Second midterm FYS4480 – Quantum mechanics for many-particle systems

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The following is my submitted solution proposal for the second midterm in FYS4480

Task 1

The Hamiltonian is given by:

$$\hat{H} = \hat{H}_0 + \hat{V},$$

where:

$$\hat{H}_0 = \sum_{p\sigma} \epsilon_p \, a^\dagger_{p\sigma} a_{p\sigma}, \quad \text{with} \quad \epsilon_p = p - 1, \tag{1}$$

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

$$P^+_p = a^\dagger_{p+} a^\dagger_{p-}, \quad P^-_q = a_{q-} a_{q+}. \tag{3}$$

The spin operators are defined as:

$$\hat{S}_z = \frac{1}{2} \sum_{p\sigma} \sigma \, a^\dagger_{p\sigma} a_{p\sigma}, \tag{4}$$

$$\hat{S}^2 = \hat{S}^2_z + \frac{1}{2}(\hat{S}_+ \hat{S}_- + \hat{S}_- \hat{S}_+), \tag{5}$$

$$\hat{S}_+ = \sum_p a^\dagger_{p+} a_{p-}, \quad \hat{S}_- = \sum_p a^\dagger_{p-} a_{p+}. \tag{6}$$

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

$$\begin{aligned}
[\hat{H}_0, \hat{S}_z] &= \left[\sum_{p'\sigma'} \epsilon_{p'} \, a^\dagger_{p'\sigma'} a_{p'\sigma'}, \; \frac{1}{2} \sum_{p\sigma} \sigma \, a^\dagger_{p\sigma} a_{p\sigma} \right] \\
&= \frac{1}{2} \sum_{p'\sigma'} \sum_{p\sigma} \epsilon_{p'} \, \sigma \left[a^\dagger_{p'\sigma'} a_{p'\sigma'}, \; a^\dagger_{p\sigma} a_{p\sigma} \right].
\end{aligned} \tag{7}$$

We have now reduced to problem to a commuation problem between two number operator.: We therefore need to show that for any p, q and σ, σ':

$$\left[a^\dagger_{p\sigma} a_{p\sigma}, \; a^\dagger_{q\sigma'} a_{q\sigma'} \right] = 0.$$

We do this by using the anticommutation relations for fermions:

$$\{a_{p\sigma}, a^\dagger_{q\sigma'}\} = \delta_{pq} \delta_{\sigma\sigma'}, \tag{8}$$

$$\{a_{p\sigma}, a_{q\sigma'}\} = 0, \tag{9}$$

$$\{a^\dagger_{p\sigma}, a^\dagger_{q\sigma'}\} = 0. \tag{10}$$

We have:

$$a^\dagger_{p\sigma} a_{p\sigma} a^\dagger_{q\sigma'} a_{q\sigma'} - a^\dagger_{q\sigma'} a_{q\sigma'} a^\dagger_{p\sigma} a_{p\sigma}$$

This is trivially 0 if $p = q$ and $\sigma' = \sigma$. If $p = q$ and $\sigma' \neq \sigma$, or $p \neq q$ and $\sigma' = \sigma$ (or $p \neq q$ $\sigma' \neq \sigma$), we can use the anticommutation relations to get:

$$a^\dagger_{q\sigma'} a_{q\sigma'} a^\dagger_{p\sigma} a_{p\sigma} - a^\dagger_{q\sigma'} a_{q\sigma'} a^\dagger_{p\sigma} a_{p\sigma} = 0$$

We thus get that since the number operators commute, H_0 and commutes with S_z. This is also trivial to see, since we are essentially calculating the commutation between two number-operators, just scaled differently.

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

$$[\hat{H}_0, \hat{S}^2] = [\hat{H}_0, \hat{S}_z^2] + \frac{1}{2}[\hat{H}_0, \hat{S}_+\hat{S}_- + \hat{S}_-\hat{S}_+]$$

We already know that$[\hat{H}_0, \hat{S}_z] = 0$ We then need to calculate $[\hat{H}_0, \hat{S}_+]$ and $[\hat{H}_0, \hat{S}_-]$
Using the fermionic commutation relations, we find that:

$$[\hat{H}_0, \hat{S}_+] = [\hat{H}_0, \hat{S}_-] = 0$$

This is because the commutator $[\hat{H}_0, \hat{S}_+]$ can be expanded as:

$$[\hat{H}_0, \hat{S}_+] = \sum_{p\sigma} \epsilon_p [a^\dagger_{p\sigma} a_{p\sigma}, \sum_{p'} a^\dagger_{p'\uparrow} a_{p'\downarrow}]$$

We use the anticommutation relations:

$$[a^\dagger_{p\sigma} a_{p\sigma}, a^\dagger_{p'+} a_{p'-}] = (\delta_{\sigma+} a^\dagger_{p\sigma} a_{p-} + \delta_{\sigma-} a^\dagger_{p+} a_{p\sigma}) = 0$$

therefore

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

Similarly, we find:

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

Thus:

$$[\hat{H}_0, \hat{S}_+\hat{S}_-] = [\hat{H}_0, \hat{S}_+]\hat{S}_- + \hat{S}_+[\hat{H}_0, \hat{S}_-] = 0$$

