Second Midterm

Problem 1)

- **1.1)** Show $[\hat{H}_0, \hat{S}_z] = 0$

$$[\hat{H}_0, \hat{S}_z] = \frac{\xi}{2}[\sum_{p\sigma}(p-1)a^\dagger_{p\sigma}a_{p\sigma}, \sum_{q\tau}\tau a^\dagger_{q\tau}a_{q\tau}]$$

Here we can assume general terms and disregard the summations and constants. The commutation of summations will give rise to a summation of commutators. It then is sufficient to show that all of those general commutators are zero, as follows.

$$\begin{aligned}
[(p-1)a^\dagger_{p\sigma}a_{p\sigma}, \tau a^\dagger_{q\tau}a_{q\tau}] &= (p-1)\tau[a^\dagger_{p\sigma}a_{p\sigma}, a^\dagger_{q\tau}a_{q\tau}] \\
&\propto a^\dagger_{p\sigma}a_{p\sigma}a^\dagger_{q\tau}a_{q\tau} - a^\dagger_{q\tau}a_{q\tau}a^\dagger_{p\sigma}a_{p\sigma} \\
&= a^\dagger_{p\sigma}a_{p\sigma}a^\dagger_{q\tau}a_{q\tau} - \delta_{\substack{qp\\\tau\sigma}}a^\dagger_{q\tau}a_{p\sigma} + a^\dagger_{q\tau}a^\dagger_{p\sigma}a_{q\tau}a_{p\sigma} \\
&= a^\dagger_{p\sigma}a_{p\sigma}a^\dagger_{q\tau}a_{q\tau} - \delta_{\substack{qp\\\tau\sigma}}a^\dagger_{q\tau}a_{p\sigma} + a^\dagger_{p\sigma}a^\dagger_{q\tau}a_{p\sigma}a_{q\tau} \\
&= a^\dagger_{p\sigma}a_{p\sigma}a^\dagger_{q\tau}a_{q\tau} - \delta_{\substack{qp\\\tau\sigma}}a^\dagger_{q\tau}a_{p\sigma} + \delta_{\substack{qp\\\tau\sigma}}a^\dagger_{p\sigma}a_{q\tau} - a^\dagger_{p\sigma}a_{p\sigma}a^\dagger_{q\tau}a_{q\tau} \\
&= a^\dagger_{p\sigma}a_{p\sigma}a^\dagger_{q\tau}a_{q\tau} - a^\dagger_{p\sigma}a_{p\sigma}a^\dagger_{q\tau}a_{q\tau} \\
&= 0
\end{aligned} \tag{1}$$

- **1.2)** Show $[\hat{V}, \hat{S}_z] = 0$ Similarly

$$[\hat{V}, \hat{S}_z] = -\frac{g}{2}[\sum_{rs}\hat{P}^+_r\hat{P}^-_s, \sum_{q\tau}\tau a^\dagger_{q\tau}a_{q\tau}]$$

For the same arguments, we disregard constants and sums, resulting

$$\begin{aligned}
[\hat{P}^+_r\hat{P}^-_s, a^\dagger_{q\tau}a_{q\tau}] &= [\hat{P}^+_r\hat{P}^-_s, a^\dagger_{q\tau}a_{q\tau}] \\
&= \hat{P}^+_r[\hat{P}^-_s, a^\dagger_{q\tau}a_{q\tau}] + [\hat{P}^+_r, a^\dagger_{q\tau}a_{q\tau}]\hat{P}^-_s
\end{aligned}$$

Let us first look at the first one

$$\begin{aligned}
[\hat{P}^-_s, a^\dagger_{q\tau}a_{q\tau}] &= [a_{s-}a_{s+}, a^\dagger_{q\tau}a_{q\tau}] \\
&= a_{s-}a_{s+}a^\dagger_{q\tau}a_{q\tau} - a^\dagger_{q\tau}a_{q\tau}a_{s-}a_{s+} \\
&= a_{s-}a_{s+}a^\dagger_{q\tau}a_{q\tau} - a^\dagger_{q\tau}a_{s-}a_{s+}a_{q\tau} \\
&= a_{s-}a_{s+}a^\dagger_{q\tau}a_{q\tau} + a_{s-}a^\dagger_{q\tau}a_{s+}a_{q\tau} - \delta_{sq-\tau}a_{s+}a_{q\tau} \\
&= a_{s-}a_{s+}a^\dagger_{q\tau}a_{q\tau} - a_{s-}a_{s+}a^\dagger_{q\tau}a_{q\tau} + \delta_{sq+\tau}a_{s-}a_{q\tau} - a_{s+}a_{s-} \\
&= a_{s-}a_{s+} - a_{s+}a_{s-}
\end{aligned}$$

Similarly, the second one,

$$\begin{aligned}
[\hat{P}_r^+, a_{q\tau}^\dagger a_{q\tau}] &= [a_{r+}^\dagger a_{r-}^\dagger, a_{q\tau}^\dagger a_{q\tau}] \\
&= a_{r+}^\dagger a_{r-}^\dagger a_{q\tau}^\dagger a_{q\tau} - a_{q\tau}^\dagger a_{q\tau} a_{r+}^\dagger a_{r-}^\dagger \\
&= a_{r+}^\dagger a_{r-}^\dagger a_{q\tau}^\dagger a_{q\tau} + a_{q\tau}^\dagger a_{r+}^\dagger a_{q\tau} a_{r-}^\dagger - \delta_{qr\tau+} a_{q\tau}^\dagger a_{r-}^\dagger \\
&= a_{r+}^\dagger a_{r-}^\dagger a_{q\tau}^\dagger a_{q\tau} - a_{q\tau}^\dagger a_{r+}^\dagger a_{r-}^\dagger a_{q\tau} + \delta_{qr\tau-} a_{q\tau}^\dagger a_{r+}^\dagger - a_{r+}^\dagger a_{r-}^\dagger \\
&= a_{r-}^\dagger a_{r+}^\dagger - a_{r+}^\dagger a_{r-}^\dagger
\end{aligned}$$

So putting it back together, it follows

$$\begin{aligned}
[\hat{P}_r^+ \hat{P}_s^-, a_{q\tau}^\dagger a_{q\tau}] &= \hat{P}_r^+ (a_{s-} a_{s+} - a_{s+} a_{s-}) + (a_{r-}^\dagger a_{r+}^\dagger - a_{r+}^\dagger a_{r-}^\dagger) \hat{P}_s^- \\
&= a_{r+}^\dagger a_{r-}^\dagger (a_{s-} a_{s+} - a_{s+} a_{s-}) + (-a_{r+}^\dagger a_{r-}^\dagger + a_{r+}^\dagger a_{r-}^\dagger) a_{s-} a_{s+} \\
&= 0
\end{aligned} \tag{2}$$

- **1.3)** Show $[\hat{H}_0, \hat{S}^2] = 0$

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

$$\hat{S}_\pm := \sum_p a_{p\pm}^\dagger a_{p\mp}.$$

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

But the first term is immediately zero since

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

The second term follows

$$\begin{aligned}
[\hat{H}_0, (\hat{S}_+ \hat{S}_- + \hat{S}_- \hat{S}_+)] &= [\hat{H}_0, \hat{S}_+ \hat{S}_-] + [\hat{H}_0, \hat{S}_- \hat{S}_+] \\
&= [\hat{H}_0, \hat{S}_+] \hat{S}_- + \hat{H}_0 [\hat{S}_-, \hat{S}_+] + [\hat{H}_0, \hat{S}_-] \hat{S}_+ + \hat{H}_0 [\hat{S}_+, \hat{S}_-]
\end{aligned}$$

Clearly, $H_0[\hat{S}_+, \hat{S}_-] + \hat{H}_0[\hat{S}_-, \hat{S}_+] = 0$, since $[A, B] + [B, A] = AB - BA + BA - AB$. Now let us see $[\hat{H}_0, \hat{S}_+] = 0$.

