Second Midterm

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Contents

This midterm contains Problem 1) through 7).
Everything is answered (unless I missed something) with the exception of the comparison in Problem 6) with the results of Problem 3).
Repository with all code is at https://github.com/simloken/FYS4480, wherein we have `main.py`, which contains functions for solving problem 2, 3, 5 and 7 respectively.

Problem 1

With the definitions given in the midterm, we have then that:

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

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

and the spin operators:

$$\hat{S}_z = \frac{1}{2}\sum_{p\sigma} \sigma a_{p\sigma}^\dagger a_{p\sigma}$$

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

where

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

We need also a number operator $\hat{N}$ such that:

$$\hat{N}_{p\sigma} = a_{p\sigma}^\dagger a_{p\sigma}$$

which also means:

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

We now check that the commutation relations between the unperturbed Hamiltonian and $\hat{S}_z$. We have then that:

$$\left[\hat{H}_0, \hat{S}_z\right] = \frac{1}{2}\sum_{p\sigma}(p-1)\sum_{q\mu}\mu\left[a_{p\sigma}^\dagger a_{p\sigma}, a_{q\mu}^\dagger a_{q\mu}\right]$$

We recognize the latter sum as two number operators N, respectively $N_{p\sigma}$ and $N_{p\mu}$, which commute, meaning that:

$$\left[\hat{H}_0, \hat{S}_z\right] = 0 \tag{1}$$

Moving now onto the total spin $\hat{S}^2$ with the unperturbed Hamiltonian, which is defined as:

$$\left[\hat{H}_0, \hat{S}^2\right] = \left[\hat{H}_0, S_Z^2\right] + \left[\hat{H}_0, \frac{1}{2}\left(\hat{S}_+\hat{S}_- + \hat{S}_-\hat{S}_+\right)\right] = 0 + \left[\hat{H}_0, \frac{1}{2}\left(\hat{S}_+\hat{S}_- + \hat{S}_-\hat{S}_+\right)\right]$$

Note that the first term becomes 0 as we know $\hat{S}_z$ commutes with $\hat{H}_0$. We have then

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

rewritten as:

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

Here, we can employ a simple trick, since we know that $\hat{H}_0$ is hermitian, and that $\hat{S}_+$ is the hermitian adjoint of $\hat{S}_-$. As such, it follows that:

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

and therefore:

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

We move now onto the perturbation $\hat{V}$, first starting with $\hat{S}_z$. We have then:

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

We note that $\hat{V}$ contains $\hat{P}$, and rewrite:

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

from which we get:

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

Here we again employ the same trick as before. Since we know that $\hat{S}_z$ is hermitian, and that, similar to $S_\pm$, the hermitian adjoint of P_p^+ is P_p^-, we again use that we know these must commute, giving:

$$\left[\hat{V}, \hat{S}_z\right] = 0 \tag{3}$$

We now move onto the last commutation relation, that of $\left[\hat{V}, \hat{S}^2\right]$. We get:

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

$$\left[\hat{V},\hat{S}^2\right] = 0 + \frac{1}{2}\left(\left[\hat{V},\hat{S}_+\hat{S}_-\right] + \left[\hat{V},\hat{S}_-\hat{S}_+\right]\right)$$

Sadly, we cannot employ the same trick as last time. Instead, we find respectively the commutations of $\left[P_p^+, S_+\right]$ and $\left[P_p^-, S_-\right]$

$$\left[P_p^+, S_+\right] = \left[a_{p+}^\dagger a_{p-}^\dagger, \sum_q a_{q+}^\dagger a_{q-}\right] = a_{p+}^\dagger \left[a_{p-}^\dagger, \sum_q a_{q+}^\dagger a_{q-}\right] + \left[a_{p+}^\dagger, \sum_q a_{q+}^\dagger a_{q-}\right] a_{p-}^\dagger$$

Summing now over everything, we find that every commutator besides $p = q$ are 0, meaning:

$$\left[P_p^+, S_+\right] = \sum_q \left(a_{p+}^\dagger a_{q+}^\dagger \left[a_{p-}^\dagger, a_{q-}\right] + a_{p+}^\dagger \left[a_p-^\dagger, a_{q+}^\dagger\right] a_{q-} + a_{q+}^\dagger \left[a_{p+}^\dagger, a_{q-}\right] a_{p-} + \left[a_{p+}^\dagger, a_{q+}^\dagger\right] a_{q-} a_{p-}\right)$$