We get in total:

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

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

Compute the commutator:

$$[\hat{V}, \hat{S}_z] = -\frac{1}{2} g \sum_{pq} \left[P^+_p P^-_q,\ \hat{S}_z \right]$$

We do this by examining the following:

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

$$= a^\dagger_{k+} a^\dagger_{k-} a_{q-} (\delta_{pq}\delta_{\sigma+} - a^\dagger_{p\sigma} a_{q+}) a_{p\sigma} - a^\dagger_{p\sigma} (\delta_{pk}\delta_{\sigma+} - a^\dagger_{k+} a_{p\sigma}) a^\dagger_{k-} a_{q-} a_{q+}$$

$$= a^\dagger_{k+} a^\dagger_{k-} a_{q-} a_{q+} - a^\dagger_{k+} a^\dagger_{k-} (\delta_{pq}\delta_{\sigma-} - a^\dagger_{p\sigma} a_{q-}) a_{q+} a_{p\sigma} - a^\dagger_{k+} a^\dagger_{k-} a_{q-} a_{q+} + a^\dagger_{p\sigma} a^\dagger_{k+} (\delta_{pk}\delta_{\sigma-} - a^\dagger_{k-} a_{p\sigma}) a_{q-} a_{q+}$$

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

$$= a^\dagger_{p\sigma} a^\dagger_{k+} a^\dagger_{k-} a_{q-} a_{q+} a_{p\sigma} - a^\dagger_{p\sigma} a^\dagger_{k+} a^\dagger_{k-} a_{q-} a_{q+} a_{p\sigma} = 0$$

The operators $\hat{V}$ and $\hat{S}_z$ therefore commute.

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

We already know V commute with S_z and therefore commutes with S_z^2 as well. We thus proceed with the second term: Using $[A, BC] = [A, B]C + B[A, C]$,

$$[\hat{V}, \hat{S}_+\hat{S}_-] = [\hat{V}, \hat{S}_+]\hat{S}_- + \hat{S}_+[\hat{V}, \hat{S}_-]$$

We try to compute $[\hat{V}, \hat{S}_+]$:

$$[\hat{V}, \hat{S}_+] = -\frac{1}{2}g\sum_{pq}\left[P_p^+P_q^-,\ \sum_k a_{k+}^\dagger a_{k-}\right]$$

Using commutator identities and recognizing that $[P_p^+,\ a_{k+}^\dagger a_{k-}] = 0$ and $[P_q^-,\ a_{k+}^\dagger a_{k-}] = 0$, we find:

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

This is because we have a commutator on the form $[P_p^+,\ a_{k+}^\dagger a_{k-}] = [\ a_{p+}^\dagger a_{p-}^\dagger,\ a_{k+}^\dagger a_{k-}] = \delta_{pk}a_{p+}^\dagger a_{k+}^\dagger = a_{k+}^\dagger a_{k+}^\dagger$ We get similar contributions from $[P_p^+, S_-], [P_p^-, S_+], [P_p^-, S_-]$. All these are zero due to duplicated like $a_j a_j = 0$ when applied to any state. It must also be zero due to the anticommutation rules. Since any combination for $[P^\pm, S_\pm] = 0$, the operators must commute. $[\hat{V}, \hat{S}^2] = 0$

Hence the Hamiltonian, both the interaction term and H_0 term commutes with both spin operator $\hat{S}_z$ and the total spin $\hat{S}^2$. This is important because it means that the total spin magnitude and its z-component are conserved quantities in the system. This conservation implies that energy eigenstates can be labeled by definite spin quantum numbers, simplifying the analysis.

Task 2

We have to construct the Hamiltonian FCI matrix with no broken pairs and total spin S=0. This automatically means that any 1p1h or 3p3h, etc... states are disallowed since they break a pair. It also means thatany 2p2h or 4p4h state must excite/de-excite a *pair* of electrons. We hence define the possible states:

$$|^{34}_{12}\rangle, |^{56}_{12}\rangle, |^{56}_{34}\rangle, |^{78}_{12}\rangle, |^{78}_{34}\rangle |^{78}_{56}\rangle = |\Phi_0\rangle, |\Phi_1\rangle, |\Phi_2\rangle, |\Phi_3\rangle, |\Phi_4\rangle |\Phi_5\rangle$$

This notation may be confusing, but $|^{rs}_{pq}\rangle$ refers to states p, q, r, s being occupied, since the reference state is the pure vacuum state (for now). The Associated Hamiltonian Matrix is calculated by finding the elements $H_{ij} = \langle\Phi_i|\hat{H}|\Phi_j\rangle$.

$$\begin{aligned}\langle\Phi_i|\hat{H}|\Phi_j\rangle &= \langle\Phi_i|\sum_{p\sigma}(p-1)a_{p\sigma}^\dagger a_{p\sigma}|\Phi_j\rangle - \langle\Phi_i|\frac{1}{2}g\sum_{pq}\hat{P}_p^+\hat{P}_q^-|\Phi_j\rangle \\ &= \sum_{p\sigma}(p-1)\langle\Phi_i|a_{p\sigma}^\dagger a_{p\sigma}|\Phi_j\rangle - \frac{1}{2}g\sum_{pq}\langle\Phi_i|\hat{P}_p^+\hat{P}_q^-|\Phi_j\rangle\end{aligned}$$

The first summation is equivalent to the number operator, and counts the occupied states. This will only give a contribution if the states are identical, hence only along the diagonal. The contribution will depend on which states are occupied, and teh corresponding energy-level p.

