Midterm 2

Hishem Kløvnes

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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:

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

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

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

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

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

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

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

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

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

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

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

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

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

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:

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

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

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

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

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

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 $\hat{S}_z$:

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

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

The first term:

$$[a_{q-} a_{q+}, a_{r\sigma}^\dagger a_{r\sigma}] = a_{q-}[a_{q+}, a_{r\sigma}^\dagger] a_{r\sigma} + a_{q-} a_{r\sigma}^\dagger [a_{q+}, a_{r\sigma}]$$

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

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

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

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

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Now the second term:

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

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

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

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

$$= a_{p+}^\dagger a_{p-} + a_{p-}^\dagger a_{p+}$$

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

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

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

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

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

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

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

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

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

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

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

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

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

The second term:

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

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

The third term:

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

$$= -a_{p+}^\dagger a_{r+}^\dagger \delta_{pr} \delta_{--} - a_{r+}^\dagger \delta_{pr} \delta_{+-} a_{p-}^\dagger = -a_{p+}^\dagger a_{p+}^\dagger$$

The fourth term:

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

$$= -a_{p+}^\dagger a_{r-}^\dagger \delta_{pr}\delta_{-+} - a_{r-}^\dagger \delta_{pr}\delta_{++}a_{p-}^\dagger = -a_{p-}^\dagger a_{p-}^\dagger$$

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:

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

$$+a_{p+}^\dagger a_{p-}^\dagger a_{q+}^\dagger a_{q-}a_{q+}a_{q+}$$

$$-a_{p+}^\dagger a_{p+}^\dagger a_{p-}^\dagger a_{p+}a_{q-}a_{q+}$$

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

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:

$$\hat{P_p^+} = a_{p+}^\dagger a_{p-}^\dagger$$

$$\hat{P_p^-} = a_{p-}a_{p+}$$

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

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

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:

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

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

$$[\hat{P_p^+}, \hat{P_q^+}] = [a_{p+}^\dagger a_{p-}^\dagger, a_{q+}^\dagger a_{q-}^\dagger]$$

$$a_{p+}^\dagger[a_{p-}^\dagger, a_{q+}^\dagger]a_{q-}^\dagger + a_{p+}^\dagger a_{q+}^\dagger[a_{p-}^\dagger, a_{q-}^\dagger] + [a_{p+}^\dagger, a_{q+}^\dagger]a_{q-}^\dagger a_{p-}^\dagger + a_{q+}^\dagger[a_{p+}^\dagger, a_{q-}^\dagger]a_{p-}^\dagger$$

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 $S = 0$:

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

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.

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

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

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

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

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:

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

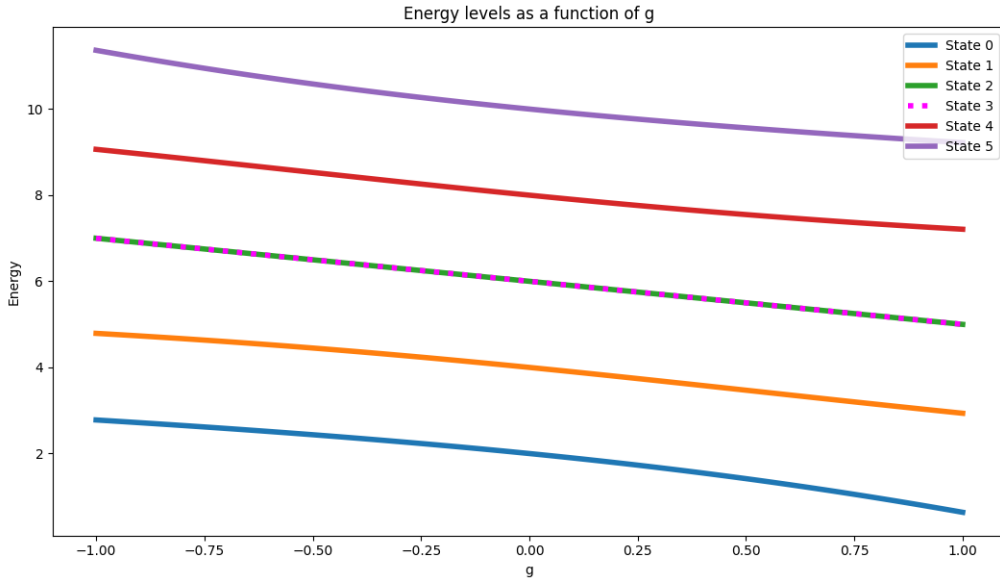The following plot and the matrix elements are calculated with the code in `energies.py`