Giving finally:

$$\left[\hat{P}_p, \hat{S}_+\right] = a_{p+}^\dagger a_{p+}^\dagger \left[a_{p-}^\dagger, a_{p-}\right] + a_{p+}^\dagger \left[a_{p-}^\dagger, a_{p+}^\dagger\right] a_{p-} + a_{p+}^\dagger \left[a_{p+}, a_{p-}\right] a_{p-} + \left[a_{p+}^\dagger a_{p+}^\dagger\right] a_{p-} a_{p-}$$

$$\left[\hat{P}_p, \hat{S}_+\right] = 0 \rightarrow \left[\hat{V}, \hat{S}^2\right] = 0 \tag{4}$$

Note that I omitted the calculation of $\left[\hat{P}_p, S_-\right]$ (which is necessary for the result above to be true), but it is done the same way as that of our above calculations.
Lastly, we were asked to find $\left[P_p^+, P_p^+\right]$:

$$\left[P_p^+, P_p^+\right] = a_{p+}^\dagger a_{p-}^\dagger a_{p+}^\dagger a_{p-}^\dagger - a_{p+}^\dagger a_{p-}^\dagger a_{p+}^\dagger a_{p-}^\dagger = 0 \tag{5}$$

and $\left[P_p^-, P_p^-\right]$:

$$\left[P_p^-, P_p^-\right] = a_{p-}^\dagger a_{p+}^\dagger a_{p-}^\dagger a_{p+}^\dagger - a_{p-}^\dagger a_{p+}^\dagger a_{p-}^\dagger a_{p+}^\dagger = 0 \tag{6}$$

Problem 2

We define the ground state by:

$$|\Phi_0\rangle = a_{1+}^\dagger a_{1-}^\dagger a_{2+}^\dagger a_{2-}^\dagger |0\rangle = \hat{P}_1^+ \hat{P}_2^+ |0\rangle$$

leading to the other Slater determinants:

$$|\Phi_1\rangle = \hat{P}_1^+ \hat{P}_3^+ |0\rangle$$

$$|\Phi_2\rangle = \hat{P}_1^+ \hat{P}_4^+ |0\rangle$$

$$|\Phi_3\rangle = \hat{P}_2^+ \hat{P}_3^+ |0\rangle$$

$$|\Phi_4\rangle = \hat{P}_2^+ \hat{P}_4^+ |0\rangle$$

$$|\Phi_5\rangle = \hat{P}_3^+ \hat{P}_4^+ |0\rangle$$

Now onto finding the matrix. We must now find the contributions of generic states $\alpha, \beta, \gamma, \delta$ on $\hat{H}_0$ and $\hat{V}$ respectively. We start with $\hat{H}_0$:

$$\langle(\alpha)(-\alpha)(\beta)(-\beta)|\hat{H}_0|(\gamma)(-\gamma)(\delta)(-\delta)\rangle = \sum_{p\sigma}(p-1)\langle(\alpha)(-\alpha)(\beta)(-\beta)|\hat{N}_{p\sigma}|(\gamma)(-\gamma)(\delta)(-\delta)\rangle$$

We can then sum over σ and get:

$$\langle(\alpha)(-\alpha)(\beta)(-\beta)|\hat{H}_0|(\gamma)(-\gamma)(\delta)(-\delta)\rangle = 2\sum_{p}(p-1)(\delta_{p\gamma}+\delta_{p\delta})\langle(\alpha)(-\alpha)(\beta)(-\beta)|(\gamma)(-\gamma)(\delta)(-\delta)\rangle$$

Employing then Wicks Theorem we find that:

$$\langle(\alpha)(-\alpha)(\beta)(-\beta)|\hat{H}_0|(\gamma)(-\gamma)(\delta)(-\delta)\rangle = 2(r+2-2)(\delta_{\alpha\gamma}\delta_{\beta\delta}+\delta_{\alpha\delta}\delta_{\beta\gamma}) \tag{7}$$

We do now the same for $\hat{V}$, resulting in:

$$\langle(\alpha)(-\alpha)(\beta)(-\beta)|\hat{V}|(\gamma)(-\gamma)(\delta)(-\delta)\rangle = -\frac{1}{2}g(\delta_{\beta\delta}+\delta_{\beta\gamma}+\delta_{\alpha\delta}+\delta_{\alpha\gamma}) \tag{8}$$