The second term is a pair-wise 2p2h operator, and thus gives contributions when the two states can be related to eachother through a pair-wise 2p2h excitation. Along the diagonal, it will give two contributions, since both states occupy the same pairs $-\frac{g}{2} - \frac{g}{2} = -g$ (Example: If the state is occupying p=1 (s+-) and p=3 (s+-), we get contributions from P=q=1 and p=q=3).

If however, the two states occupy only one shared state (off diagonal), we only get a contribution $-\frac{g}{2}$.

Along the opposite diagonal, however (lower left to upper right part of the Hamiltonian matrix) no state pairs are shared, and we will get 0 contributions here since it would require more than a two-pair operator.

$$H_{FCI} = \begin{bmatrix} 2-g & -\frac{g}{2} & -\frac{g}{2} & -\frac{g}{2} & -\frac{g}{2} & 0 \\ -\frac{g}{2} & 4-g & -\frac{g}{2} & -\frac{g}{2} & 0 & -\frac{g}{2} \\ -\frac{g}{2} & -\frac{g}{2} & 6-g & 0 & -\frac{g}{2} & -\frac{g}{2} \\ -\frac{g}{2} & -\frac{g}{2} & 0 & 6-g & -\frac{g}{2} & -\frac{g}{2} \\ -\frac{g}{2} & 0 & -\frac{g}{2} & -\frac{g}{2} & 8-g & -\frac{g}{2} \\ 0 & -\frac{g}{2} & -\frac{g}{2} & -\frac{g}{2} & -\frac{g}{2} & 10-g \end{bmatrix}$$

Diagonalizing this matrix corresponds to a Full Configuration Interaction Calculation, and we do it numerically. The results are presented in Figure 1. We see here that the energy decreases for increasing values of g. When there is 0 interaction between the particles, the energy is 2. When the interaction has a negative coefficient, the energy increases, possibly making the system more unstable and indicating a repulsive interaction. When g increases to 1, the ground state energy decreases, indicating that the interaction is attractive.

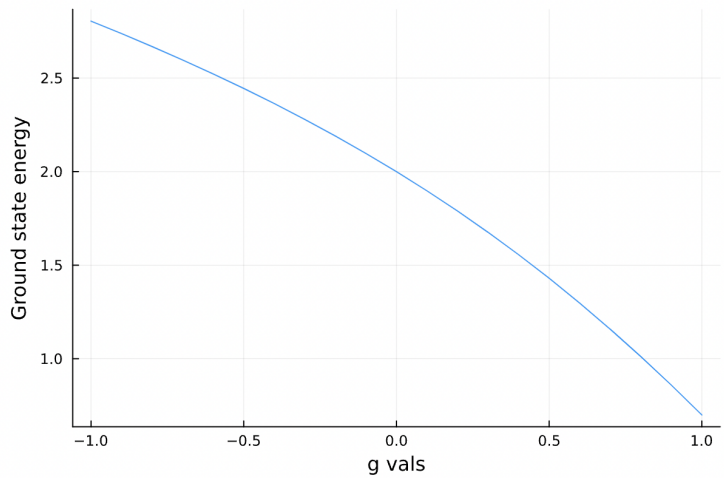

Figure 1: Ground State energy of FCI wrt various g values

Task 3

Allowing only 2p2h states, we truncate the Hamiltonian matrix to a 5x5 matrix, corresponding to a Configuration interaction (CI) calculation omitting the state $|\Phi_5\rangle$

$$H_{CI} = \begin{bmatrix} 2-g & -\frac{g}{2} & -\frac{g}{2} & -\frac{g}{2} & 0 \\ -\frac{g}{2} & 4-g & -\frac{g}{2} & 0 & -\frac{g}{2} \\ -\frac{g}{2} & -\frac{g}{2} & 6-g & 0 & -\frac{g}{2} \\ -\frac{g}{2} & -\frac{g}{2} & 0 & 6-g & -\frac{g}{2} \\ 0 & -\frac{g}{2} & -\frac{g}{2} & -\frac{g}{2} & 8-g \end{bmatrix}$$

Diagonalizing this matrix numerically, yields the comparative results in Figure 2. We see that the results are very good for g values between -1 and 1. As g increases to -5 and 5 however, the results start to diverge slightly. This indicates that the mixing from the 4p4h state has a stronger effect on the ground state energy when the interactions are stronger, and it is more negligible when the interactions are weak. This makes sense, since a stronger interaction would mean that the higher energy states interact more with the lower energy states, hence removing a high order term yields good results only when this interaction is weak.