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

Again, ignoring the sum and constant for now

$$\begin{aligned}
[\hat{H}_0, \hat{S}_+] &\to [a^\dagger_{p\sigma} a_{p\sigma}, a^\dagger_{q+} a_{q-}] \\
&\to a^\dagger_{p\sigma} a_{p\sigma} a^\dagger_{q+} a_{q-} + a^\dagger_{p\sigma} a^\dagger_{q+} a_{p\sigma} a_{q-} - \delta_{qp\sigma-} a^\dagger_{q+} a_{p\sigma} \\
&\to a^\dagger_{p\sigma} a_{p\sigma} a^\dagger_{q+} a_{q-} + a^\dagger_{p\sigma} (\delta_{pq\sigma+} - a_{p\sigma} a^\dagger_{q+}) a_{q-} - \delta_{qp\sigma-} a^\dagger_{q+} a_{p\sigma} \\
[\hat{H}_0, \hat{S}_+] &= \sum_{p\sigma} (p-1)(a^\dagger_{p+} a_{p-} - a^\dagger_{p+} a_{p-}) = 0
\end{aligned} \tag{3}$$

Therefore it follows that $[\hat{H}_0, \hat{S}_-] = 0$ also, since both $\hat{H}_0$ is hermitian and $\hat{S}^\dagger_- = \hat{S}_+$

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

So now we have shown all terms following the expansion of $[\hat{H}_0, \hat{S}^2]$ are zero.

- **1.4)** Show $[\hat{V}, \hat{S}^2] = 0$

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

But we have shown $[V, \hat{S}_z] = 0$, so again, the first term vanishes. The second term follows,

$$\begin{aligned}
[V, (\hat{S}_+ \hat{S}_- + \hat{S}_- \hat{S}_+)] &= [V, \hat{S}_+ \hat{S}_-] + [V, \hat{S}_- \hat{S}_+] \\
&= [V, \hat{S}_+] \hat{S}_- + V[\hat{S}_-, \hat{S}_+] + [V, \hat{S}_-] \hat{S}_+ + V[\hat{S}_+, \hat{S}_-]
\end{aligned}$$

Similarly to the last case, it is clear $V[\hat{S}_-, \hat{S}_+] + V[\hat{S}_+, \hat{S}_-] = 0$. Analyzing the remaining terms,

$$\begin{aligned}
[\hat{V}, \hat{S}_+] &\to [\hat{P}^+_p \hat{P}^-_q, a^\dagger_{s+} a_{s-}] \\
&= a^\dagger_{p+} a^\dagger_{p-} a_{q-} a_{q+} a^\dagger_{s+} a_{s-} + a^\dagger_{s+} a^\dagger_{p+} a_{s-} a^\dagger_{p-} a_{q-} a_{q+} \\
&= a^\dagger_{p+} a^\dagger_{p-} a_{q-} a_{q+} a^\dagger_{s+} a_{s-} + a^\dagger_{p+} a^\dagger_{s+} a^\dagger_{p-} a_{s-} a_{q-} a_{q+} - a^\dagger_{s+} a^\dagger_{s+} a_{q-} a_{q+} \\
&= a^\dagger_{p+} a^\dagger_{p-} a_{q-} a_{q+} a^\dagger_{s+} a_{s-} - a^\dagger_{p+} a^\dagger_{p-} a^\dagger_{s+} a_{q-} a_{q+} a_{s-} - a^\dagger_{s+} a^\dagger_{s+} a_{q-} a_{q+} \\
&= a^\dagger_{p+} a^\dagger_{p-} a_{q-} a_{q+} a^\dagger_{s+} a_{s-} + a^\dagger_{p+} a^\dagger_{p-} a_{q-} a^\dagger_{s+} a_{q+} a_{s-} - a^\dagger_{s+} a^\dagger_{s+} a_{q-} a_{q+} \\
&= a^\dagger_{p+} a^\dagger_{p-} a_{q-} a_{q+} a^\dagger_{s+} a_{s-} - a^\dagger_{p+} a^\dagger_{p-} a_{q-} a_{q+} a^\dagger_{s+} a_{s-} + a^\dagger_{p+} a^\dagger_{p-} a_{q-} a_{q-} - a^\dagger_{s+} a^\dagger_{s+} a_{q-} a_{q+} \\
&= 0 \\
[\hat{V}, \hat{S}_+] &= -\frac{1}{2} g \sum_{pq} [\hat{P}^+_p \hat{P}^-_q, a^\dagger_{s+} a_{s-}] = 0
\end{aligned} \tag{4}$$

Again, this forces $[\hat{V}, \hat{S}_-] = 0$ because $\hat{S}^\dagger_+ = \hat{S}_-$ and $\hat{V}$ is hermitian, concluding the demonstration.

- **1.5)** Show that if $\xi = 1$ then $\hat{H} = \sum_{p\sigma}(p-1)a^\dagger_{p\sigma}a_{p\sigma} - \frac{1}{2}g\sum_{pq}\hat{P}^+_p\hat{P}^-_q$

  Indeed, given

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

  where

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

  It suffices to plug the definitions of

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

  and sum the operators.

- **1.6)** The new enunciation is actually to show $[\hat{P}^\pm_p, \hat{P}^\pm_q] = 0$

  This is immediate from the anti-commutation rules.

  $$\begin{aligned}[\hat{P}^\pm_p, \hat{P}^\pm_q] &= a^\dagger_{p\pm}a^\dagger_{p\mp}a^\dagger_{q\pm}a^\dagger_{q\mp} - a^\dagger_{q\pm}a^\dagger_{q\mp}a^\dagger_{p\pm}a^\dagger_{p\mp} \\ &= a^\dagger_{p\pm}a^\dagger_{p\mp}a^\dagger_{q\pm}a^\dagger_{q\mp} - (-1)^4 a^\dagger_{p\pm}a^\dagger_{p\mp}a^\dagger_{q\pm}a^\dagger_{q\mp} = 0\end{aligned}$$

Problem 2) This system, given its constraints, exhibits one possible zero-particle zero-hole configuration, one possible four-particle four-hole excitation, and four possible two-particle two-hole excitations. Therefore, the hamiltonian is 6×6. Since we are never breaking spin pairs, and fermions are indistinguishable, we can denote the ansatz for our ground state as

$$|\Phi_0\rangle = |12\rangle = \hat{P}^+_1\hat{P}^+_2|0\rangle$$

Where this denotes that $p = 1$ and $p = 2$ are filled with opposite spin fermions, and therefore, it is not important to denote the spin since we don't break pairs. We then construct the hamiltonian. Let us start by analyzing a general element of the hamiltonian.

$$\begin{aligned}\langle kl|\,H\,|nm\rangle &= \langle 0|\,\hat{P}^-_l\hat{P}^-_k H \hat{P}^+_n\hat{P}^+_m\,|0\rangle \\ &= \sum_{p\sigma}(p-1)\,\langle 0|\,\hat{P}^-_l\hat{P}^-_k a^\dagger_{p\sigma}a_{p\sigma}\hat{P}^+_n\hat{P}^+_m\,|0\rangle - \frac{1}{2}g\sum_{rs}\langle 0|\,\hat{P}^-_l\hat{P}^-_k\hat{P}^+_r\hat{P}^-_s\hat{P}^+_n\hat{P}^+_m\,|0\rangle \end{aligned} \tag{5}$$

