}a_{q+} + a_{q+}a_{q-}$$

Now the second term:

$$[a^\dagger_{p+}a^\dagger_{p-}, a^\dagger_{r\sigma}a_{r\sigma}] = a^\dagger_{p+}[a^\dagger_{p-}, a^\dagger_{r\sigma}]a_{r\sigma} + a^\dagger_{p+}a^\dagger_{r\sigma}[a^\dagger_{p-}, a_{r\sigma}]$$

$$+[a^\dagger_{p+}, a^\dagger_{r\sigma}]a_{r\sigma}a^\dagger_{p-} + a^\dagger_{r\sigma}[a^\dagger_{p+}, a_{r\sigma}]a^\dagger_{p-}$$

Where the only surviving therm, the ones with one creation and one annihilation operator, are:

$$= -a^\dagger_{p+}\delta_{pr}\delta_{\sigma-}a_{r\sigma} - a^\dagger_{p-}\delta_{pr}\delta_{\sigma+}a_{r\sigma}$$

$$= a^\dagger_{p+}a_{p-} + a^\dagger_{p-}a_{p+}$$

Now we can put the two results back into the first expression, and we can see that it simply reduces to zero.

$$= \frac{1}{4}g\sum_{pq}\sigma\Big(a^\dagger_{p+}a^\dagger_{p-}(a_{q-}a_{q+} + a_{q-}a_{q+}) - a_{q-}a_{q+}(a^\dagger_{p+}a^\dagger_{p-} + a^\dagger_{p+}a^\dagger_{p-})\Big) = 0$$

And now we can check if $\hat{V}$ commutes with $\hat{S}^2$:

$$[\hat{V}, \hat{S}^2] = [\hat{V}, \hat{S}^2_z] + \frac{1}{2}\Big([\hat{V}, S_+\hat{S}_-] + [\hat{V}, S_-\hat{S}_+]\Big)$$

The first term is zero from the fact that $\hat{V}$ commutes with $\hat{S}_z$. The second term is:

$$[\hat{V}, \hat{S}_+\hat{S}_-] = -\frac{1}{2}g\sum_{pq}[a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}, \sum_r a^\dagger_{r+}a_{r-}a^\dagger_{r-}a_{r+}]$$

$$= -\frac{1}{2}g\sum_{pqr}\Big(a^\dagger_{p+}a^\dagger_{p-}[a_{q-}a_{q+}, a^\dagger_{r+}a_{r-}]a^\dagger_{r-}a_{r+}$$

$$+a^\dagger_{p+}a^\dagger_{p-}a^\dagger_{r+}a_{r-}[a_{q-}a_{q+}, a^\dagger_{r-}a_{r+}]$$

$$+[a^\dagger_{p+}a^\dagger_{p-}, a^\dagger_{r+}a_{r-}]a^\dagger_{r-}a_{r+}a_{q-}a_{q+}$$

$$+a^\dagger_{r+}a_{r-}[a^\dagger_{p+}a^\dagger_{p-}, a^\dagger_{r-}a_{r+}]a_{q-}a_{q+}\Big)$$

I will seperate the commutations and look at them one by one. The first term:

$$[a_{q-}a_{q+}, a^\dagger_{r+}a_{r-}] = a_{q-}[a_{q+}, a^\dagger_{r+}]a_{r-} + a_{q-}a^\dagger_{r+}[a_{q+}, a_{r-}] + [a_{q-}, a^\dagger_{r+}]a_{r-}a_{q+} + a_{r-}[a_{q-}, a^\dagger_{r+}]a_{q+}$$

$$= a_{q-}\delta_{qr}\delta_{++}a_{r-} + \delta_{qr}\delta_{+-}a_{r-}a_{q+} = a_{q-}a_{q-}$$

The second term:

$$[a_{q-}a_{q+}, a^\dagger_{r-}a_{r+}] = a_{q-}[a_{q+}, a^\dagger_{r-}]a_{r+} + a_{q-}a^\dagger_{r-}[a_{q+}, a_{r-}] + [a_{q-}, a^\dagger_{r-}]a_{r+}a_{q+} + a^\dagger_{r-}[a_{q-}, a_{r+}]a_{q+}$$

$$= a_{q-}\delta_{qr}\delta_{+-}a_{r+} + \delta_{qr}\delta_{+-}a_{r+}a_{q+} = a_{q+}a_{q+}$$

The third term:

$$[a^\dagger_{p+}a^\dagger_{p-}, a^\dagger_{r+}a_{r-}] = a^\dagger_{p+}[a^\dagger_{p-}, a^\dagger_{r+}]a_{r-} + a^\dagger_{p+}a^\dagger_{r+}[a^\dagger_{p-}, a_{r-}] + [a^\dagger_{p+}, a^\dagger_{r+}]a_{r-}a^\dagger_{p-} + a^\dagger_{r+}[a^\dagger_{p+}, a_{r-}]a^\dagger_{p-}$$

$$= -a^\dagger_{p+}a^\dagger_{r+}\delta_{pr}\delta_{--} - a^\dagger_{r+}\delta_{pr}\delta_{+-}a^\dagger_{p-} = -a^\dagger_{p+}a^\dagger_{p+}$$

The fourth term:

$$[a^\dagger_{p+}a^\dagger_{p-}, a^\dagger_{r-}a_{r+}] = a^\dagger_{p+}[a^\dagger_{p-}, a^\dagger_{r-}]a_{r+} + a^\dagger_{p+}a^\dagger_{r-}[a^\dagger_{p-}, a_{r+}] + [a^\dagger_{p+}, a^\dagger_{r-}]a_{r+}a^\dagger_{p-} + a^\dagger_{r-}[a^\dagger_{p+}, a_{r+}]a^\dagger_{p-}$$

$$= -a^\dagger_{p+}a^\dagger_{r-}\delta_{pr}\delta_{-+} - a^\dagger_{r-}\delta_{pr}\delta_{++}a^\dagger_{p-} = -a^\dagger_{p-}a^\dagger_{p-}$$

Now we can put the results back into the expression, and since r is equal to either p or q, we can adjust acording to this:

$$= -\frac{1}{2}g\sum_{pq}\Big(a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q-}a^\dagger_{q-}a_{q+}$$

$$+a^\dagger_{p+}a^\dagger_{p-}a^\dagger_{q+}a_{q-}a_{q+}a_{q+}$$

$$-a^\dagger_{p+}a^\dagger_{p+}a^\dagger_{p-}a_{p+}a_{q-}a_{q+}$$

$$-a^\dagger_{p+}a_{p-}a^\dagger_{p-}a^\dagger_{p-}a_{q-}a_{q+}\Big)$$

All of these terms are zero, because if we look closely, we can either see that each term is trying to annihilate the same state twice. For the seconf and third term this happens directly, while for the first and last term, this happens when trying to normal order the operators.
The last term is the same as the second term, because of the commutation relations between $\hat{S}_+$ and $\hat{S}_-$, and therefor the result is zero.
This means that $\hat{V}$ commutes with $\hat{S}^2$.
We can now introduce the pair-creation and pair-annihilation operators:

$$\hat{P^+_p} = a^\dagger_{p+}a^\dagger_{p-}$$

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

Lets re-introduce the $\hat{V}$ operator:

$$\hat{V} = -\frac{1}{2}g\sum_{pq}a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}$$

From this we can easily see that we can write $\hat{V}$ as:

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

And therefor we can write the $\hat{H}$, with $\xi = 1$ as:

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

And laslty we want to show that the pair creation operators commutes among themselves:

$$[\hat{P^+_p}, \hat{P^+_q}] = [a^\dagger_{p+}a^\dagger_{p-}, a^\dagger_{q+}a^\dagger_{q-}]$$

$$a^\dagger_{p+}[a^\dagger_{p-}, a^\dagger_{q+}]a^\dagger_{q-} + a^\dagger_{p+}a^\dagger_{q+}[a^\dagger_{p-}, a^\dagger_{q-}] + [a^\dagger_{p+}, a^\dagger_{q+}]a^\dagger_{q-}a^\dagger_{p-} + a^\dagger_{q+}[a^\dagger_{p+}, a^\dagger_{q-}]a^\dagger_{p-}$$