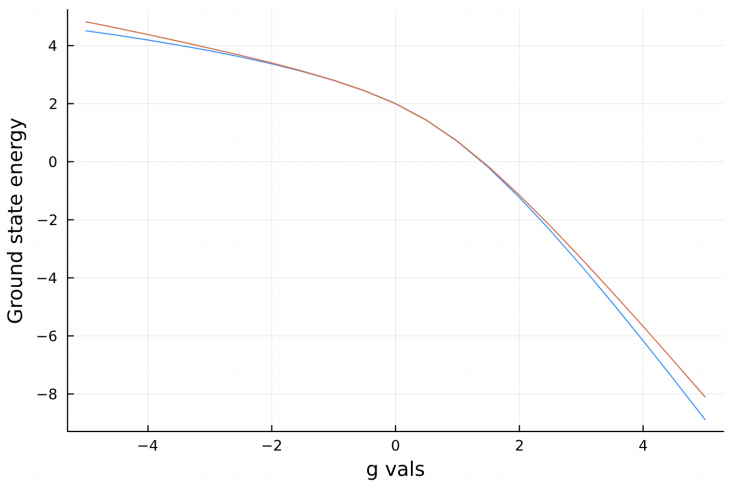

Figure 2: Ground State energy of FCI and 2p2h truncation wrt various g values

In Figure 3, the diagrams corresponding to the truncated FCI (CI) are shown. The two top diagrams represent an incoming particle (or hole,right diagram) pair, with an outgoing particle (or hole) pair. The two middle diagrams represent a pairwise particle→ hole (left) de-excitation or pairwise hole→particle (right)excitation. The two lowest diagrams represent the first term in the Hamiltonian, which counts the occupied states and returns the associated energy $p-1$ which is represented by the X in the figure. The state remains unchanged. Hence, for this hamiltonian, the diagrams show that all excitations are pairwise, and conserves the spin.

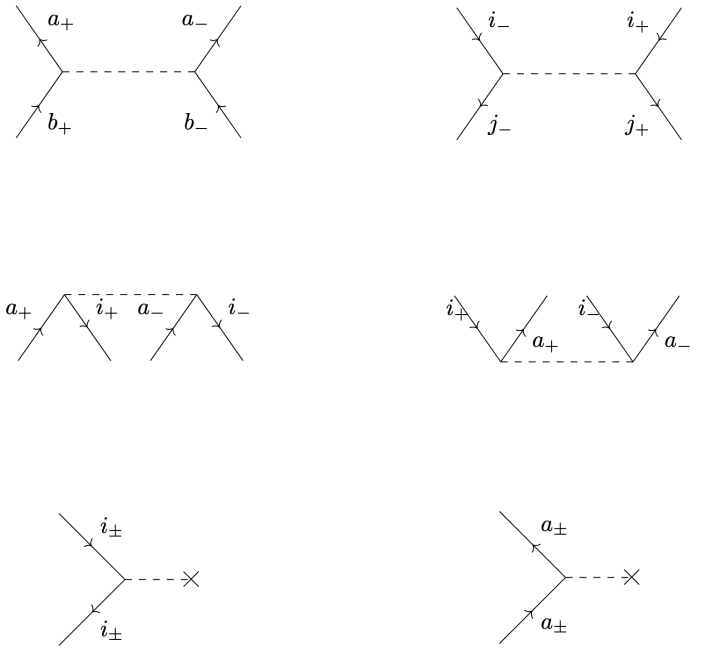

Figure 3: Diagrams for CI (Truncated FCI without 4p4h states)

Technically, we are not yet in the particle-hole formalism, so only the top left and bottom right diagrams are representative for now. The diagrams are illustrated in this way for clarity, since we will now move on to the particle-hole picture with Hartree Fock.

Task 4 / 5

We now move on to the particle hole formalism, this includes us finding a new vacuum state $|0\rangle \rightarrow |\Phi_0\rangle = a^\dagger_{1+}a^\dagger_{1-}a^\dagger_{2+}a^\dagger_{2-}|0\rangle$. We also need to define new normal orderings with respect to this basis, thin involves us first calculating the term $\langle\Phi_0|\hat{H}|\Phi_0\rangle$. As stated previously, the first term in the Hamiltonian is equivalent to the number operator acting on the state $|\Phi_0\rangle$. This will count states 1 and 2 twice (for spin up and down), resulting in $2(1-1)+2(2-1)=2$. The second term accounts for all possible 2p2h states from the ground state. When we apply this operator on $|\Phi_0\rangle$, we get two contributions, which is when p=q=1, and p=q=2. Then the operator will de-excite and excite back the same pair, and we get the original state $|\Phi_0\rangle$ back. Any other combination will automatically be 0. This means that we get a term $-g/2 - g/2 = -g$.

In total we have a ground state refrence energy: $E_0^{ref} = 2-g$. And the two terms are now normalized wrt the vaccuum state $|\Phi_0\rangle$.

$$\hat{H} = E_0^{ref} + \sum_{p\sigma}(p-1) : a^\dagger_{p\sigma}a_{p\sigma} : -\frac{1}{2}g\sum_{pq} : \hat{P}^+_p\hat{P}^-_q :$$

The first sum excludes p=1,2, and the second sum excludes p=q=1, and p=1=2.