Starting with the leftmost term, we see that it requires $(p = n \vee p = m) \wedge (p = k \vee p = l)$ in order to not be immediately zero. It is clear that this term only contributes in the diagonals, meaning $kl = nm$ (or permutations of nm and kl, which for us is meaningless for the expected value). Thence,

$$\sum_{p\sigma}(p-1)\langle 0|\hat{P}_m^-\hat{P}_n^- a_{p\sigma}^\dagger a_{p\sigma}\hat{P}_n^+\hat{P}_m^+|0\rangle =$$

$$(n-1)\langle 0|\overbrace{a_{m-}a_{m+}a_{n-}a_{n+}a_{n+}^\dagger a_{n+}^\dagger a_{n+}^\dagger a_{n-}^\dagger a_{m+}^\dagger a_{m-}^\dagger}|0\rangle$$

$$(n-1)\langle 0|\overbrace{a_{m-}a_{m+}a_{n-}a_{n+}a_{n-}^\dagger a_{n-}a_{n+}^\dagger a_{n-}^\dagger a_{m+}^\dagger a_{m-}^\dagger}|0\rangle$$

$$(m-1)\langle 0|\overbrace{a_{m-}a_{m+}a_{n-}a_{n+}a_{m+}^\dagger a_{m+}a_{n+}^\dagger a_{n-}^\dagger a_{m+}^\dagger a_{m-}^\dagger}|0\rangle$$

$$(m-1)\langle 0|\overbrace{a_{m-}a_{m+}a_{n-}a_{n+}a_{m-}^\dagger a_{m-}a_{n+}^\dagger a_{n-}^\dagger a_{m+}^\dagger a_{m-}^\dagger}|0\rangle)$$

$$= 2(n-1)+2(m-1)$$

Similarly, for the rightmost term of 5,

$$\begin{aligned}
-\frac{g}{2}\sum_{rs}\langle 0|P_l^-P_k^-\hat{P}_r^+\hat{P}_s^-\hat{P}_n^+\hat{P}_m^+|0\rangle &= -\frac{g}{2}\sum_{rs}\langle 0|\overbrace{P_l^-P_k^-P_r^+P_s^-P_n^+P_m^+}|0\rangle \\
&\quad -\frac{g}{2}\langle 0|\overbrace{P_l^-P_k^-P_r^+P_s^-P_n^+P_m^+}|0\rangle \\
&\quad -\frac{g}{2}\langle 0|\overbrace{P_l^-P_k^-P_r^+P_s^-P_n^+P_m^+}|0\rangle \\
&\quad -\frac{g}{2}\langle 0|\overbrace{P_l^-P_k^-P_r^+P_s^-P_n^+P_m^+}|0\rangle \\
&= -\frac{g}{2}\sum_{rs}(\delta_{kr}\delta_{sn}\delta_{lm}+\delta_{kr}\delta_{sm}\delta_{ln}+\delta_{kn}\delta_{sm}\delta_{lr}+\delta_{km}\delta_{sr}\delta_{lm})
\end{aligned} \tag{6}$$

From this we know that all the secondary diagonal has to be zero since they imply $k! = l! = n! = m$. Similarly, the diagonal contribution forces $k = n \wedge l = m$, but in our system, $n! = m$ and $k! = l$ so they account for a contribution of

$$-\frac{g}{2}\sum_{rs}(\delta_{nr}\delta_{sn}+\delta_{sm}\delta_{mr}) = -g$$

Now we are left only with the task of analyzing the terms off-diagonal. But that is easy because, in each column of the hamiltonian, only one delta survives because of the constraint $n! = m$ and $k! = l$, giving only $-g/2$.

This reasoning was possible because we can contract the pair creation and pair operators like in the wicks theorem seamlessly, except for the fact that crossing lines do not give rise to a minus sign since we showed that the product of pair creation and pair annihilation operators commute.

After all this, we can write the hamiltonian, ordering the diagonal elements.

$$\begin{bmatrix} 2-g & -g/2 & -g/2 & -g/2 & -g/2 & 0 \\ -g/2 & 4-g & -g/2 & -g/2 & 0 & -g/2 \\ -g/2 & -g/2 & 6-g & 0 & -g/2 & -g/2 \\ -g/2 & -g/2 & 0 & 6-g & -g/2 & -g/2 \\ -g/2 & 0 & -g/2 & -g/2 & 8-g & -g/2 \\ 0 & -g/2 & -g/2 & -g/2 & -g/2 & 10-g \end{bmatrix}$$

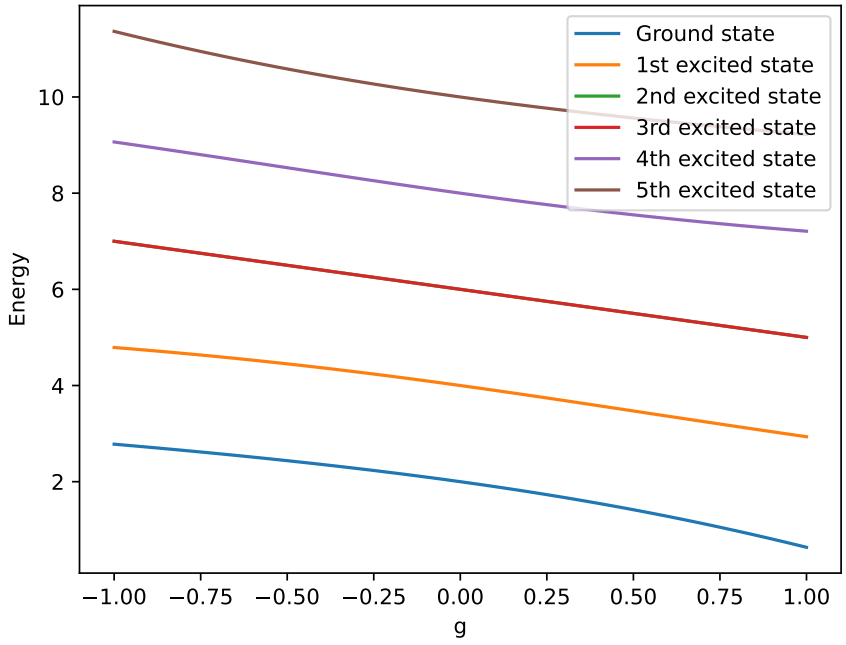

Figure 1: Energies of the ground state and excited states of the system varying the parameter g from -1 to 1 with 100 points in between. We here see the energy of the ground state behave monotonically decreasing with the strength of the interaction.

Problem 3)

If we make the approximation where we consider only two-particle two-hole excitations happen, then our hamiltonian becomes

$$\begin{bmatrix} 2-g & -g/2 & -g/2 & -g/2 & -g/2 \\ -g/2 & 4-g & -g/2 & -g/2 & 0 \\ -g/2 & -g/2 & 6-g & 0 & -g/2 \\ -g/2 & -g/2 & 0 & 6-g & -g/2 \\ -g/2 & 0 & -g/2 & -g/2 & 8-g \end{bmatrix}$$