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.

c)

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

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

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

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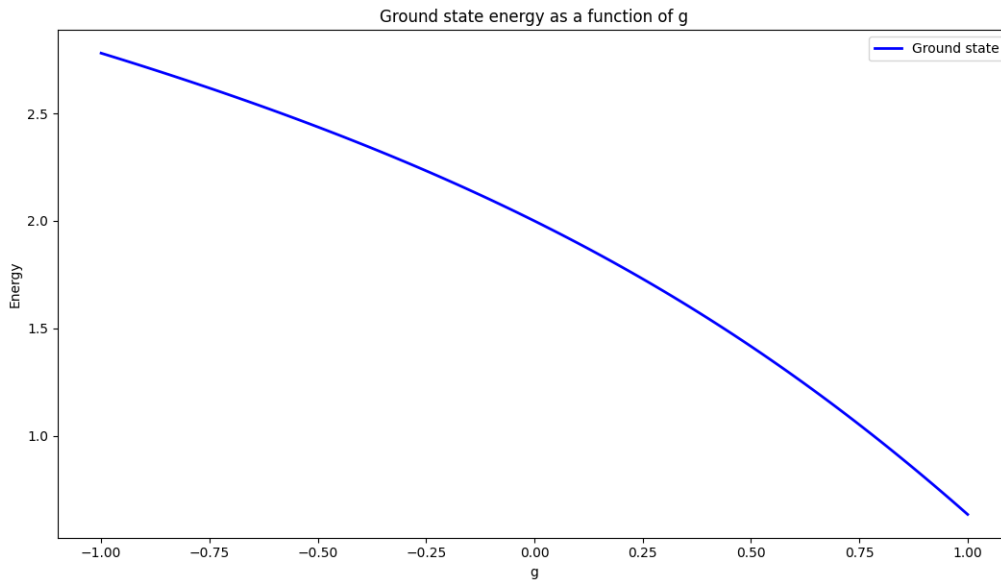
Figure 2: Ground state energy as a function of the interraction strength g.

ground state energy by only using the states $|\Phi_0\rangle$ and $|\Phi_4\rangle$.

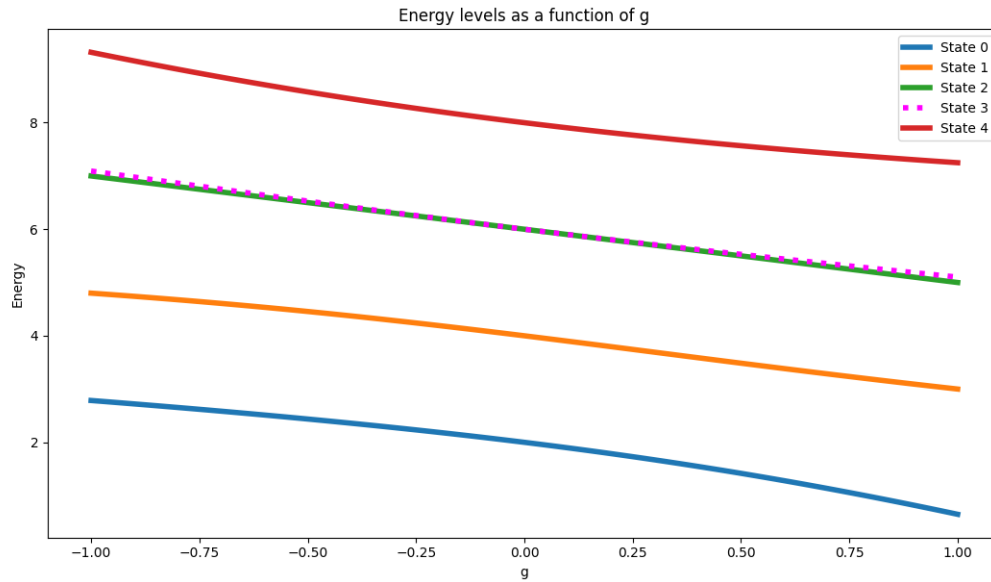In 5 we show the energy difference between the approximation and the ground state