We can now attempt to do a Hartree Fock calculation with this Hamiltonian in mind. In the FCI picture, a hartree fock calculation is equivalent with evaluating

$$\langle\Phi_0|\hat{f}|1p1h\rangle = \langle 1p1h|\hat{f}|\Phi_0\rangle = 0$$

This is already trivially 0, since we have by assumption excluded all possible 1p1h states. Hence We already are in a Hartree fock basis. We can also show this easily by using the Hartree Fock operator from the first midterm.

$$h^{HF}_{\alpha\gamma} = \langle\alpha|h_0|\gamma\rangle + \sum_p\sum_{\beta\delta} C^*_{p\beta}C_{p\delta}\langle\alpha\beta|V|\gamma\delta\rangle_{AS},$$

If we first assum $C = I$, we get

$$h^{HF}_{\alpha\gamma} = \langle\alpha|h_0|\gamma\rangle + \sum_p\sum_{\beta\delta}\langle\alpha p|V|\gamma p\rangle_{AS},$$

We get elements proportional to:

$$\delta_{\alpha\gamma} + \sum_p\sum_{\beta\delta}\langle\alpha p|V|\gamma p\rangle_{AS},$$

Along the off-diagonal, the double summation will always give 0, since p will be recquired to associated as the spin pair to α and the spin pair to γ at the same time. This is due to the nature of the pair-wise 2p2h excitation Hamiltonian-term. If α (or γ) and p has different energy values, then they are not a pair, and the interaction will be 0, because it is an excluded state. Hence both terms will only contribute along the diagonal of the Hartree Fock matrix. This means that the iteration scheme for Hartree Fock is already done, and we are in a Hartree Fock basis. The Ground state energy is as before given by $2-g$, with single-particle energies $(p-1)-\frac{g}{2}$). This can be seen in the code as well.

The diagrams Hartree Fock can affect is: 1, 3, 4, 5. These are the only ones in Figure 2 (from problem sheet) that do not include a $\langle\Phi_0|\hat{f}|1p1h\rangle$ term, which is set to zero by Hartree Fock.

Task 5: diagrams

The diagrams that will contribute from Figure 2 (problem sheet) are the ones that do not introduce any intermediate 1p1h, or 3p3h states. The only diagrams that do not do this are 1, 4, 5, 8 and 9. However, diagram 9 will not contribute. The diagram first creates a 2p2h state, but the leftmost particle state additionally interacts with another particle state. This is not possible and requires a pair-braking to get three particles (intermediately). Diagram 8 is similar, but will contribute. The loop here will sum over hole states, and does not require and additional excitation, hence does not break any pairs.

Diagram 1

This is a simple 2p2h diagram. First, we see that there are two closed loops, and 2 hole states, inducing $(-)^4 = +$, then we see that there are two identical lines, inducing a factor $\frac{1}{4}$. Combining all this and the intermediate state energies, we get:

$$\frac{1}{4}\sum_{ijab}\frac{\langle ij|v|ab\rangle\langle ab|v|ij\rangle}{\epsilon_i+\epsilon_j-\epsilon_a-\epsilon_b} = \frac{1}{4}\sum_{ia}\frac{\langle i\bar{i}|v|a\bar{a}\rangle\langle a\bar{a}|v|i\bar{i}\rangle}{2\epsilon_i-2\epsilon_a} = \frac{1}{4}\left(-\frac{g}{2}\right)^2\sum_{ia}\frac{1}{2\epsilon_i-2\epsilon_a}$$

Diagram 4

This is similar, but we have two intermediate particle states. We have two loops, two hole states: $+$. We have three identical lines: $\frac{1}{8}$. And we since there are three interaction vertices, we will have three contributions, and two energy denominators:

$$\frac{1}{8}\sum_{ijabcd}\frac{\langle ij|v|ab\rangle\langle ab|v|cd\rangle\langle cd|v|ij\rangle}{(\epsilon_i+\epsilon_j-\epsilon_a-\epsilon_b)(\epsilon_i+\epsilon_j-\epsilon_c-\epsilon_d)} = \frac{1}{8}\sum_{iac}\frac{\langle i\bar{i}|v|a\bar{a}\rangle\langle a\bar{a}|v|b\bar{b}\rangle\langle b\bar{b}|v|i\bar{i}\rangle}{(2\epsilon_i-2\epsilon_a)(2\epsilon_i-2\epsilon_b)} = \frac{1}{8}\left(-\frac{g}{2}\right)^3\sum_{iac}\frac{1}{4(\epsilon_i-\epsilon_a)(\epsilon_i-\epsilon_b)}$$

Diagram 5

Instead of an intermediate additional two-particle excitation, we have an additional two-hole excitation. With two loops and four hole states we get a $+$, and with three identical lines here as well, we get a factor $\frac{1}{8}$ too. The term becomes:

$$\frac{1}{8}\sum_{ijklab}\frac{\langle ij|v|ab\rangle\langle kl|v|ij\rangle\langle ab|v|kl\rangle}{(\epsilon_i+\epsilon_j-\epsilon_a-\epsilon_b)(\epsilon_k+\epsilon_l-\epsilon_a-\epsilon_b)} = \frac{1}{8}\sum_{ija}\frac{\langle i\bar{i}|v|a\bar{a}\rangle\langle j\bar{j}|v|i\bar{i}\rangle\langle a\bar{a}|v|j\bar{j}\rangle}{4(\epsilon_i-\epsilon_a)(\epsilon_k-\epsilon_a)} = \frac{1}{8}\left(-\frac{g}{2}\right)^3\sum_{iac}\frac{1}{4(\epsilon_i-\epsilon_a)(\epsilon_k-\epsilon_a)}$$