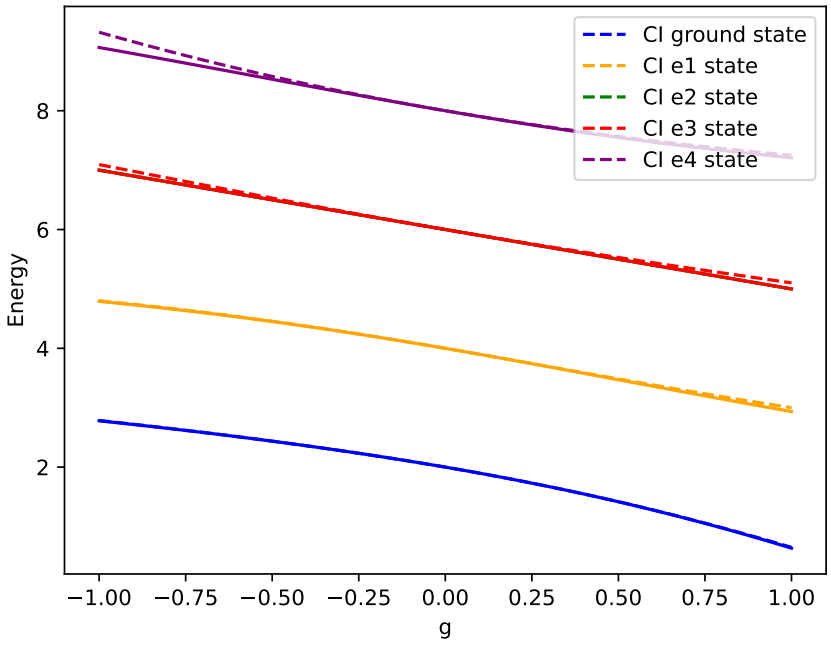

Figure 2: Energies of the ground state and excited states of the approximate system varying the parameter g from -1 to 1 with 100 points in between. We here consider only up to two-particle two-hole excitations. The energy is grouped by colors, but the approximate system energies are dashed, while the continuous line corresponds to our exact solution. It is evident that the approximation becomes worse the higher the excited level.

Problem 4) We can, as we have done in the previous midterm, define the normal ordered hamiltonian operator as

$$\hat{H}_N = \sum_{\alpha\beta}\langle\alpha|\hat{h}_0|\beta\rangle\{a^\dagger_\alpha a_\beta\} + \frac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|V|\gamma\delta\rangle_{AS}\{a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma\} + \sum_{\alpha\beta i}\langle\alpha i|V|\beta i\rangle\{a^\dagger_\alpha a_\beta\} + \\ + \frac{1}{2}\sum_{ij}\langle ij|V|ij\rangle_{AS} + \sum_i\langle i|\hat{h}_0|i\rangle$$

Where the labels i, j are explicitly below the Fermi Level. The two last elements then are defined as the E_0^{ref}. This normal-ordered hamiltonian is more usually written as

$$\hat{H}_N = E_0^{ref} + \hat{F}_N + \hat{V}_N$$

$$\hat{F}_N = \sum_{\alpha\beta}\langle\alpha|\hat{f}|\beta\rangle\{a^\dagger_\alpha a_\beta\}, \quad \hat{V}_N = \frac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|\hat{V}|\gamma\delta\rangle_{AS}\{a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma\},$$

$$\langle\alpha|\hat{f}|\beta\rangle = \langle\alpha|h_0|\beta\rangle + \sum_{i\leq F}\langle\alpha i|\hat{V}|\beta i\rangle_{AS}$$

So for our problem, we have $i, j \in \{1_-, 1_+, 2_-, 2_+\}$ and we know also the matrix elements. Since the single particle states are eigenstates of $\hat{h}_0$, $\langle p_\sigma|\hat{h}_0|q_\tau\rangle = (p-1)\delta_{pq}\delta_{\sigma\tau}$. We then know the reference energy to be

$$E_0^{ref} = 2 - g.$$

Moreover, $\langle\alpha\beta|V|\gamma\delta\rangle_{AS}$ will only be different from zero in the following cases

$$\begin{aligned} \langle p_+p_-|V|q_+q_-\rangle_{AS} &= -g/2, \qquad \langle p_-p_+|V|q_-q_+\rangle_{AS} = -g/2 \\ \langle p_+p_-|V|q_-q_+\rangle_{AS} &= g/2, \qquad \langle p_-p_+|V|q_+q_-\rangle_{AS} = g/2 \end{aligned}$$

So that

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

Notice that whenever we were to plug the positive $g/2$ in the sum, we actually perform a flip in the operators at the expense of a minus sign and allowing us to group the sum. In analogy to this analysis, but now opening the spin degrees of freedom, we can investigate the Hartree-Fock matrix elements considering $\langle p_\sigma r_\zeta|V|q_\tau s_\omega\rangle_{AS} = (-g/2)\delta_{pr}\delta_{qs}\delta_{\sigma\tau}\delta_{\zeta\omega}$ and also adding the constraint δ_{rs}.

$$\begin{aligned} \langle p_\sigma|\hat{f}|q_\tau\rangle &= (p-1)\delta_{pq}\delta_{\sigma\tau} - \frac{g}{2}\frac{1}{2}\sum_{\substack{s\leq 2\\ \omega\in\{-,+\}}}\sum_{\substack{r\leq 2\\ \zeta\in\{-,+\}}}\delta_{pr}\delta_{qs}\delta_{\sigma\tau}\delta_{\zeta\omega}\delta_{rs} \\ &= (p-1)\delta_{pq}\delta_{\sigma\tau} - \frac{g}{4}\delta_{\sigma\tau}\sum_{\substack{s\leq 2\\ \omega\in\{-,+\}}}\sum_{\substack{r\leq 2\\ \zeta\in\{-,+\}}}\delta_{pr}\delta_{qs}\delta_{\zeta\omega}\delta_{rs} \\ &= (p-1)\delta_{pq}\delta_{\sigma\tau} - \frac{g}{4}\delta_{\sigma\tau}\sum_{\substack{s\leq 2\\ \omega\in\{-,+\}}}\sum_{\zeta\in\{-,+\}}\delta_{qs}\delta_{\zeta\omega}\delta_{ps} \\ &= \begin{cases} (p-1)\delta_{pq}\delta_{\sigma\tau} - \frac{g}{2}\delta_{pq}\delta_{\sigma\tau}, & p,q\leq 2 \\ (p-1)\delta_{pq}\delta_{\sigma\tau}, & \text{else} \end{cases} \end{aligned}$$

This tells us that we are already in a Hartree-Fock basis since the Hartree-Fock Hamiltonian expressed by the elements $\langle p_\sigma|\hat{f}|q_\tau\rangle$ is already diagonal.

The terms of $\hat{F}_N$ then follow

$$\hat{F}_N = \sum_{p_\sigma q_\tau}((p-1)\delta_{pq}\delta_{\sigma\tau} - \frac{g}{2}\delta_{\sigma\tau}\delta_{pq})\{a^\dagger_{p_\sigma}a_{q_\tau}\} + \sum_{\substack{p_\sigma q_\tau\\ p,q>2}}\frac{g}{2}\delta_{\sigma\tau}\delta_{pq}\{a^\dagger_{p_\sigma}a_{q_\tau}\},$$

A canonical Hartree-Fock approach is one in which the matrix representation of the Fock operator $\hat{f}$ is diagonal in the Hartree-Fock basis ($\langle\psi_i|\hat{f}|\psi_j\rangle = \epsilon_i\delta_{ij}$). We know that the Slater

determinants obtained by the wave functions are unchanged by unitary transformations of the wave functions, and therefore we can give different representations for the Hartree-Fock eigenvalue equations $\hat{f}\psi_i = \epsilon_i\psi_i$. The representations which leave the matrix form of $\hat{f}$ non-diagonal but block-diagonal in terms of the particles and holes spinorbitals are called non-canonical Hartree-Fock. In those cases, the Fock operator matrix elements are then $f_{ia} = 0$.