All these terms are zero, because commuting two creation or annihilation operators will give zero.

b)

For this part we want to construct the Hamiltonian matrix for a system with no broken pairs and total spin of $S = 0$, for the case of the four lowest single-particle states.
We can start by defining a state with total spin $S = 0$:

$$\left|\Phi_{\alpha\beta}\right\rangle = P_\alpha^+ P_\beta^+ \left|0\right\rangle$$

For our case, the slater determinants will be:

$$\begin{aligned}
\left|\Phi_0\right\rangle &= P_1^+ P_2^+ \left|0\right\rangle \\
\left|\Phi_1\right\rangle &= P_1^+ P_3^+ \left|0\right\rangle \\
\left|\Phi_2\right\rangle &= P_1^+ P_4^+ \left|0\right\rangle \\
\left|\Phi_3\right\rangle &= P_2^+ P_3^+ \left|0\right\rangle \\
\left|\Phi_4\right\rangle &= P_2^+ P_4^+ \left|0\right\rangle \\
\left|\Phi_5\right\rangle &= P_3^+ P_4^+ \left|0\right\rangle
\end{aligned}$$

We will start by finding the expectation value of the one body term:

$$\left\langle\Phi_{\alpha\beta}\right| \hat{H}_0 \left|\Phi_{\alpha\beta}\right\rangle = \left\langle\Phi_{\alpha\beta}\right| \sum_{p\sigma} (p-1) a_{p\sigma}^\dagger a_{p\sigma} \left|\Phi_{\alpha\beta}\right\rangle$$

$$= \sum_{p\sigma} (p-1) \left\langle\Phi_{\alpha\beta}\right| a_{p\sigma}^\dagger a_{p\sigma} \left|\Phi_{\alpha\beta}\right\rangle$$

Here $\sigma = \pm 1$ and p can have the values $p = \alpha, \beta$, and therefor we can write the expression as:

$$\left\langle\Phi_{\alpha\beta}\right| \hat{H}_0 \left|\Phi_{\alpha\beta}\right\rangle = 2(\alpha - 1) + 2(\beta - 1) = 2(\alpha + \beta - 2)$$

For the interraction term $\hat{V}$, we will use the indexes $\alpha, \beta, \gamma, \delta$ to represent the four lowest single-particle states. We can write the expectation value as:

$$\left\langle\Phi_{\alpha\beta}\right| \hat{V} \left|\Phi_{\alpha\beta}\right\rangle = -\frac{1}{2} g \left\langle\Phi_{\alpha\beta}\right| \sum_{pq} \hat{P_p^+} \hat{P_q^-} \left|\Phi_{\gamma\delta}\right\rangle$$

$$= -\frac{1}{2} g \sum_{pq}^{\infty} \left\langle 0\right| P_\beta^- P_\alpha^- P_p^+ P_q^- P_\gamma^+ P_\delta^+ \left|0\right\rangle$$

For this we will need to use contractions.

$$\overbrace{P_\beta^- P_\alpha^- P_p^+ P_q^- P_\gamma^+ P_\delta^+} = \delta_{\beta\delta}\delta_{\alpha p}\delta_{q\gamma}$$

$$\overbrace{P_\beta^- P_\alpha^- P_p^+ P_q^- P_\gamma^+ P_\delta^+} = \delta_{\beta\gamma}\delta_{\alpha p}\delta_{q\delta}$$

$$\overbrace{P_\beta^- P_\alpha^- P_p^+ P_q^- P_\gamma^+ P_\delta^+} = \delta_{\beta p}\delta_{\alpha\gamma}\delta_{q\delta}$$

$$\overbrace{P_\beta^- P_\alpha^- P_p^+ P_q^- P_\gamma^+ P_\delta^+} = \delta_{\beta p}\delta_{\alpha\delta}\delta_{q\gamma}$$

Usually, when we work with contraction, we will notice how many of the lines cross to determine if the term is negative or positive. One cross, and the term is negative, while

two crosses and the term is positive.
For these operators, each of them contain either two creation or two annihilation operators, and therefor the result will always be positive.
Now we can set up the matrices:

$$\hat{H}_0 = \begin{bmatrix} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 6 & 0 & 0 & 0 \\ 0 & 0 & 0 & 6 & 0 & 0 \\ 0 & 0 & 0 & 0 & 8 & 0 \\ 0 & 0 & 0 & 0 & 0 & 10 \end{bmatrix}$$

$$\hat{V} = -\frac{1}{2}g \begin{bmatrix} 2 & 1 & 1 & 1 & 1 & 0 \\ 1 & 2 & 1 & 1 & 0 & 1 \\ 1 & 1 & 2 & 0 & 1 & 1 \\ 1 & 1 & 0 & 2 & 1 & 1 \\ 1 & 0 & 1 & 1 & 2 & 1 \\ 0 & 1 & 1 & 1 & 1 & 2 \end{bmatrix}$$

The total Hamiltonian matrix will be:

$$\hat{H} = \hat{H}_0 + \hat{V} = \begin{bmatrix} 2-g & -\frac{1}{2}g & -\frac{1}{2}g & -\frac{1}{2}g & -\frac{1}{2}g & 0 \\ -\frac{1}{2}g & 4-g & -\frac{1}{2}g & -\frac{1}{2}g & 0 & -\frac{1}{2}g \\ -\frac{1}{2}g & -\frac{1}{2}g & 6-g & 0 & -\frac{1}{2}g & -\frac{1}{2}g \\ -\frac{1}{2}g & -\frac{1}{2}g & 0 & 6-g & -\frac{1}{2}g & -\frac{1}{2}g \\ -\frac{1}{2}g & 0 & -\frac{1}{2}g & -\frac{1}{2}g & 8-g & -\frac{1}{2}g \\ 0 & -\frac{1}{2}g & -\frac{1}{2}g & -\frac{1}{2}g & -\frac{1}{2}g & 10-g \end{bmatrix}$$

The following plot and the matrix elements are calculated with the code in `energies.py`
As we can see in 1 and 2, the ground state energy is decreasing as the interaction strength g increases. This is expected, as the interaction term is negative, and therefor the total energy will decrease as the interaction strength increases. While at $g = 0$ the ground state energy is $\langle \Phi_0 | \hat{H}_0 | \Phi_0 \rangle$ 2.

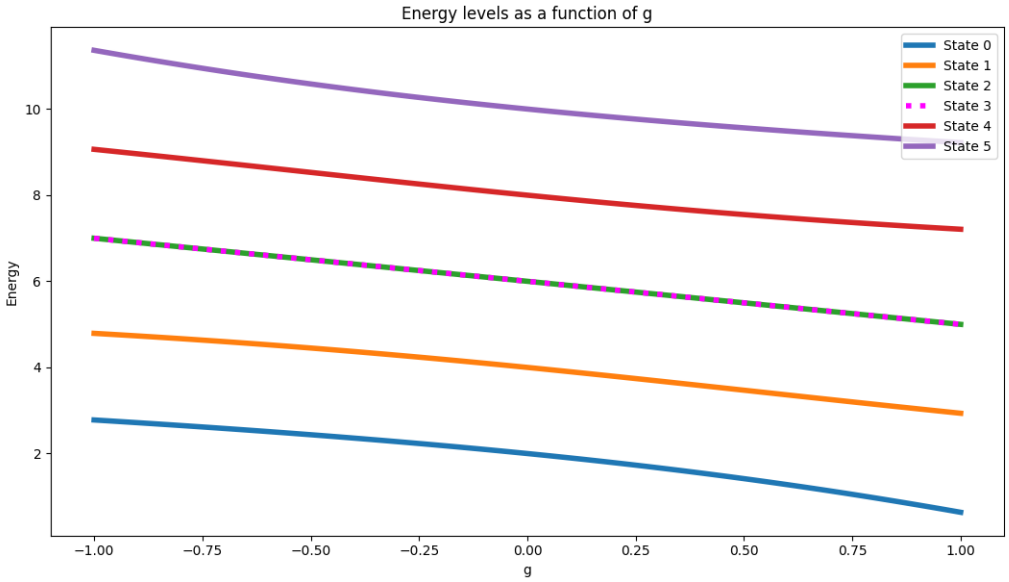

Figure 1: The Hamiltonian matrix for a system with no broken pairs and total spin of $S = 0$, for the case of the four lowest single-particle states. Energies as a function of the strength of the interaction g.The dashed lines is to show the degeneracy of the states.