Diagram 8

This is nearly the same as diagram 1, but at the left hand side, there is an additional interaction. We have two identical lines, two hole lines, and three closed loops, meaning we get a factor $-\frac{1}{4}$. In total:

$$-\frac{1}{4}\sum_{ijkab}\frac{\langle ij|v|ab\rangle\langle ki|v|ki\rangle\langle ab|v|ij\rangle}{(\epsilon_i+\epsilon_j-\epsilon_a-\epsilon_b)(\epsilon_i+\epsilon_j-\epsilon_a-\epsilon_b)} = -\frac{1}{4}\sum_{ia}\frac{\langle i\bar{i}|v|a\bar{a}\rangle\langle i\bar{i}|v|i\bar{i}\rangle\langle a\bar{a}|v|j\bar{j}\rangle}{4(\epsilon_i-\epsilon_a)(\epsilon_i-\epsilon_a)} = -\frac{1}{4}\left(-\frac{g}{2}\right)^3\sum_{iac}\frac{1}{4(\epsilon_i-\epsilon_a)^2}$$

Ground State Energy

We put everything together, and get the results presented in Figure 4. It is clear that this method works very well! It is interesting however, that the energy estimate is too large for $g \approx -1$, but too little for $g \approx 1$. This is an indicator for a potential problem with MBPT, which is that it is not a variational approach. Introducing more terms, will not guarantee a better result, which we will see.

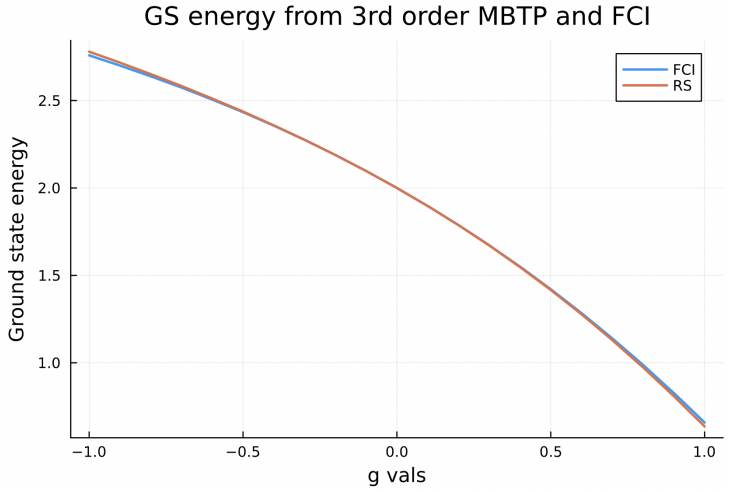

Figure 4: RS MBPT 3rd order results compared to FCI

Task 6

The 2p2h diagram is associated with second order pertubation theory. The Wave operator is in this case in first order, and is given in the following way.

$$\Delta E^{(2)} = \langle\Phi_0|\hat{H}_I \frac{Q}{E^{ref} - \hat{H}_0}\hat{H}_I|\Phi_0\rangle = \langle\Phi_0|\hat{H}_I \frac{Q}{E^{ref} - \hat{H}_0}\sum_{i,j,a,b}\langle ij|v|ab\rangle|\Phi_{ij}^{ab}\rangle = \langle\Phi_0|\hat{H}_I \frac{1}{E^{ref} - \hat{H}_0}Q\sum_i \frac{-g}{2}|\Phi_i\rangle$$

$$= \langle\Phi_0|\hat{H}_I \frac{1}{E^{ref} - \hat{H}_0}\sum_i \frac{-g}{2}|\Phi_i\rangle = -\frac{g}{2}\sum_i \frac{\langle\Phi_0|\hat{H}_I|\Phi_i\rangle}{E^{ref} - (E^{ref} - \epsilon_i - \epsilon_j + \epsilon_a + \epsilon_b)} = \left(-\frac{g}{2}\right)^2 \sum_{ia}\frac{1}{2\epsilon_i - 2\epsilon_a}$$

An interesting observation can be made by relating this to the original CI (FCI truncated to only 0p0h and 2p2h states) calculations which relates the ground state to the higher energy ones

$$|\Psi_0\rangle = \sum_{i=0}^{5} C_i|\Phi_0\rangle = \sum_{ijab}^{5} C_{ij}^{ab}|\Phi_{ij}^{ab}\rangle$$

We get the second equality by considering that 1p1h, and 3p3h states are excluded by the hamiltonian, and 4p4h is truncated from FCI to CI. The mixing can therefore only come from 2p2h contributions. We also know from FCI with hartree fock that the correlation energy is given:

$$\Delta E = \sum_{ijab}\langle ij|v|ab\rangle C_{ij}^{ab} = \sum_{ia}\langle i\hat{i}|v|a\hat{a}\rangle C_{i\hat{i}}^{a\hat{a}}$$