This gives rise to two matrices, where the columns correspond to the states Φ_0 through Φ_5:

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

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

Adding these together gives us the resulting matrix:

$$\hat{H} = \begin{bmatrix} 2-g & -\frac{g}{2} & -\frac{g}{2} & -\frac{g}{2} & -\frac{g}{2} & 0 \\ -\frac{g}{2} & 4-g & -\frac{g}{2} & -\frac{g}{2} & 0 & -\frac{g}{2} \\ -\frac{g}{2} & -\frac{g}{2} & 6-g & 0 & -\frac{g}{2} & -\frac{g}{2} \\ -\frac{g}{2} & -\frac{g}{2} & 0 & 6-g & -\frac{g}{2} & -\frac{g}{2} \\ -\frac{g}{2} & 0 & -\frac{g}{2} & -\frac{g}{2} & 8-g & -\frac{g}{2} \\ 0 & -\frac{g}{2} & -\frac{g}{2} & -\frac{g}{2} & -\frac{g}{2} & 10-g \end{bmatrix} \tag{9}$$

which when diagonalizing and varying g gives us the plot:

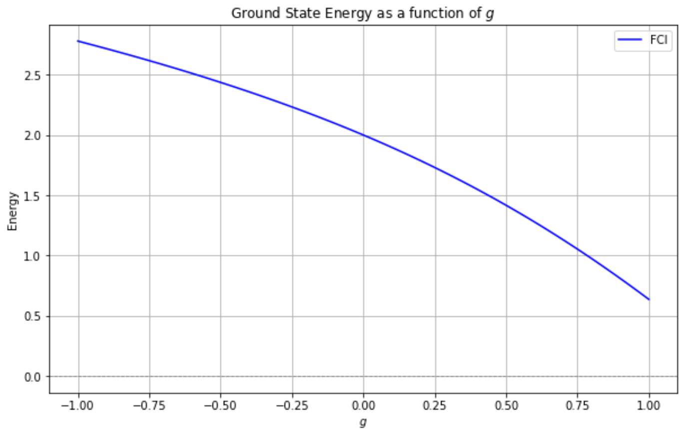

Figure 1: A FCI plot as we vary the coupling strength g

We note that the ground state energy decreases as we increase the coupling strength. Additionally, we have the eigenvalues as a function of g:

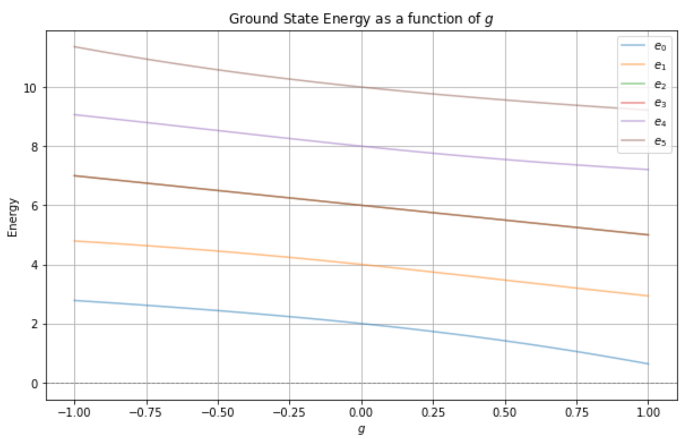

Figure 2: An eigenvalue plot as we vary the coupling strength g

We note that we only see five distinct lines, despite six eigenvalues. This is because we have degeneracy for e_2, e_3.

Problem 3

This means that we will have to remove the state(s) where the four particles are not in the two lowest orbits. This is only the case for the state Φ_5, ie the final column (and row), giving us a new matrix:

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

and associated plot:

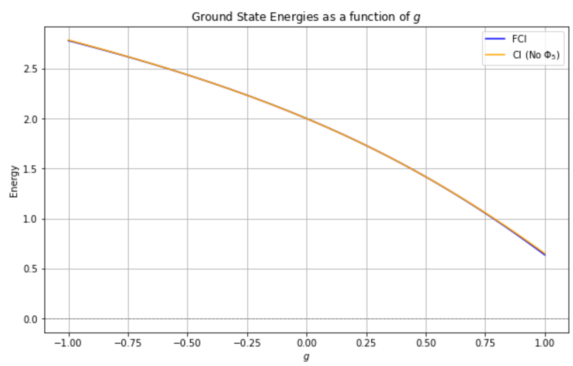

Figure 3: A CI plot as we vary the coupling strength g, without Φ_5

A direct comparison between FCI and CI can be seen in the plot, but it can be a bit hard to see properly as they overlap so closely. We therefore look at the difference between the two plots instead:

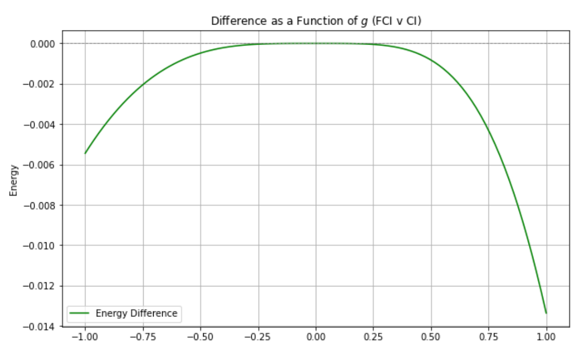

Figure 4: A comparison of energy calculation between FCI and CI

We see here that, although the differences are small, CI makes for a good method values of g close to 0. However, we see also a steep drop-off in accuracy as g increases. This is perhaps related to the fact that we see the ground state energy increase sharply as we increase g for the FCI method.

Problem 4

We set the Fermi level to include the model space, $p = 1, 2$. This allows us to use the creation and annihilation operators $P_p^{\pm}$ to achieve to achieve the excluded space $p = 3, 4$. We move also to particle-hole formalism, where the fermi level states are indicated by $i, j, k... \in \{1, 2\}$ and the states above the fermi level are indicated by $a, b, c... \in \{3, 4\}$
For our reference state $|\Phi_0\rangle$, the unperturbed Hamiltonian is given by:

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

$$\sum_{p\sigma} (p-1)\hat{N}_{p\sigma} = \langle \Phi_0 | \hat{H}_0 | \Phi_0 \rangle + \sum_{p\sigma} (p-1)\hat{N}_{p\sigma}$$

For the perturbation, we get:

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

Which in turn gives us the Fermi vacuum energy and $\hat{H}_0^N, \hat{V}^N$ from above:

$$E_0^{\text{ref}} = 2 \sum_{i} (i-1) - \frac{1}{2} gM, \xrightarrow{M=2} E_0^{\text{ref}} = 2 - g$$

Note that M is the number of pair states *below* the Fermi level.

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

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

We then have the Fock operator:

$$f_{pq} = \langle p | \hat{f} | q \rangle = \langle p | \hat{H}_0 | q \rangle + \sum_{j} \langle pj | \hat{V} | qj \rangle_{AS}$$

and it's second quantization:

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

Normally, this would be quite a troublesome calculation, but we can again employ a trick. We note that our Hamiltonian is 0 outside of the diagonal, meaning that $p = q$, and thus we only have one sum:

$$\hat{F} = \sum_{p} \langle p | \hat{f} | p \rangle a_p^\dagger a_p$$

which then, writing in normal order gives rise to:

$$\hat{F} \sum_{p} \langle p | \hat{f} | p \rangle a_p^\dagger a_p + \sum_{i} \langle i | \hat{f} | i \rangle$$

and finally the Canonical Hartree-Fock:

$$\hat{f} |p\rangle = \sum_{q} \epsilon_{qp} |q\rangle \tag{11}$$

Problem 5

We use the equation found in the previous midterm (and/or lectures):

$$\sum_{\beta} h^{\mathcal{HF}}_{\alpha\beta} C_{i\beta} = \epsilon_i C_{i\alpha}$$

While initially daunting, there are some things we can do to make this easier on ourselves. We note that, given the orthonormal basis, the one-body contribution $\hat{h}_0$ is actually entirely diagonal:

$$\langle \alpha | \hat{h}_0 | \beta \rangle = (\alpha - 1)\delta_{\alpha\beta}$$

Now we need to find the contribution from the two-body. Keeping in mind the restraints of our system, we note that a particular particle may be described by two quantum numbers, it's energy e and its spin σ, thus a given configuration is just a sum over four quantum numbers, the energies and the spins of two particles respectively. We note also that the particles must *share* energy level and that the spins *have to* be opposite. With this in mind, we find again an entirely diagonal contribution.