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. TODO: add diagrammatic representation
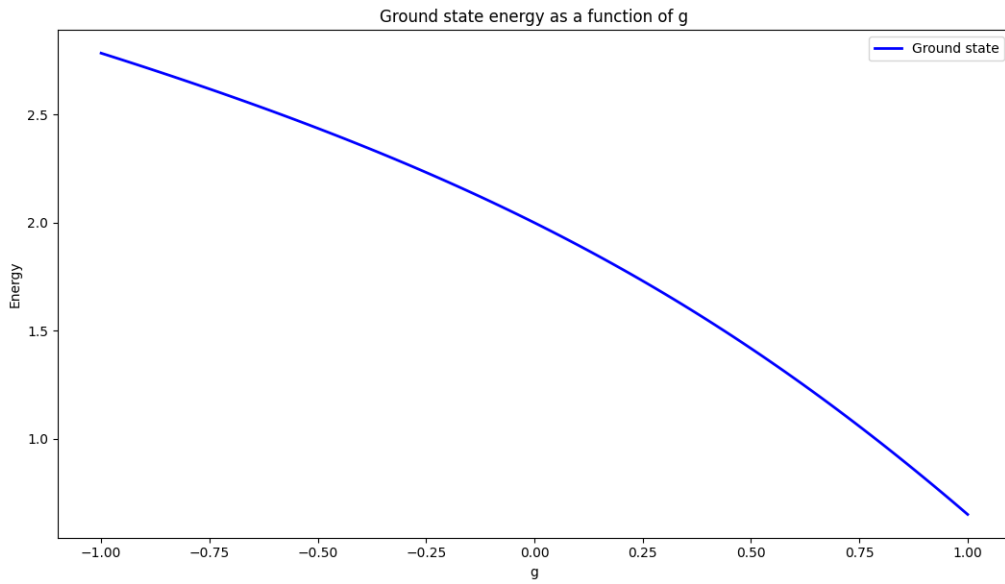
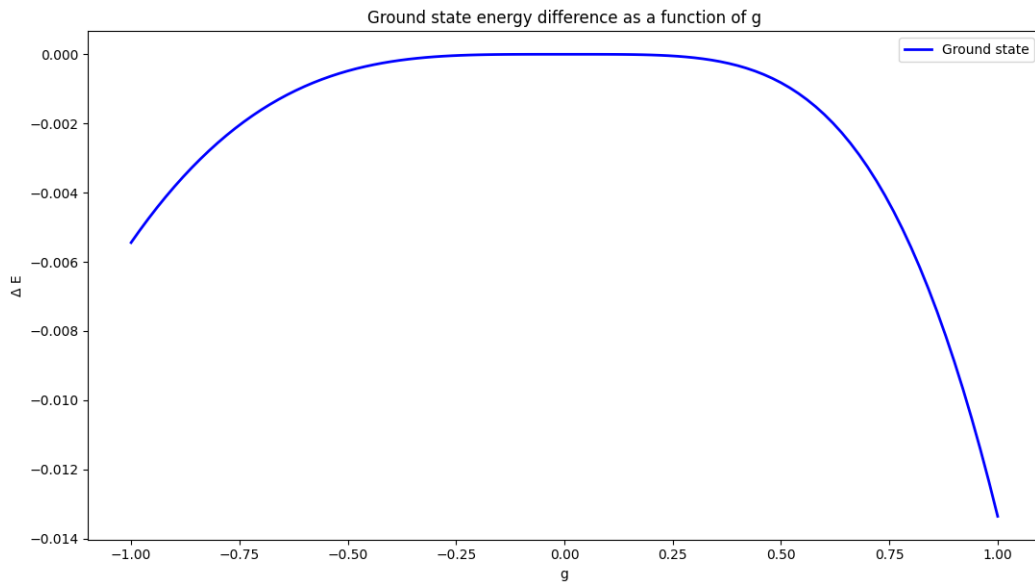Figure 4: Ground state energy approximation as a function of the interaction strength g.

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

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:

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

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

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 $|\psi_p\rangle$, 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)

$$C_{p\lambda}^* C_{p\lambda'} \left(\overbrace{a_{\alpha\sigma_1} \overbrace{a_{\lambda\sigma} a_{\lambda'\sigma}^\dagger}} a_{\beta\sigma_2}^\dagger + \overbrace{a_{\alpha\sigma_1} \overbrace{a_{\lambda\sigma} a_{\lambda'\sigma}^\dagger} a_{\beta\sigma_2}^\dagger} \right)$$

$$= C_{p\lambda}^* C_{p\lambda'} \left(\delta_{\sigma_1\sigma_2} \delta_{\alpha\beta} \delta_{\lambda\lambda'} \delta_{\sigma\sigma} - \delta_{\sigma_1\sigma} \delta_{\alpha\lambda} \delta_{\beta\lambda'} \delta_{\sigma\sigma_2} \right)$$