From $\Delta E^{(2)}$, we get

$$C_{i\hat{i}}^{a\hat{a}} = -\frac{g}{2}\frac{1}{2\epsilon_i - 2\epsilon_a}$$

This means that we get:

$$|\Psi_0\rangle = \sum_{ia} -\frac{g}{2}\frac{1}{2\epsilon_i - 2\epsilon_a}|\Phi_{i\hat{i}}^{a\hat{a}}\rangle$$

Now We just need to see that the states $|\Phi_{i\hat{i}}^{a\hat{a}}\rangle$ are the already defined 2p2h states $|\Phi_1\rangle, |\Phi_2\rangle, |\Phi_3\rangle, |\Phi_4\rangle$. This means that we get finally

$$|\Psi_0\rangle = C_0|\Phi_0\rangle - \frac{g}{2}\frac{1}{2\epsilon_2 - 2\epsilon_3}|\Phi_1\rangle - \frac{g}{2}\frac{1}{2\epsilon_2 - 2\epsilon_4}|\Phi_2\rangle - \frac{g}{2}\frac{1}{2\epsilon_1 - 2\epsilon_3}|\Phi_3\rangle - \frac{g}{2}\frac{1}{2\epsilon_1 - 2\epsilon_4}|\Phi_4\rangle$$

$$|\Psi_0\rangle = C_0|\Phi_0\rangle + \frac{g}{4}|\Phi_1\rangle + \frac{g}{8}|\Phi_2\rangle + \frac{g}{8}|\Phi_3\rangle + \frac{g}{12}|\Phi_4\rangle$$

There is a certain arbitrary-ness over the sign, therefore, we plot the error of the absolute values $|C_i|^2$ from CI and MBPT in Figure 5.

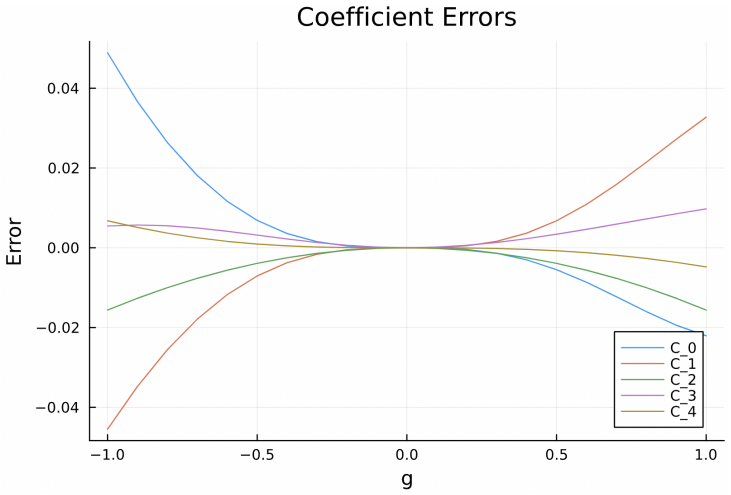

Figure 5: Error of Coefficients from CI and the estimated ones from 2nd order MBPT

It is clear, that when the interaction is small, corresponding to $g \in [-0.5, 0.5]$, the errors of MBPT are small. When g increases, meaning that the interactions are stronger, the theory struggles more, which is as expected, since pertubation theories thrive the most when the pertubations are small.

Task 7

In principle, there are a lot of diagrams to be considered here. But most of them can be easily disregarded. All four diagrams in Figure 3 (in the problem sheet) become 0 due to intermediate 1p1h excitations violating the pairing condition. In the same way, all diagrams from Figure 5 are also zero. From Figure 4, most diagrams will also vanish due to a pair-breaking. This is a different form of breaking, since here, the breaking is not due to exciting only one particle, but exciting two particles to different destinations. In for example diagram 12, we get a interaction int the third vertix from the top on the form $\langle ph|v|ph\rangle$ (p=particle, h=hole). In other words, a particle state comes in and out on one end of the vertix, and a hole state comes in and out from the other end. This means that a particle-hole pair goes in and out, which recquires a pair breaking. The only diagrams in figure 4 that does not do this are 5, 6, 14 and 15.

In Figure 6, we need to use the linked diagram theorem, which tells us automatically, that any unlinked diagrams are 0 in RS pertubation theory. This means that diagrams 33 and 41 is zero. The other diagrams contribute. The result can be seen in Figure 6.