Problem 5)

Again, as was done in midterm 1, given $\psi_p = \sum_\lambda C_{p\lambda}\phi_\lambda$, we can write E_0^{ref} as

$$\langle\psi_0|\hat{H}|\psi_0\rangle = \sum_{i\leq F}\sum_{\alpha\beta} C^*_{i\alpha}C_{i\beta}\langle\alpha|\hat{h}_0|\beta\rangle + \frac{1}{2}\sum_{i,j\leq F}\sum_{\alpha\beta\gamma\delta} C^*_{i\alpha}C^*_{j\beta}C_{i\gamma}C_{i\delta}\langle\alpha\beta|V|\gamma\delta\rangle_{AS},$$

which we want to minimize. For that we then introduced the functional $F(\psi_0)$ and Lagrangian multiplier ϵ_i such that

$$F(\psi_0) = E_0^{HF} - \sum_i^N \epsilon_i \sum_\alpha C^*_{i\alpha}C_{i\alpha}$$

we then minimize with respect to any of the coefficients

$$\begin{aligned}\frac{d}{dC^*_{i\alpha}}F(\psi_0) &= \frac{d}{dC^*_{i\alpha}}(E_0^{HF} - \sum_i^N \epsilon_i \sum_\alpha C^*_{i\alpha}C_{i\alpha}) \\ &= \sum_\beta C_{i\beta}\langle\alpha|\hat{h_0}|\beta\rangle + \sum_{j\leq F}\sum_{\beta\gamma\delta} C^*_{j\beta}C_{i\gamma}C_{j\delta}\langle\alpha\beta|V|\gamma\delta\rangle_{AS} - \epsilon_i C_{i\alpha} = 0\end{aligned}$$

Then, we change dummy variables $\beta \leftrightarrow \gamma$ for the first sum and $j \leftrightarrow p$ and $i \leftrightarrow p$ in general.

$$\sum_\gamma C_{p\gamma}\langle\alpha|\hat{h_0}|\gamma\rangle + \sum_{p\leq F}\sum_{\beta\gamma\delta} C^*_{p\beta}C_{p\gamma}C_{p\delta}\langle\alpha\beta|V|\gamma\delta\rangle_{AS} = \epsilon_p C_{p\alpha}$$

But we saw that $h^{HF}_{\alpha\gamma}$ is already diagonal, meaning that the coefficients resume to deltas. More specifically,

$$\sum_\gamma \delta_{p\gamma}\langle\alpha|\hat{h_0}|\gamma\rangle + \sum_{p\leq F}\sum_{\beta\gamma\delta} \delta_{p\beta}\delta_{p\gamma}\delta_{p\delta}\langle\alpha\beta|V|\gamma\delta\rangle_{AS} = \epsilon_p \delta_{p\alpha}$$

So if we call the Fock operator matrix elements

$$
\begin{aligned}
h^{HF}_{\alpha\gamma} &= \langle\alpha|\hat{h}_0|\gamma\rangle + \sum_{p\leq F}\sum_{\beta\delta}\delta_{p\beta}\delta_{p\delta}\langle\alpha\beta|V|\gamma\delta\rangle_{AS} \\
&= \langle\alpha|\hat{h}_0|\gamma\rangle + \sum_{\beta,\delta\leq F}\delta_{\beta\delta}\langle\alpha\beta|V|\gamma\delta\rangle_{AS} \\
&= \begin{cases} (p-1)\delta_{\alpha\gamma} - \frac{g}{2}\delta_{\alpha\gamma}, & \alpha,\gamma \leq F \\ (p-1)\delta_{\alpha\gamma}, & \text{else} \end{cases}
\end{aligned}
$$

with p being the level of the quantum number $\alpha = p_\sigma$, for example. So we write the Hartree-Fock equations as

$$
\begin{aligned}
\epsilon^{HF}_p\delta_{p\alpha} &= \sum_\gamma h^{HF}_{\alpha\gamma}\delta_{p\gamma} \\
&= \begin{cases} \sum_\gamma (p-1)\delta_{\alpha\gamma}\delta_{p\gamma} - \frac{g}{2}\delta_{\alpha\gamma}\delta_{p\gamma}, & \alpha,\gamma \leq F \\ \sum_\gamma (p-1)\delta_{\alpha\gamma}\delta_{p\gamma}, & \text{else} \end{cases} \\
&= \begin{cases} (p-1)\delta_{\alpha p} - \frac{g}{2}\delta_{\alpha p}, & \alpha \leq F \\ (p-1)\delta_{\alpha p}, & \text{else} \end{cases}
\end{aligned}
$$

Which is what we had to begin with. If we then run our Hartree-Fock code, it stops after one iteration, since the matrix is already diagonal. However we can still get back the energy from the ground state as in the first midterm, generating the plot in Figure 3.

Since the HF transformation is equivalent to setting the one particle one hole excitations contributions to be 0, the only diagrams in Figure 2 from the project description which could be affected are those which correspond to 1p1h interaction. Those are diagrams 2, 6, and 7.

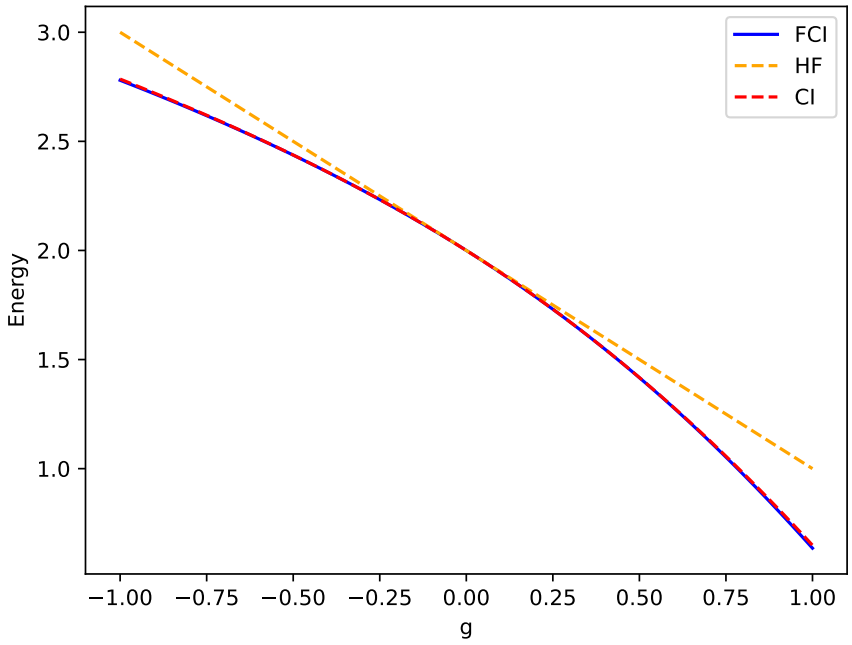

Figure 3: Energies of the ground state for the FCI, HF approximation, and truncation approximation. Here we see that even the truncation case approximates better our ground-state energy. That makes sense because Hartree-Fock transformation is analogous to setting one-particle one-hole contributions in FCI to 0. In our problem, we do not have one-particle one-hole excitations, and so HF does not do better than the initial guess of the ground state energy, which is the straight line $2 - g$.

Problem 6)

The energy of the system up to second-order RS perturbation theory is given by

$$E^{(2)} = W_0 + \Delta E^{(1)} + \Delta E^{(2)}$$

Where W_0 is the sum of the unperturbed energies of the system, which we already know to be

$$W_0 = \sum_{\substack{p \leq 2 \\ \sigma \in \{-,+\}}} (p - 1) = 2$$

And

$$\Delta E^{(1)} = \langle \Phi_0 | H_I | \Phi_0 \rangle = \frac{1}{2} \sum_{ij \leq F} \langle ij | V | ij \rangle_{AS} = -g$$

Which makes sense as we know that $E_0^{ref} = W_0 + \Delta E^{(1)} = 2 - g$ from FCI.