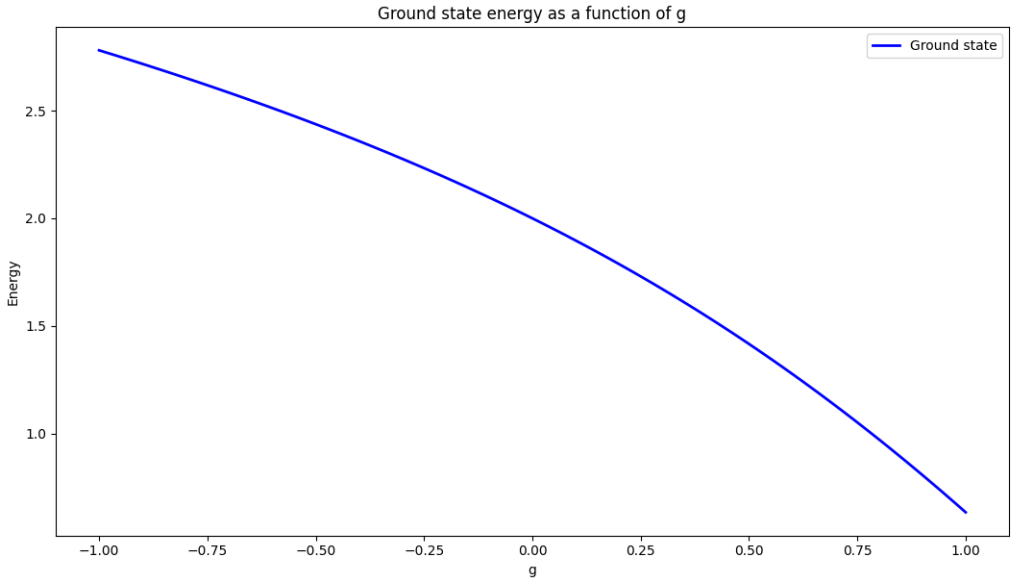

Figure 2: Ground state energy as a function of the interraction strength g.

c)

In 1 the energy levels i show are from states $|\Phi_0\rangle$ to $|\Phi_5\rangle$, more explicitly:

$$|\Phi_0\rangle = P_1^+ P_2^+ |0\rangle \, |\Phi_1\rangle = P_1^+ P_3^+ |0\rangle \, |\Phi_2\rangle = P_1^+ P_4^+ |0\rangle$$

$$|\Phi_3\rangle = P_2^+ P_3^+ |0\rangle \, |\Phi_4\rangle = P_2^+ P_4^+ |0\rangle \, |\Phi_5\rangle = P_3^+ P_4^+ |0\rangle$$

For this part we want to make an approximation to the ground state energy. For this we will use at most two-particle two-holes excitations. Hence we will approximate the ground state energy by only using the states $|\Phi_0\rangle$ and $|\Phi_4\rangle$.

In 5 we show the energy difference between the approximation and the ground state

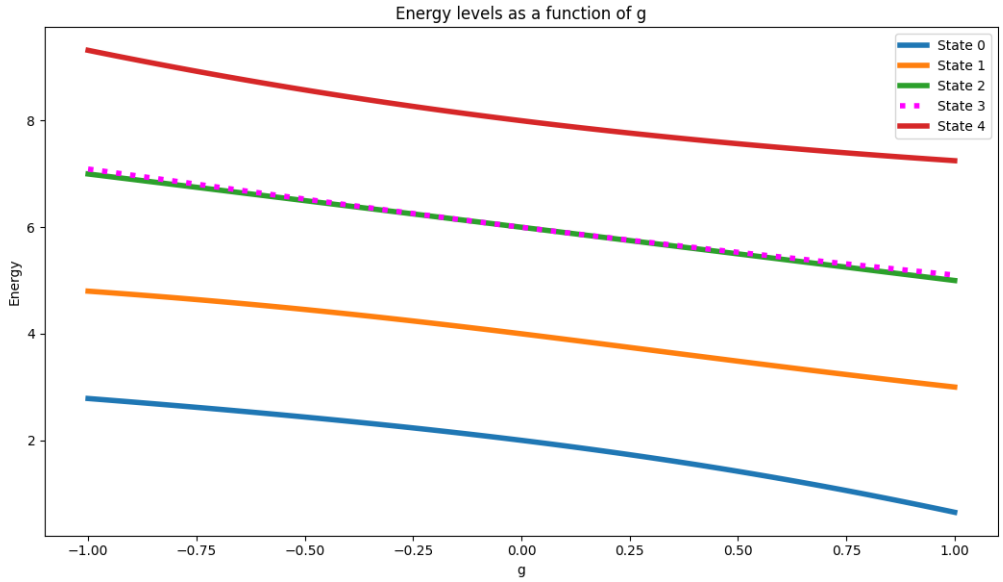

Figure 3: Excluding $|\Phi_5\rangle$. The Hamiltonian matrix for a system with no broken pairs and total spin of $S = 0$, for the case of the four lowest single-particle states. Energies as a function of the strength of the interaction g

energy. We can see that the approximation is very close to the ground state energy as the difference is very small. We can see that the energy difference is negative, meaning the approximated ground state has slightly higher energy than the true ground state energy.

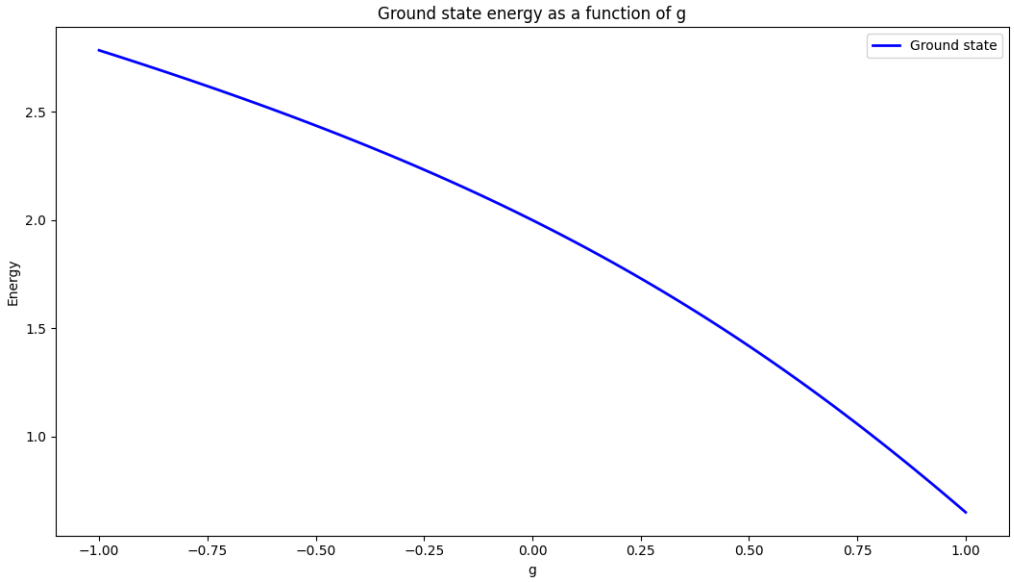

Figure 4: Ground state energy approximation as a function of the interraction strength g.