$$\rho_{\alpha\beta} \langle \alpha_+ \alpha_- | V | \beta_+ \beta_- \rangle = -\frac{1}{2} g \rho_{\alpha\beta}$$

where the subscript $+, -$ indicate the spin.
As is customary, we assume $C^*_{i\alpha} = \delta_{i\alpha}$, or $C = I$. We note now that given C, the associated density matrix ρ is diagonal, as is both the one-body and two-body contributions. Thus we already have a Hartree-Fock basis (!!!), and we don't really even need to do anything else. No explicit calculation or iteration is needed. The energy by our Hartree-Fock method then becomes a simple:

$$E[\Phi_0^{\mathcal{HF}}] = 2 - g \tag{12}$$

in other words entirely linear with g. Perhaps this is "cheating" in the sense that we don't "solve" our Hartree-Fock model iteratively, but it is a welcome discovery!
Although not strictly necessary, we include here also the Hartree-Fock matrix:

$$H^{\mathcal{HF}} = \begin{bmatrix} 0 - \frac{1}{2}g & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 - \frac{1}{2}g & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 - \frac{1}{2}g & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 - \frac{1}{2}g & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 \end{bmatrix}$$

with the associated plot:

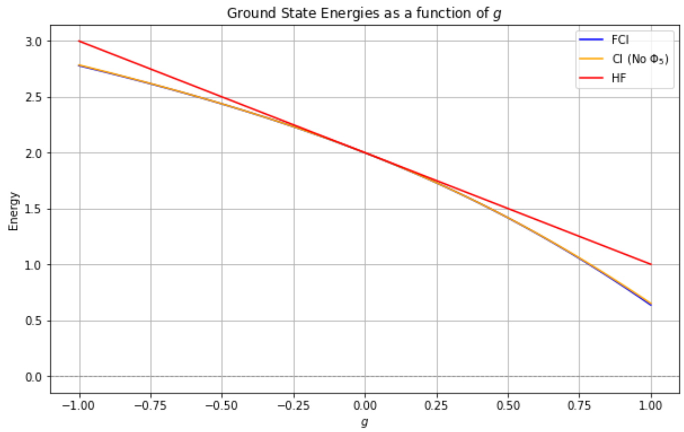

Figure 5: Comparing the ground state energy calculation using both FCI, CI and HF.

We note that HF is adequate in and around g, but as g increases (or decreases), HF fails us. This isn't exactly much of a surprise, considering the linear nature of HF.
We again get a closer look with looking at the difference:

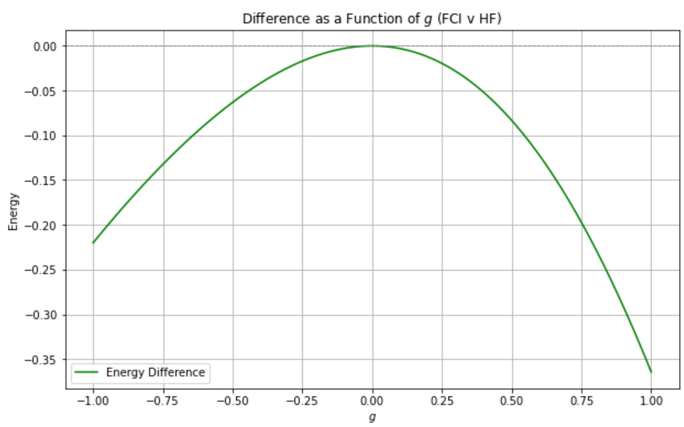

Figure 6: The difference between FCI and HF

Again, we see that HF is perfectly suitable when $g \approx 0$, but for any other value of g we cannot realistically use this, especially given its linear nature.