- (2)

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

- (3)

$$C_{p\lambda}^* C_{p\lambda'} \left(\overbrace{a_{\alpha\sigma_1} \overbrace{a_{\lambda\sigma} a_{\lambda'\sigma}^\dagger}} a_{\beta\sigma_2}^\dagger + \overbrace{a_{\alpha\sigma_1} \overbrace{a_{\lambda\sigma} a_{\lambda'\sigma}^\dagger} a_{\beta\sigma_2}^\dagger} \right)$$

$$= C_{p\lambda}^* C_{p\lambda'} \left(\delta_{\sigma_1\sigma_2} \delta_{\alpha\beta} \delta_{\lambda\lambda'} \delta_{\sigma\sigma} - \delta_{\sigma_1\sigma} \delta_{\alpha\lambda} \delta_{\beta\lambda'} \delta_{\sigma\sigma_2} \right)$$

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

$$\langle \alpha | \hat{h}_{HF} | \beta \rangle = (2 - g)\delta_{\alpha\beta} - 2\delta_{\sigma_1\sigma_2} \delta_{\alpha\beta} \sum_{p=1}^{2} \sum_{\lambda} (p-1)|C_{p\lambda}|^2$$

$$+ \delta_{\sigma_1\sigma_2} \sum_{p=1}^{2} (p-1) C_{p\alpha}^* C_{p\beta} + \sum_{p=3}^{4} (p-1) C_{p\beta}^* C_{p\alpha}$$

$$+ \frac{g}{2} \left[2\delta_{\sigma_1\sigma_2} \delta_{\alpha\beta} \sum_{p=1}^{2} \sum_{\lambda} |C_{p\lambda}|^2 - \delta_{\sigma_1\sigma_2} \sum_{p=1}^{2} C_{p\beta} C_{p\alpha}^* \right]$$
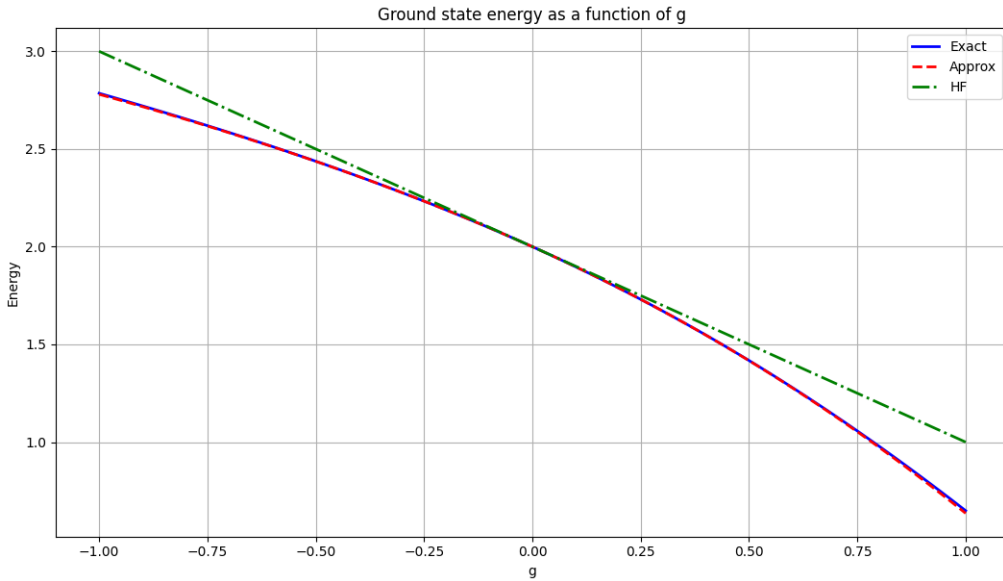
TODO: make this expression more readable

Figure 6: Comparison of HF, exact solution and the approximation. Energies as a function of the strength of the interaction g

In figure 6 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:

$$|p+p-\rangle = a_{p+}^\dagger a_{p-}^\dagger |0\rangle$$

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 has $(h, l, p) = (2, 2, 2)$, diagram 4 has $(h, l, p) = (2, 2, 3)$, diagram 5 has $(h, l, p) = (4, 2, 3)$ and diagram 8 has $(h, l, p) = (4, 3, 1)$.

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

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

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

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

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

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

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

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

Where the sums over equivalent spins are implied, so we could simplify the expressions by removing pre-factors of 2^{-p}.

f)

g)