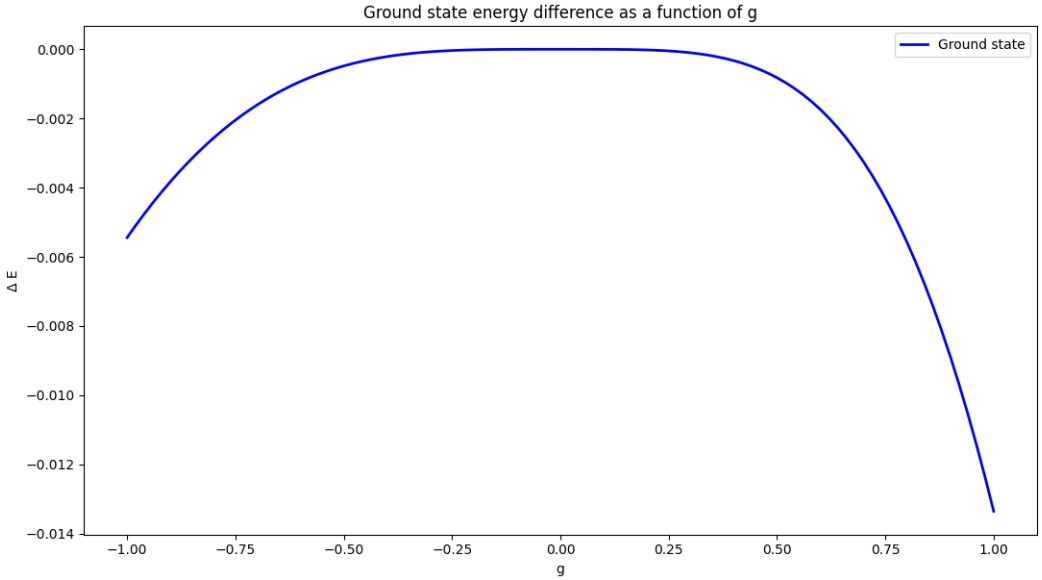

Figure 5: Difference between the ground state energy and the approximation as a function of the interraction strength g.

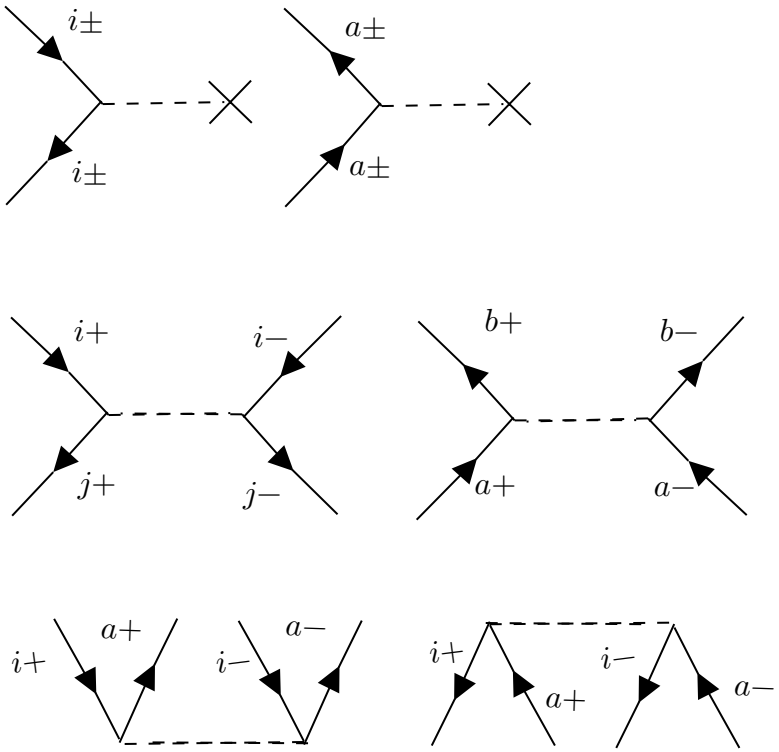

Figure 6: Diagrammatic representation corresponding to the approximation of the ground state up to two-particle two-hole excitations.

d)

The one-body operator $\hat{H}_0$ can be typically be expressed in terms of matrix elements $\langle p|\,\hat{h}_0\,|q\rangle$ as:

$$\hat{H}_0 = \sum_{pq} \langle p|\,\hat{h}_0\,|q\rangle\, a_p^\dagger a_q$$

When normal ordering, we can adjust the term to:

$$a_p^\dagger a_q = \{a_p^\dagger a_q\} + \delta_{pq\in i}$$

And from this we can write the one-body term as:

$$\hat{H}_0 = \sum_{pq} \langle p|\,\hat{h}_0\,|q\rangle\, \{a_p^\dagger a_q\} + \sum_{pq} \langle p|\,\hat{h}_0\,|q\rangle\, \delta_{pq\in i}$$

Where the second term is a constant that represents the expectation value of the one-body operator in the refrence state:

$$\sum_{pq} \langle p|\,\hat{h}_0\,|q\rangle\, \delta_{pq\in i} = \langle \Phi_0|\,\hat{H}_0\,|\Phi_0\rangle$$

From this we get

$$\hat{H}_0 = \sum_{pq} \langle p|\,\hat{h}_0\,|q\rangle\, \{a_p^\dagger a_q\} + \langle \Phi_0|\,\hat{H}_0\,|\Phi_0\rangle$$

Now applying the spesific case where $\langle p|\,\hat{h}_0\,|q\rangle = (p-1)\delta_{pq}$ and find that

$$\hat{H}_0 = \sum_{p\sigma} (p-1)\{a_p^\dagger a_q\} + \langle \Phi_0|\,\hat{H}_0\,|\Phi_0\rangle$$

For the interraction term we will approach the normal ordering in a similar way. We can write the interraction term as:

$$\hat{H}_I = \frac{1}{4}\sum_{pqrs} \langle pq|\,\hat{v}\,|rs\rangle\, a_p^\dagger a_q^\dagger a_s a_r$$

where we can re-write the creation and annihilation operators as:

$$a_p^\dagger a_q^\dagger a_s a_r = \{a_p^\dagger a_q^\dagger a_s a_r\} + a_p^\dagger \overbrace{a_q^\dagger a_s} a_r$$

$$+ a_p^\dagger \overbrace{a_q^\dagger a_s a_r} + \overbrace{a_p^\dagger a_q^\dagger} a_s a_r + \overbrace{a_p^\dagger a_q^\dagger a_s} a_r + \overbrace{a_p^\dagger a_q^\dagger a_s a_r} + \overbrace{a_p^\dagger a_q^\dagger a_s a_r}$$

For this spesific case we will substitute $\frac{1}{4}\langle pq|\,\hat{v}\,|rs\rangle$ with $-\frac{g}{2}\delta_{pq}\delta_{rs}$. The interraction term can now be seperated into three parts:

- 1. The two body term, which arrises from the normal ordering of the creation and annihilation operators.
- 2. The one body term, which comes from the single contractions.
- 3. The constant term, which comes from the double contractions.