Now we are left with the task of finding $\Delta E^{(2)}$. We saw we could obtain contributions to the energies order by order by

$$\Delta E^{(i)} = \langle \Phi_0 | H_I \Omega^{(i)} | \Phi_0 \rangle.$$

Where $H_I = \hat{V}_N + \hat{F}_N$ with $\hat{V}_N$, $\hat{F}_N$ defined in the previous problems, and normal-ordered with respect to the new vacuum which we will define below. We have seen that the wave operator to second order can be written

$$\Omega^{(2)} |\Phi_0\rangle = \sum_{m!=0} \frac{|\Phi_m\rangle \langle \Phi_m | H_I | \Phi_m \rangle \langle \Phi_m | H_I | \Phi_0 \rangle}{W_0 - \omega_m} - \sum_{m!=0} \frac{|\Phi_m\rangle \langle \Phi_m | H_I | \Phi_0 \rangle \langle \Phi_0 | H_I | \Phi_0 \rangle}{(W_0 - \omega_m)^2}$$

Where the $|\Phi_m\rangle$ are the Slater determinants of our excluded space, meaning, the excited levels we have (4 2p2h and 1 4p4h) and ω_m are simply the eigenvalues of

$$\hat{H}_0 |\Phi_m\rangle = \omega_m |\Phi_m\rangle .$$

For our problem, we can define the general SD's as

$$\begin{aligned} |\Phi_0\rangle &:= \hat{P}_1^+ \hat{P}_2^+ |0\rangle \\ |\Phi_1\rangle := \left|\Phi_{11}^{33}\right\rangle = \hat{P}_1^+ \hat{P}_3^+ |\Phi_0\rangle, &\qquad |\Phi_2\rangle := \left|\Phi_{11}^{44}\right\rangle = \hat{P}_1^+ \hat{P}_4^+ |\Phi_0\rangle \\ |\Phi_3\rangle := \left|\Phi_{22}^{33}\right\rangle = \hat{P}_2^+ \hat{P}_3^+ |\Phi_0\rangle, &\qquad |\Phi_4\rangle := \left|\Phi_{22}^{44}\right\rangle = \hat{P}_2^+ \hat{P}_4^+ |\Phi_0\rangle \\ |\Phi_5\rangle &:= \left|\Phi_{33}^{44}\right\rangle = \hat{P}_3^+ \hat{P}_4^+ |\Phi_0\rangle \end{aligned}$$

Where I omitted the spin degrees of freedom for simplicity. Then, the contributions of the energy to the second order can be more succinctly written

$$\Delta E^{(2)} = \sum_{m!=0} \frac{\langle \Phi_0 | H_I | \Phi_m \rangle \langle \Phi_m | H_I | \Phi_0 \rangle}{W_0 - \omega_m}$$

We could now proceed to sum over all the possible excited states, expanding the definition of H_I and taking the possible contractions (and this is what we will do when moving above the second order). However, since we were told which diagram contributes to the second-order perturbation in energy, we can use the diagram rules to immediately calculate the energy contributions from diagram 1. The denominator will be of the form

$$\frac{1}{\sum_{j=1}^{2} \epsilon_j - \sum_{a=1}^{2} \epsilon_a}$$

given that we have two particle lines and two hole lines. The number of equivalent pairs of lines is 2, giving rise to a 1/4 term. Moreover, we also know we are supposed to sum over all intermediate states (a, b, i, j) in our 2p2h case. This diagram then contributes a term of

$$\Delta E^{(2)} = \frac{1}{4} \sum_{a,b,i,j} \frac{\langle ij | V | ab \rangle_{AS} \langle ab | V | ij \rangle_{AS}}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}$$

with the sign of this sum given by $(-1)^{loops+holes} = (-1)^4$, which is positive.

Notice, however, that we already have the matrix elements $\langle ab|V|ij\rangle$ from the FCI calculation, and so we use that to calculate the energy of the ground state to second order in perturbation.

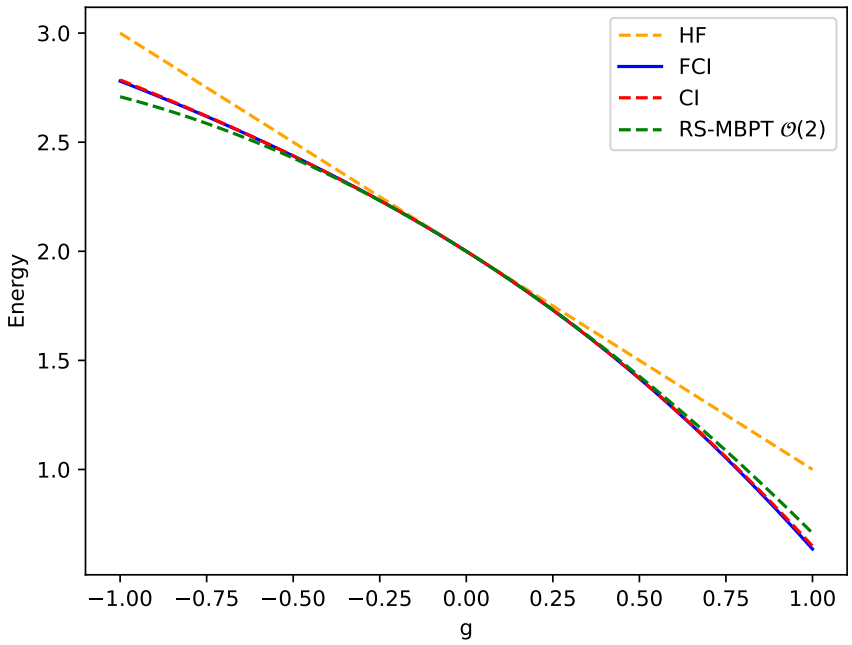

Figure 4: Energies of the ground state for the FCI, CI, HF approximation, and $\mathcal{O}(2)$ RS-MBPT. While better than the HF approximation, the second order in perturbation still yields worse results than CI.

Problem 7 (a continuation of problem 6)

In many-body perturbation theory, we use diagrams to represent perturbations in the energy levels as interactions of particle and hole states via excitations defined by operators. Diagrams are then said to be linked when multiple operators "contract", in the sense that particle and hole lines connect them.

Unlinked diagrams are exactly what the name says: at least two diagrams that are themselves closed by particle or hole lines but which do not connect their operators by particle or hole lines. In a graph theory approach, we can think of them as disjoint graphs. In Rayleigh–Schrodinger's perturbation theory, when we expand the energies and write those in a diagrammatic way, unlinked diagrams appear. Those represent unphysical diagrams, as they do not depend on the number of particles, while energy is an extensive property. They should, therefore, not contribute to the final energy approximation, and that is exactly what Goldstone's linked-diagram guarantees. That theorem states that all unlinked diagrams, in the end, cancel each other. It is then possible for us to simply take into account the linked diagrams when calculating the energy contributions of the perturbations.

Then, based on the linked diagram theorem, up to fourth-order perturbation, we can say that diagrams 33 and 41 in Figure 6 of the project description will not contribute. Given the fact that the hamiltonian does not break pairs, we can also safely say that all diagrams from Figures 3 and 5 of the project description vanish, as they are all 1p1h or 3p3h diagrams.

We are then left to analyze figure 4 and the linked diagrams in figure 6. After carefully drawing the labels of particles and lines, it becomes clear which diagrams do not contribute, as I did in figures 5 and 6. In resume, the diagrams that do contribute to the fourth order are diagrams 5, 6, 14, 15, 34, 35, 36, 37, 38, 39, 40.

To generate plots of the energy contributions up to fourth order in the perturbation then, we could do as in problem 6 and get the interaction terms from the diagrams. We will not do that, however. Here we opt to use the formalism of Shavitt and Bartlett, ch. 2.4: General derivation of formal perturbation theories.