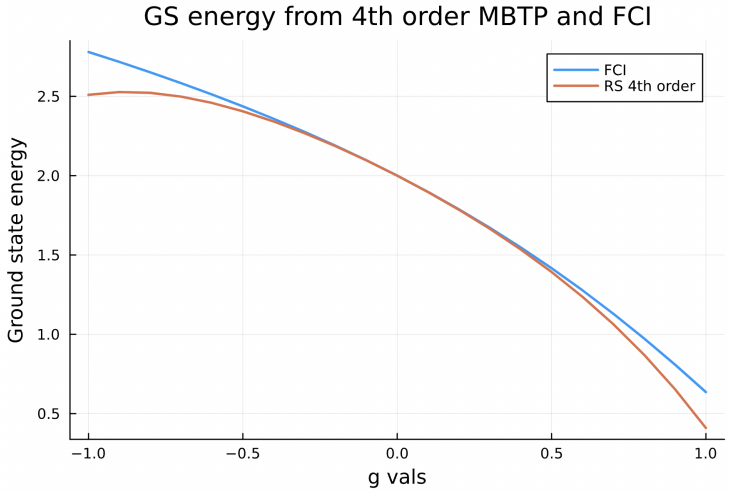

Figure 6: 4th order MBPT results compared with FCI for $g \in [-1, 1]$

Bellow in Figure 7, a comparison of all techniques are shown. It is clear that CI and third order MBPT theory are the best approximations for this system (and for this range of g values). It is also an interesting result that fourth order MBPT performs significantly worse than the other methods. The reason for this is that MBPT is not a variational method, meaning that the theory can both overestimate and underestimate the energy (which we saw in Figure 4). Including more terms will therefore not generally increase it's accuracy, but *can* diminish it. This is in contrast to variational methods which always approach the ground state energy.

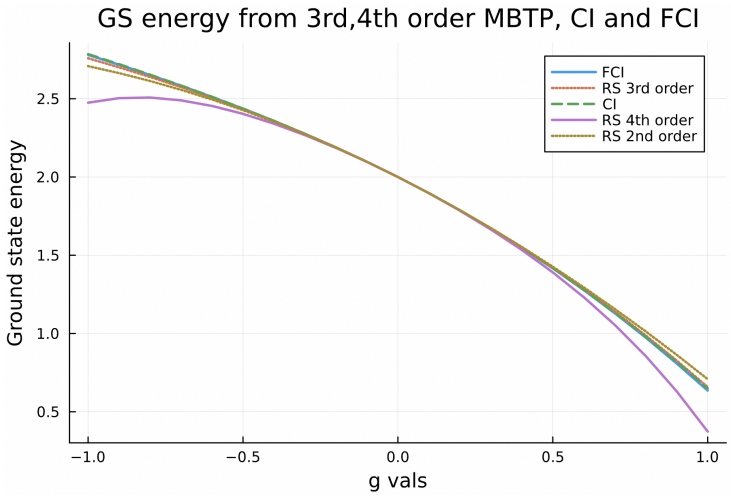

Figure 7: 2nd, 3rd, 4th order MBPT results compared with FCI and CI for $g \in [-1, 1]$

Task 7 diagram expressions

These are the final expressions of the fourth order MBPT for the system in this project. Note that i, j and k represent hole states, a, b and c represent particle states. For the calculation, we sum over all of them.

Diagram 5/6

$$E+ = 2\left(\frac{1}{2}\right)^4\left(-\frac{g}{2}\right)^4 \frac{1}{2^3(\epsilon_i-\epsilon_a)(\epsilon_j-\epsilon_a)(\epsilon_j-\epsilon_b)}$$

Diagram 14

$$E+ = \left(\frac{1}{2}\right)^4\left(-\frac{g}{2}\right)^4 \frac{1}{2^3(\epsilon_i-\epsilon_a)(\epsilon_i-\epsilon_b)(\epsilon_i-\epsilon_c)}$$

Diagram 15

$$E+ = \left(\frac{1}{2}\right)^4\left(-\frac{g}{2}\right)^4 \frac{1}{2^3(\epsilon_i-\epsilon_a)(\epsilon_j-\epsilon_a)(\epsilon_k-\epsilon_a)}$$

Diagram 34

$$E+ = \left(\frac{1}{2}\right)^2\left(-\frac{g}{2}\right)^2 \frac{1}{2^3(\epsilon_i-\epsilon_a)(2\epsilon_i-\epsilon_a-\epsilon_b)(\epsilon_i-\epsilon_b)}$$

Diagram 35

$$E+ = \left(\frac{1}{2}\right)^2\left(-\frac{g}{2}\right)^4 \frac{1}{2^3(\epsilon_i-\epsilon_a)(\epsilon_i+\epsilon_j-2\epsilon_a)(\epsilon_j-\epsilon_a)}$$

Diagram 36/37

$$E+ = 2\left(\frac{1}{2}\right)^4\left(-\frac{g}{2}\right)^4\frac{1}{2^3(\epsilon_i-\epsilon_a)(\epsilon_j+\epsilon_i-\epsilon_a-\epsilon_b)(\epsilon_j-\epsilon_b)}$$

Diagram 38

$$E+ = \left(-\frac{g}{2}\right)^4\frac{1}{2^4(\epsilon_i-\epsilon_a)^3}$$

Diagram 39

$$E+ = \left(\frac{1}{2}\right)^2\left(-\frac{g}{2}\right)^4\frac{1}{2^3(\epsilon_i-\epsilon_a)(\epsilon_i+\epsilon_j-2\epsilon_a)(\epsilon_i-\epsilon_a)}$$

Diagram 40

$$E+ = \left(\frac{1}{2}\right)^2\left(-\frac{g}{2}\right)^4\frac{1}{2^3(\epsilon_i-\epsilon_a)(2\epsilon_i-\epsilon_a-\epsilon_b)(\epsilon_i-\epsilon_a)}$$

Code

My code is available in my github, which can be found here at [1]. The code is under FYS4480 / Project 2.

References

[1] Aleksander Sekkelsten. *UIO Numerical work*. URL: https://github.com/Im2ql4u/Machine-learning-UIO.