From this we can construct a new normal ordered interraction term:

$$\hat{H}_I = -\frac{g}{2}\sum_{pq}\{a_p^\dagger a_q^\dagger a_q a_p\} - \frac{g}{2}\sum_{pq} a_{p\sigma}^\dagger a_{p\sigma} + -\frac{g}{2}(\delta_{pr}\delta_{qs} + \delta_{ps}\delta_{qr})$$

We can combine the one-body term into the first one we found, and we get:

$$\hat{H}_0^N = \sum_{p\sigma}(p-1)\{a_{p\sigma}^\dagger a_{p\sigma}\} - \frac{g}{2}\sum_{p\sigma} a_{p\sigma}^\dagger a_{p\sigma}$$

The normal ordered interraction term is:

$$\hat{V}^N = -\frac{g}{2}\sum_{pq}\{a_p^\dagger a_q^\dagger a_q a_p\}$$

and the refrence energy:

$$E_0^{ref} = \langle\Phi_0|\,\hat{H}_0\,|\Phi_0\rangle - \frac{g}{2}\sum_{pq}(\delta_{pr}\delta_{qs} + \delta_{ps}\delta_{qr}) = 2 - g$$

where the values were obtained in the previous task.
The total normal ordered Hamiltonian is:

$$\hat{H}^N = \hat{H}_0^N + \hat{V}^N + E_0^{ref}$$

We now want to set up the standard Hartree-Fock equations for the system, also known as the canonical Hartree-Fock equations equations. We begin by defining the single-particle operator $\hat{f}$, which for a general case is given by:

$$\langle p|\,\hat{f}\,|q\rangle = \langle p|\,\hat{H}_0\,|q\rangle + \sum_j \langle pj|\,\hat{V}\,|qj\rangle_{AS}$$

where the subscript AS indicates thath the matrix elements are antisymmetrized:

$$\langle pj|\,\hat{V}\,|qj\rangle_{AS} = \langle pj|\,\hat{V}\,|qj\rangle - \langle pj|\,\hat{V}\,|jq\rangle$$

Since $\langle p|\,\hat{f}\,|q\rangle = 0$ for $p \neq q$ due to the orthaogonality of the Hartree-Fock orbitals, we are left with only diagonal contributions, $p = q$.
In second quantization, we can write the single-particle operator as:

$$\hat{F} = \sum_{pq}\langle p|\,\hat{f}\,|q\rangle\, a_p^\dagger a_q = \sum_p \langle p|\,\hat{f}\,|p\rangle\, a_p^\dagger a_p$$

To express the normal-ordered form, we write:

$$\overbrace{a_p^\dagger a_p} = \{a_p^\dagger a_p\} + \delta_{pp}$$

Which leads to:

$$\hat{F} = \sum_p \langle p|\,\hat{f}\,|p\rangle\,\{a_p^\dagger a_p\} + \sum_p \langle p|\,\hat{f}\,|p\rangle\,\delta_{pp}$$

Finally, the canonical Hartree-Fock equations are:

$$\hat{f}\,|p\rangle = \epsilon_p\,|p\rangle$$

where the single-particle energies ϵ_p is the single-particle energy, and $|p\rangle$ ar the Hartree-Fock orbitals. these equations represent an eigenvalue problem, where the Fock operator $\hat{f}$ contains both the one-body contributions and the two-body contributions.

e)

In the previous exam we showed that the HF equations can be written as:

$$\sum_{\gamma} h^{HF}_{\alpha\gamma} C_{p\gamma} = \epsilon_p C_{p\alpha}$$

where

$$h^{HF}_{\alpha\gamma} = \langle\alpha| h |\gamma\rangle + \sum_{q} \sum_{\beta\delta} C^*_{q\beta} C_{q\delta} \langle\alpha\beta| V |\gamma\delta\rangle_{AS}$$

To find the HF equations for the spesific case, we do an operator basis transformation:

$$a^\dagger_{p\sigma} = \sum_{\lambda} C_{p\lambda} a^\dagger_{\lambda\sigma}$$

$$a_{p\sigma} = \sum_{\lambda} C^*_{p\lambda} a_{\lambda\sigma}$$

This transformation expresses the operators in terms of the new basis $\left|\psi_p\right\rangle$, where $p = 1, 2, 3, 4$.
The HF Hamiltonian can be written in terms of creation and annihilation operators as:

- 1. The one-body term:

$$\sum_{p=1}^{2} \sum_{\sigma} (p-1) a^\dagger_p a_p - \sum_{p=3}^{4} \sum_{\sigma} (p-1) a_p a^\dagger_p$$

- 2. The two-body term:

$$\frac{1}{2} \sum_{p=1}^{2} \sum_{\sigma} a_p a^\dagger_p$$

Now we can substitute to the new basis

- Term 1:

$$\sum_{p=1}^{2} \sum_{\sigma} (p-1) a^\dagger_p a_p \Rightarrow \sum_{p=1}^{2} \sum_{\sigma} (p-1) \sum_{\lambda\lambda'} C_{p\lambda} C^*_{p\lambda'} a^\dagger_{\lambda\sigma} a_{\lambda'\sigma}$$

- Term 2:

$$\sum_{p=3}^{4} \sum_{\sigma} (p-1) a_p a^\dagger_p \Rightarrow \sum_{p=3}^{4} \sum_{\sigma} (p-1) \sum_{\lambda\lambda'} C^*_{p\lambda} C_{p\lambda'} a_{\lambda\sigma} a^\dagger_{\lambda'\sigma}$$

- Term 3:

$$\frac{1}{2} \sum_{p=1}^{2} \sum_{\sigma} a_p a^\dagger_p \Rightarrow \frac{1}{2} \sum_{p=1}^{2} \sum_{\sigma} \sum_{\lambda\lambda'} C^*_{p\lambda} C_{p\lambda'} a_{\lambda\sigma} a^\dagger_{\lambda'\sigma}$$

Now, we would like to find the matrix elements of the transformed Hamiltonian. Which means calculating $\langle aplha| \hat{h}^{HF} |\beta\rangle$, where $|\alpha\rangle = a^\dagger_{\alpha\sigma} |0\rangle$.

TWe will now apply wicks theorem term by term.:

- (1)

$$C^*_{p\lambda}C_{p\lambda'}\left(\overbrace{a_{\alpha\sigma_1}a_{\lambda\sigma}a^\dagger_{\lambda'\sigma}a^\dagger_{\beta\sigma_2}}+\overbrace{a_{\alpha\sigma_1}a_{\lambda\sigma}a^\dagger_{\lambda'\sigma}a^\dagger_{\beta\sigma_2}}\right)$$
$$=C^*_{p\lambda}C_{p\lambda'}\left(\delta_{\sigma_1\sigma_2}\delta_{\alpha\beta}\delta_{\lambda\lambda'}\delta_{\sigma\sigma}-\delta_{\sigma_1\sigma}\delta_{\alpha\lambda}\delta_{\beta\lambda'}\delta_{\sigma\sigma_2}\right)$$

- (2)

$$C_{p\lambda}C^*_{p\lambda'}\left(\overbrace{a_{\alpha\sigma_1}a^\dagger_{\lambda\sigma}}\overbrace{a_{\lambda'\sigma}a^\dagger_{\beta\sigma_2}}\right)=C_{p\lambda}C^*_{p\lambda'}\delta_{\alpha\lambda}\delta_{\beta\lambda'}\delta_{\sigma\sigma_1}\delta_{\sigma\sigma_2}$$

- (3)

$$C^*_{p\lambda}C_{p\lambda'}\left(\overbrace{a_{\alpha\sigma_1}a_{\lambda\sigma}a^\dagger_{\lambda'\sigma}a^\dagger_{\beta\sigma_2}}+\overbrace{a_{\alpha\sigma_1}a_{\lambda\sigma}a^\dagger_{\lambda'\sigma}a^\dagger_{\beta\sigma_2}}\right)$$
$$=C^*_{p\lambda}C_{p\lambda'}\left(\delta_{\sigma_1\sigma_2}\delta_{\alpha\beta}\delta_{\lambda\lambda'}\delta_{\sigma\sigma}-\delta_{\sigma_1\sigma}\delta_{\alpha\lambda}\delta_{\beta\lambda'}\delta_{\sigma\sigma_2}\right)$$