We then use the matrix elements defined by:

$$\langle \Phi_n | V | \Phi_m \rangle = \langle \Phi_0 | \hat{P}_a^- \hat{P}_i^- V \hat{P}_b^+ \hat{P}_j^+ | \Phi_0 \rangle \coloneqq \langle ai | V | bj \rangle$$

Where a and b represent particle levels and i and j hole levels, including the spin degree of freedom. The useful thing here is that we already made the contractions of the pair creation pair annihilation operators in the FCI calculations in 6.

Then using the formulas from Shavitt and Bartlett:

$$\begin{aligned}
E^{(1)} &= V_{00} \\
E^{(2)} &= \sum_{i \neq 0} \frac{V_{0i} V_{i0}}{D_{0i}} \\
E^{(3)} &= \sum_{ij \neq 0} \frac{V_{0i} W_{ij} V_{j0}}{D_{0i} D_{0j}} \\
E^{(4)} &= \sum_{ijk \neq 0} \frac{V_{0i} W_{ij} W_{jk} V_{k0}}{D_{0i} D_{0j} D_{0k}} - E^{(2)} \sum_{i \neq 0} \frac{V_{0i} V_{0i}}{D_{0i}^2}
\end{aligned}$$

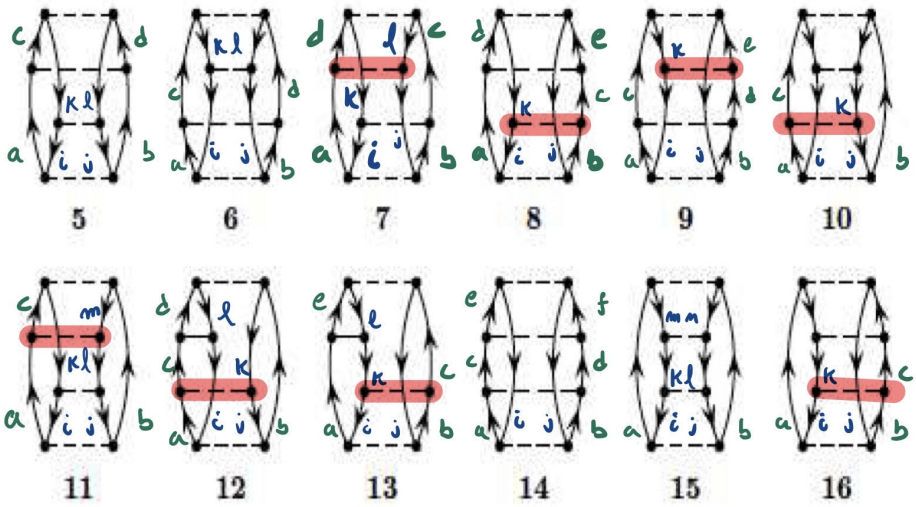

FIG. 4: Two-particle-two-hole excitations to fourth order.

Figure 5: Two particle two hole excitations to fourth order. Here I show with a red line which interactions should not contribute due to representing broken pairs in our model. Note that some labels are not included because as soon as I encountered a broken pair, I stopped the labeling.

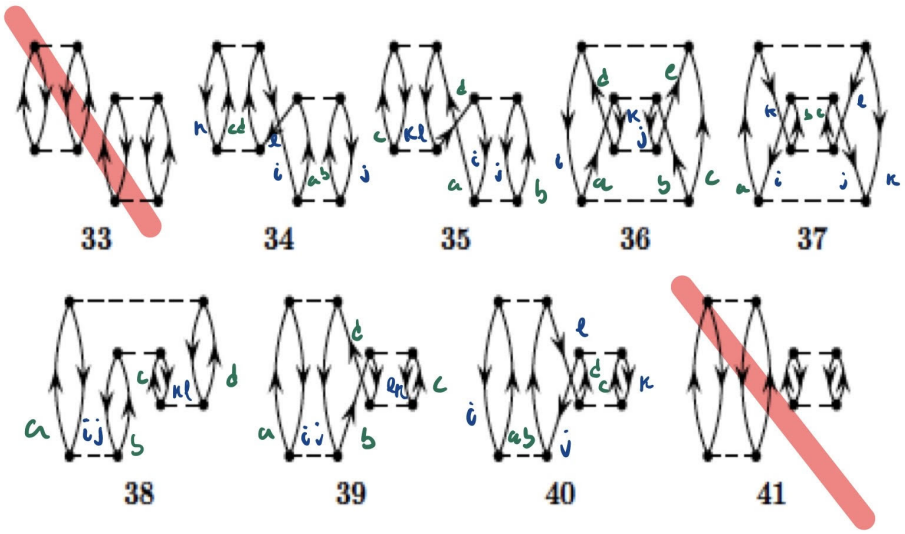

FIG. 6: Four-particle-four-hole excitations to fourth order.

Figure 6: Four particle four hole excitations to fourth order. Here the only diagrams that do not contribute are unlinked ones.

With

$$
\begin{aligned}
V_{00} &= \langle \Phi_0 | V | \Phi_0 \rangle = -g \\
V_{0i} &= \langle \Phi_0 | V | \Phi_i \rangle \\
D_{0i} &= E_0^{(0)} - E_i^{(0)} = 2 - \hat{H}_0 \, | \Phi_i \rangle \\
W_{ij} &= V_{ij} - \delta_{ij}(2 - g)
\end{aligned}
$$

Just for visualization, I draw below the V_{ij} matrix.

$$
V_{IJ} = \begin{bmatrix}
\langle \Phi_0 | V | \Phi_0 \rangle & \langle \Phi_0 | V | \Phi_1 \rangle & \langle \Phi_0 | V | \Phi_2 \rangle & \langle \Phi_0 | V | \Phi_3 \rangle & \langle \Phi_0 | V | \Phi_4 \rangle & \langle \Phi_0 | V | \Phi_5 \rangle \\
\langle \Phi_1 | V | \Phi_0 \rangle & \langle \Phi_1 | V | \Phi_1 \rangle & \langle \Phi_1 | V | \Phi_2 \rangle & \langle \Phi_1 | V | \Phi_3 \rangle & \langle \Phi_1 | V | \Phi_4 \rangle & \langle \Phi_1 | V | \Phi_5 \rangle \\
\langle \Phi_2 | V | \Phi_0 \rangle & \langle \Phi_2 | V | \Phi_1 \rangle & \langle \Phi_2 | V | \Phi_2 \rangle & \langle \Phi_2 | V | \Phi_3 \rangle & \langle \Phi_2 | V | \Phi_4 \rangle & \langle \Phi_2 | V | \Phi_5 \rangle \\
\langle \Phi_3 | V | \Phi_0 \rangle & \langle \Phi_3 | V | \Phi_1 \rangle & \langle \Phi_3 | V | \Phi_2 \rangle & \langle \Phi_3 | V | \Phi_3 \rangle & \langle \Phi_3 | V | \Phi_4 \rangle & \langle \Phi_3 | V | \Phi_5 \rangle \\
\langle \Phi_4 | V | \Phi_0 \rangle & \langle \Phi_4 | V | \Phi_1 \rangle & \langle \Phi_4 | V | \Phi_2 \rangle & \langle \Phi_4 | V | \Phi_3 \rangle & \langle \Phi_4 | V | \Phi_4 \rangle & \langle \Phi_4 | V | \Phi_5 \rangle \\
\langle \Phi_5 | V | \Phi_0 \rangle & \langle \Phi_5 | V | \Phi_1 \rangle & \langle \Phi_5 | V | \Phi_2 \rangle & \langle \Phi_5 | V | \Phi_3 \rangle & \langle \Phi_5 | V | \Phi_4 \rangle & \langle \Phi_5 | V | \Phi_5 \rangle
\end{bmatrix}
$$

$$
= \begin{bmatrix}
-g & -g/2 & -g/2 & -g/2 & -g/2 & 0 \\
-g/2 & -g & -g/2 & -g/2 & 0 & -g/2 \\
-g/2 & -g/2 & -g & 0 & -g/2 & -g/2 \\
-g/2 & -g/2 & 0 & -g & -g/2 & -g/2 \\
-g/2 & 0 & -g/2 & -g/2 & -g & -g/2 \\
0 & -g/2 & -g/2 & -g/2 & -g/2 & -g
\end{bmatrix}
$$

We can then plot the RS-MBPT energies up to fourth order in figure 7. The results are better understood if we plot the errors of the many methods we used to approximate the ground state energy, as done in figure 8.

The most important takeaway from figures 7 and 8 is that perturbative methods have a non-predictable convergence. Indeed, which was the best perturbative approximation depended on the strength of the interaction. For instance, for positive values of interaction force, RS-MBPT to third order was better than the HF method and RS-MBPT to fourth order and even better then CI, for large enough g. For negative interaction values however, this pattern between MBPT$\mathcal{O}(3)$ and CI is the opposite. As a way to try to evaluate the best method overall for our problem, I also ploted the log of the cumulative absolute error in Figure 9. Than analysis makes clear that the best method overall was configuration interaction by truncation of the hamiltonian in four particle four-hole excitations. This was unexpected since we are discarding 1 of 5 configurations of our excluded space. Nonetheless, it goes to show that the contributions of the particle-hole excitations to the ground state energy tend to decrease rapidly. One interesting point from figure 9 is that there is a small interval close to $g = 1$ for which third order perturbation achieves a smaller cumulative error then CI.

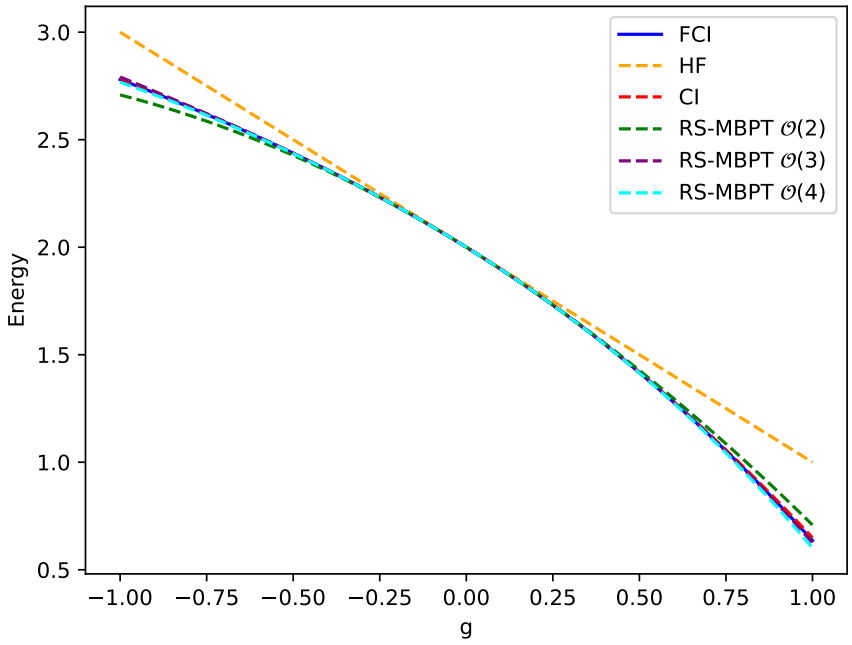

Figure 7: Comparison between all methods used to approximate the ground state energy of the pairing model.

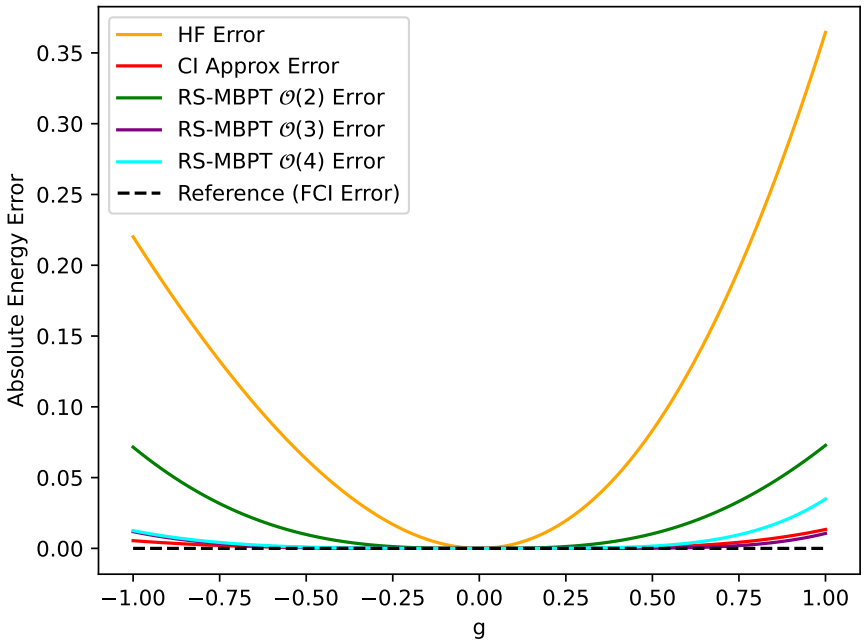

Figure 8: Absolute error comparison between all methods used to approximate the ground state energy of the pairing model.

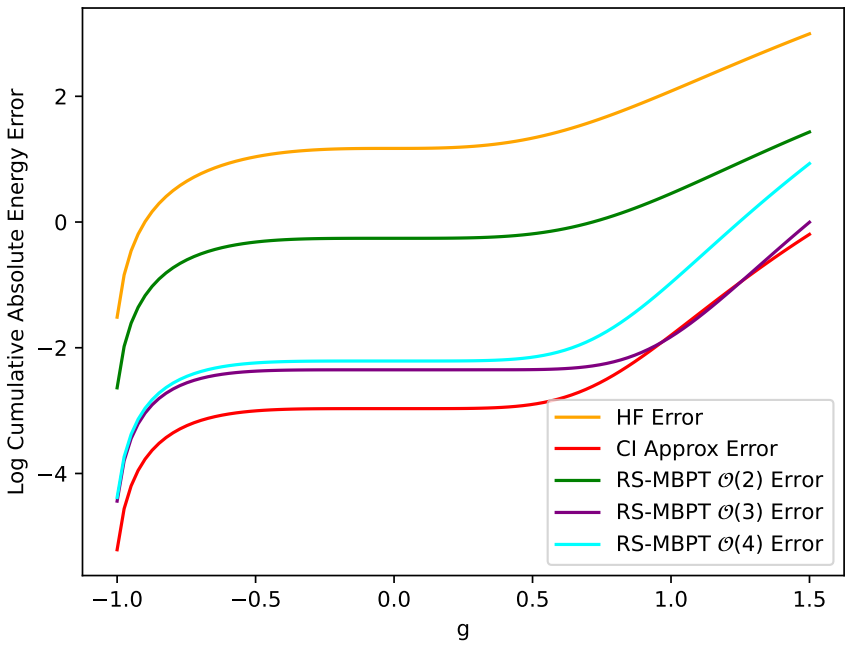

Figure 9: Log of Cumulative absolute error comparison between all methods used to approximate the ground state energy of the pairing model.