Combining all the terms and simplifying symmations, the matrix elements $\langle\alpha|\,\hat{h}_{HF}\,|\beta\rangle$ are:

$$\langle\alpha|\,\hat{h}_{HF}\,|\beta\rangle=(2-g)\delta_{\alpha\beta}-2\delta_{\sigma_1\sigma_2}\delta_{\alpha\beta}\sum_{p=1}^{2}\sum_{\lambda}(p-1)|C_{p\lambda}|^2$$
$$+\delta_{\sigma_1\sigma_2}\sum_{p=1}^{2}(p-1)C^*_{p\alpha}C_{p\beta}+\sum_{p=3}^{4}(p-1)C^*_{p\beta}C_{p\alpha}$$
$$+\frac{g}{2}\left[2\delta_{\sigma_1\sigma_2}\delta_{\alpha\beta}\sum_{p=1}^{2}\sum_{\lambda}|C_{p\lambda}|^2-\delta_{\sigma_1\sigma_2}\sum_{p=1}^{2}C_{p\beta}C^*_{p\alpha}\right]$$

TODO: make this expression more readable

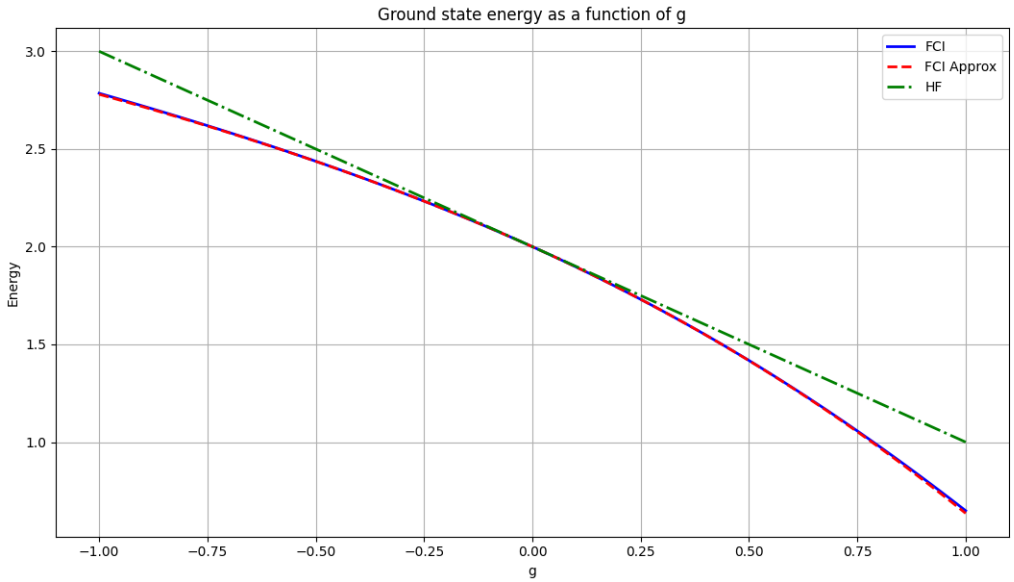

Figure 7: Comparison of HF, exact solution and the approximation. Energies as a function of the strength of the interaction g

In figure 7 we can see the comparison of the HF, exact solution and the earlier approximation. We can see that the HF solution is very close to the exact solution for g close to zero. As $|g| \to 1$ the HF solution diverges from the exact solution.

To study the perturbation system, we use none-degenerate RS perturbation theory up to third order in the interaction, excluding the first-order term. The relevant states are:

$$|1+1-\rangle, |2+2-\rangle, |3+3-\rangle, |4+4-\rangle$$

defined as:

$$|p+p-\rangle = a^\dagger_{p+} a^\dagger_{p-} |0\rangle$$

From Figure 2 in the exercise description, which displays all possible antisymmetric Goldstone diagrams to third order, we determine which diagrams contribute to the GS energy. The Hamiltonian conserves particle and hole pairs, meaning diagrams in which pairs are broken do not contribute. This leaves us with four contributing diagrams, the ones labeled 1,4,5 and 8.
For each diagram we count the number of hole states (h), loops (l) and the pair states (p).

- Diagram 1: $(h = 2, p = 2, l = 2)$
- Diagram 4: $(h = 2, p = 3, l = 2)$
- Diagram 5: $(h = 4, p = 3, l = 2)$
- Diagram 8: $(h = 4, p = 1, l = 3)$

The energy contributions for each diagram are:

- Diagram 1: $(h = 2, p = 2, l = 2)$:

$$\Delta E_1 = \frac{1}{4} \sum_{i=1}^{2} \sum_{a=3}^{4} \frac{\langle i_+ i_- | \hat{V} | a_+ a_- \rangle \langle a_+ a_- | \hat{V} | i_+ i_- \rangle}{2\epsilon_i - 2\epsilon_a}$$

- Diagram 4: $(h = 2, p = 3, l = 2)$:

$$\Delta E_4 = \frac{1}{8} \sum_{i=1}^{2} \sum_{a=3}^{4} \sum_{b=3}^{4} \frac{\langle i_+ i_- | \hat{V} | a_+ a_- \rangle \langle a_+ a_- | \hat{V} | b_+ b_- \rangle \langle b_+ b_- | \hat{V} | i_+ i_- \rangle}{(2\epsilon_i - 2\epsilon_a)(2\epsilon_i - 2\epsilon_b)}$$

- Diagram 5: $(h = 4, p = 3, l = 2)$:

$$\Delta E_5 = \frac{1}{8} \sum_{i=1}^{2} \sum_{a=3}^{4} \sum_{k=1}^{2} \frac{\langle i_+ i_- | \hat{V} | a_+ a_- \rangle \langle k_+ k_- | \hat{V} | i_+ i_- \rangle \langle a_+ a_- | \hat{V} | k_+ k_- \rangle}{(2\epsilon_i - 2\epsilon_a)(2\epsilon_k - 2\epsilon_a)}$$

- Diagram 8: $(h = 4, p = 1, l = 3)$:

$$\Delta E_8 = \frac{1}{16} \sum_{i=1}^{2} \sum_{a=3}^{4} \frac{\langle i_+ i_- | \hat{V} | a_+ a_- \rangle \langle i_+ i_- | \hat{V} | i_+ i_- \rangle \langle a_+ a_- | \hat{V} | i_+ i_- \rangle}{(2\epsilon_i - 2\epsilon_a)^2}$$

The factors before the summations come from a formula: $\frac{(-1)^{n_{loops}+n_{holes}}}{2^{n_{equivivalentpairs}}}$.
Now we want to simplify the expressions for the diagrams. And to do this we will use the fact that the interraction energy will contribute with $-\frac{g}{2}$ and that the single-particle energies are $\epsilon_i = i - 1 - \frac{g}{2}$. And so for an example case $\epsilon_i - \epsilon_a = i - a$.

- Diagram 1:
$$\Delta E_1 = \frac{1}{8}\sum_{i,a} g^2 \frac{1}{i-a}$$
- Diagram 4:
$$\Delta E_2 = -\frac{1}{32}\sum_{i,a,c} g^3 \frac{1}{(i-a)(i-c)}$$
- Diagram 5:
$$\Delta E_3 = -\frac{1}{32}\sum_{i,a,k} g^3 \frac{1}{(i-a)(k-a)}$$
- Diagram 8:
$$\Delta E_4 = \frac{1}{16}\sum_{i,a} g^3 \frac{1}{(i-a)^2}$$

For the total energy of the system, we combine the unperturbed energy $E^0 = 2 - g$, with the third order contributions:

$$E = 2 - g - \frac{7}{24}g^2 - \frac{1}{12}g^3$$

Here we can that the third order perturbation is very close to the FCI solution, and the

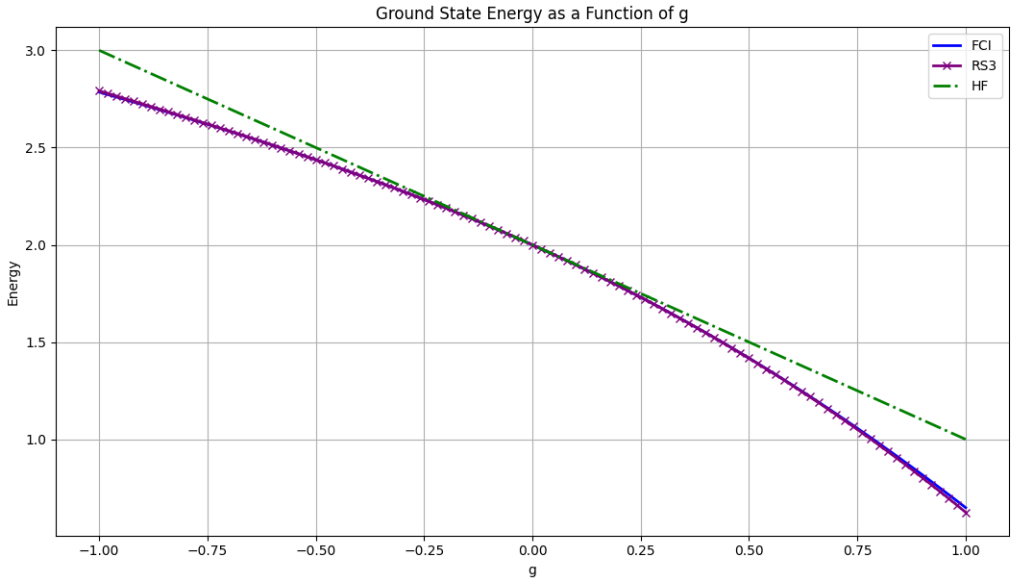

Figure 8: Comparison of HF, Rayleigh Schrödinger 3rd order perturbation, and FCI. Energies as a function of the strength of the interaction g

HF solution is not as accurate.

f)

The first order wave operator is given by:

$$\Psi^{(1)} = Q\frac{1}{E_0 - H_0}\hat{V}\Phi_{00}$$

where Q is the projection operator that excludes the ground state, and Φ_0 is the unperturbed ground state. Now we want to substitute the definitions of the operators and the wave function:

$$\Psi^{(1)} = \sum_{a,b,i,j} \frac{\langle ab|\,\hat{V}\,|ij\rangle}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}\left|\Phi_{ij}^{ab}\right\rangle$$

where $\left|\Phi_{ij}^{ab}\right\rangle$ are the 2p-2h states and the ϵ are the single-particle energies.
To simplify we reduce the summation over the indices i, j, a, b to sums over energy levels, introducing a factor of 2 per spin state:

$$\Psi^{(1)} = \frac{1}{8}\sum_{a,i} \frac{\langle i\bar{i}|\,\hat{V}\,|a\bar{a}\rangle}{\epsilon_i - \epsilon_a}\left|\Phi_{i\bar{i}}^{a\bar{a}}\right\rangle$$

where the the quantum numbers $\bar{i}$ is the opposite spin of i.
Using the interaction term $\langle i\bar{i}|\,\hat{V}\,|a\bar{a}\rangle = -\frac{g}{2}$, we can write the wave operator as:

$$\Psi^{(1)} = -\frac{g}{4}\sum_{a,i} \frac{1}{\epsilon_i - \epsilon_a}\left|\Phi_{i\bar{i}}^{a\bar{a}}\right\rangle$$

The second-order correction energy is given by:

$$E^{(2)} = \langle\Phi_0|\,\hat{V}\left|\Psi^{(1)}\right\rangle = \frac{g}{4}\sum_{a,b,i,j} \frac{\langle ij|\,\hat{V}\,|ab\rangle\,\langle ab|\,\hat{V}\,|ij\rangle}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}$$

Reducing the sum over energy levels, and accounting for spin factor, we have:

$$E^{(2)} = \frac{1}{8}\sum_{a,i} \frac{\langle i\bar{i}|\,\hat{V}\,|a\bar{a}\rangle\,\langle a\bar{a}|\,\hat{V}\,|i\bar{i}\rangle}{\epsilon_i - \epsilon_a}$$

using $\langle i\bar{i}|\,\hat{V}\,|a\bar{a}\rangle = -\frac{g}{2}$, this simplifies to:

$$E^{(2)} = -\frac{1}{8}\sum_{a,i} \frac{g^2}{\epsilon_i - \epsilon_a}$$

For a two-level spin system, summing over allowed states gives:

$$E^{(2)} = -\frac{7}{24}g^2$$

And the total energy is:

$$E = 2 - g - \frac{7}{24}g^2$$

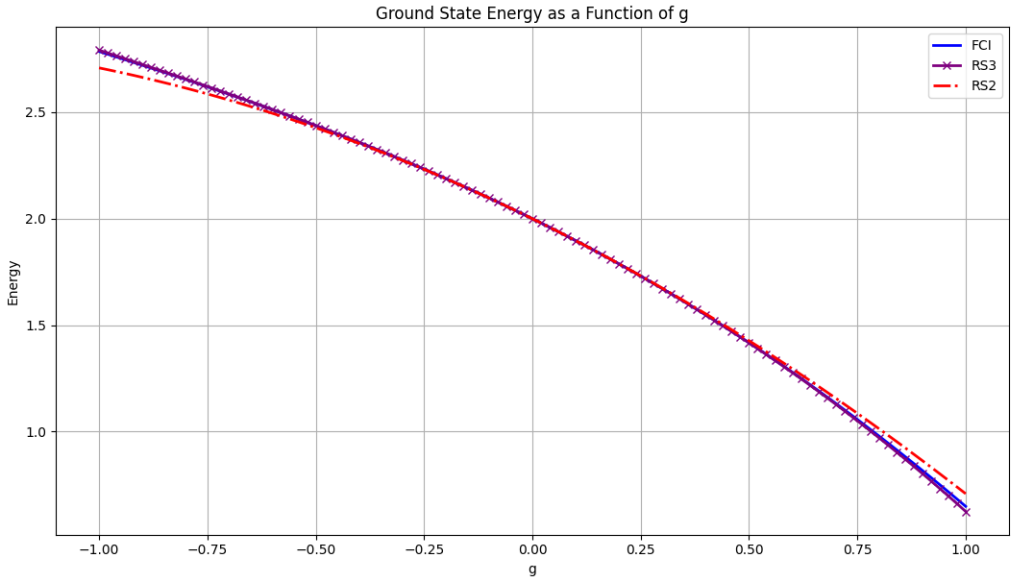

Figure 9: Comparison of Rayleigh Schrödinger 2nd and 3rd order perturbation and the FCI solution. Energies as a function of the strength of the interaction g

g)

Due to the pairing nature of our system, we can exclude the $1p-1h$ and $3p-3h$ diagrams, since they show broken pairs. We only need to look for valid diagrams with $2p-2h$ and $4p-4h$ states. The only $2p-2h$ diagrams with no broken pairs are diagram 5,6,14 and 15. And for the $4p-4h$ diagrams, the valid diagrams are 33, 41, 36 and 37 (Asssuming the outer lines of the diagrams have an arrow mistake, and they in reality should point in the same direction).
Now we can proceed with calculating the energy to fourth order with the HF basis defined earlier, with a range of g-values from -1 to 1. And again compare witht the full diagonalization from exercise b).
In the following calculations, we will adapt a new notation for the energies ϵ_i, ϵ_a etc:

$$\epsilon_{ai} = \epsilon_a - \epsilon_i, \quad \epsilon_{ij}^{ab} = \epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b$$

For diagram (5) and (6), we have $(h, l, p) = 4, 2, 4$. The contributions from these diagrams are as follows:

$$(5) = (-1)^6 \frac{1}{2^4} \sum_{abcd,ijkl} \langle ij| \hat{V} |kl\rangle \langle kl| \hat{V} |cd\rangle \langle cd| \hat{V} |ab\rangle \langle ab| \hat{V} |ij\rangle \frac{1}{\epsilon_{ij}^{ab} \epsilon_{kl}^{ab} \epsilon_{kl}^{cd}}$$

$$(6) = (-1)^6 \frac{1}{2^4} \sum_{abcd,ijkl} \langle ij| \hat{V} |kl\rangle \langle kl| \hat{V} |cd\rangle \langle cd| \hat{V} |ab\rangle \langle ab| \hat{V} |ij\rangle \frac{1}{\epsilon_{ij}^{ab} \epsilon_{ij}^{cd} \epsilon_{kl}^{cd}}$$

Which we again will simplify to:

$$(5) = \frac{1}{128} \sum_{acik} \frac{g^4}{(i-a)(k-a)(k-c)}$$

$$(6) = \frac{1}{128}\sum_{acik}\frac{g^4}{(i-a)(i-c)(k-c)}$$

For diagrams (14) we have $(h,l,p) = 2,2,4$, and (15) we have $(h,l,p) = 6,2,6$. The contributions from these diagrams are:

$$(14) = (-1)^4\frac{1}{2^4}\sum_{abcdef,ij}\langle ij|\,\hat{V}\,|ef\rangle\,\langle ef|\,\hat{V}\,|cd\rangle\,\langle cd|\,\hat{V}\,|ab\rangle\,\langle ab|\,\hat{V}\,|ij\rangle\,\frac{1}{\epsilon_{ij}^{ab}\epsilon_{ij}^{cd}\epsilon_{ij}^{cd}}$$

and

$$(15) = (-1)^8\frac{1}{2^4}\sum_{ab,ijklmn}\langle ij|\,\hat{V}\,|kl\rangle\,\langle kl|\,\hat{V}\,|mn\rangle\,\langle mn|\,\hat{V}\,|ab\rangle\,\langle ab|\,\hat{V}\,|ij\rangle\,\frac{1}{\epsilon_{ij}^{ab}\epsilon_{kl}^{ab}\epsilon_{mn}^{ab}}$$

Simplifying these expressions, we get:

$$(14) = \frac{1}{128}\sum_{ace,i}\frac{g^4}{(i-a)(i-c)(i-e)}$$

$$(15) = \frac{1}{128}\sum_{a,ikm}\frac{g^4}{(i-a)(k-a)(m-a)}$$

For diagram (36) we have $(h,l,p) = 4,0,4$, which becomes:

$$(36) = (-1)^6\frac{1}{2}\sum_{abcd,ijkl}\langle ij|\,\hat{V}\,|cd\rangle\,\langle cd|\,\hat{V}\,|kl\rangle\,\langle kl|\,\hat{V}\,|ab\rangle\,\langle ab|\,\hat{V}\,|ij\rangle\,\frac{1}{\epsilon_{ij}^{ab}\epsilon_{ijkl}^{abcd}\epsilon_{ij}^{cd}}$$

Which simplifies to:

$$(36) = \frac{1}{16}\sum_{acik}\frac{g^4}{(i-a)(i+k-a-c)(i-c)}$$

By symmetry, diagram (37) is simply:

$$(37) = \frac{1}{16}\sum_{acik}\frac{g^4}{(i-a)(i+k-a-c)(k-a)}$$

Diagram (33) and (41) are unlinked diagrams, and therefor we can exclude them as well. The final contribution to the energy is:

$$-\frac{2063}{13824}g^4 = -0.149g^4$$

And so the total fourth order energy is:

$$E = 2 - g - \frac{7}{24}g^2 - \frac{1}{12}g^3 - 0.149g^4$$

From 10 we can see the comparison of the different perturbation orders, the exact solution. We can see that the fourth order performes worse than both the third and second order, and that the third order is still the best approximation.

In figure 11 we can see the difference between the FCI solution and the different perturbation theories. We can see that the HF solution is the worst approximation, and that the third order is the best approximation. It is also worth noting that for the fourth order, the energy diverges the most from the FCI solution as $|g|$ approaches 1.

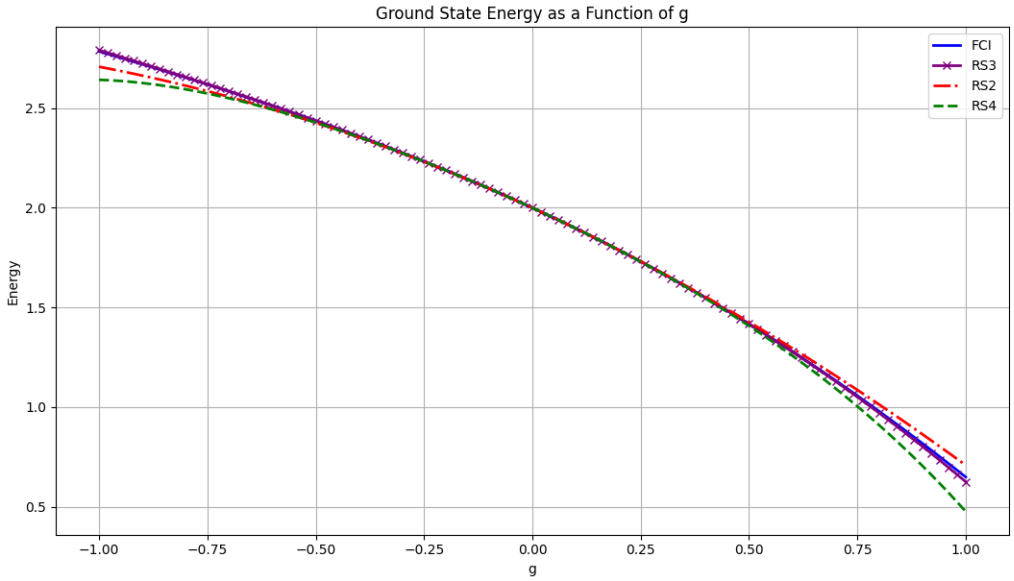

Figure 10: Comparison of Rayleigh Schrödinger 2nd, 3rd and 4th order perturbation and the FCI Energies as a function of the strength of the interaction g

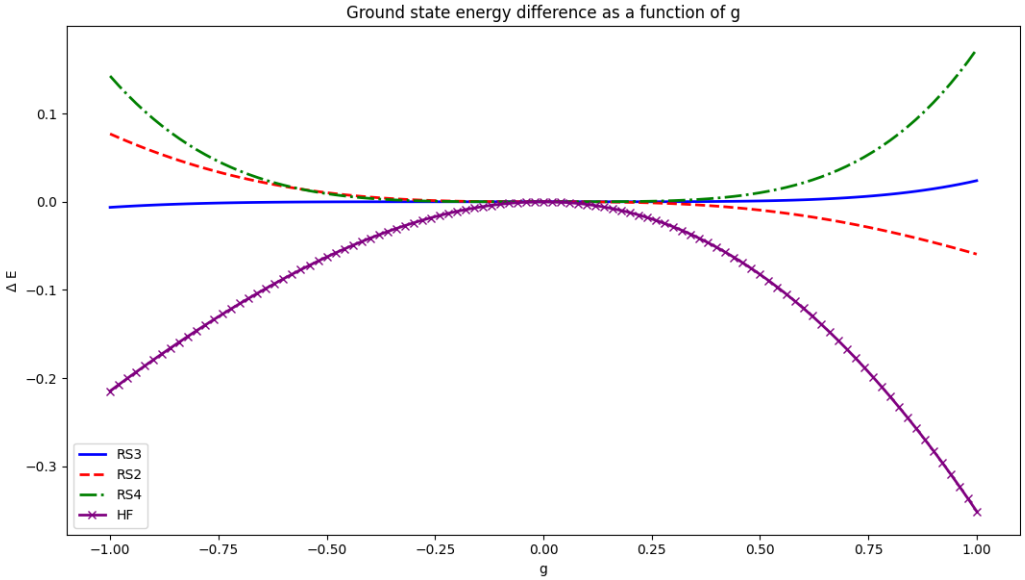

Figure 11: The plot is showing the energy difference between the FCI solution, and the HF, second, third and fourth order perturbation theory.

Github link

`https://github.com/hishemok/FYS4480/tree/main/Midterm2`