We move now onto the Rayleigh-Schrödinger perturbation theory. The diagrams that contribute to the energy of the ground state are $1, 4, 5, 8$ and 9, as these are the only unbroken pairs. Starting from the "top", we have then:

$$(1) \quad \frac{1}{4}\sum_{abij}\frac{\langle ij|V|ab\rangle\langle ab|V|ij\rangle}{\epsilon_i+\epsilon_j-\epsilon_a-\epsilon_b} = \frac{1}{8}\sum_{ai}\frac{g^2}{i-a} \tag{13}$$

$$(4) \quad \frac{1}{8}\sum_{abcdij}\frac{\langle ij|V|ab\rangle\langle ab|V|cd\rangle\langle cd|V|ij\rangle}{(\epsilon_i+\epsilon_j-\epsilon_a-\epsilon_b)(\epsilon_i\epsilon_j-\epsilon_c-\epsilon_d)} = -\frac{1}{32}\sum_{iac}\frac{g^3}{(i-a)(i-c)} \tag{14}$$

$$(5) \quad \frac{1}{8}\sum_{abijkl}\frac{\langle kl|V|ij\rangle\langle ab|V|cd\rangle\langle cd|V|ij\rangle}{(\epsilon_i+\epsilon_j-\epsilon_a-\epsilon_b)(\epsilon_k\epsilon_l-\epsilon_a-\epsilon_b)} = -\frac{1}{32}\sum_{ika}\frac{g^3}{(i-a)(k-a)} \tag{15}$$

$$(8) \quad -\frac{1}{2}\sum_{abijkl}\frac{\langle ij|V|ab\rangle\langle kl|V|ki\rangle\langle ab|V|lj\rangle}{(\epsilon_i+\epsilon_j-\epsilon_a-\epsilon_b)(\epsilon_i+\epsilon_k-\epsilon_a-\epsilon_b)} = \frac{1}{16}\sum_{ia}\frac{g^3}{(i-a)^2} \tag{16}$$

$$(9) \quad -\frac{1}{2}\sum_{abcdij}\frac{\langle ij|V|ab\rangle\langle ca|V|cd\rangle\langle db|V|ij\rangle}{(\epsilon_i+\epsilon_j-\epsilon_a-\epsilon_b)(\epsilon_i+\epsilon_j-\epsilon_a-\epsilon_c)} = \frac{1}{16}\sum_{ia}\frac{g^3}{(i-a)^2} \tag{17}$$

We then finally get our expression:

$$E^{(3)} = E^{(0)} + E^{(1)} + (1) + (4) + (5) + (8) + (9) =$$
$$2 - g + \frac{1}{8}\sum_{ai}\frac{g^2}{i-a} - \frac{1}{32}\sum_{iac}\frac{g^3}{(i-a)(i-c)} - \frac{1}{32}\sum_{ika}\frac{g^3}{(i-a)(k-a)} + \frac{1}{16}\sum_{ia}\frac{g^3}{(i-a)^2} + \frac{1}{16}\sum_{ia}\frac{g^3}{(i-a)^2}$$

We evaluate and find:

$$E^{(3)} = 2 - g - \left(\frac{3g^2}{8} - \frac{g^2}{24}\right) + \left(\frac{53g^3}{576}\right) + \left(\frac{53g^3}{576}\right) + \left(\frac{29g^3}{288}\right) + \left(\frac{29g^3}{288}\right)$$

Simplifying to the polynomial:

$$E^{(3)} = \frac{37g^3}{96} - \frac{5g^2}{12} - g + 2 \tag{18}$$

which we can plot:

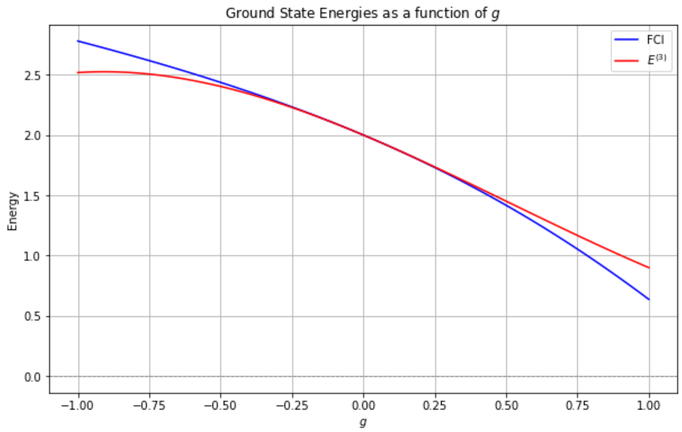

Figure 7: $E^{(3)}$ compared to FCI

We perform better than HF, as expected, but we still see poor performance in the 'extremes' of the g range. One interesting thing to note is that $E^{(3)}$ is less than FCI for small g, whereas it is bigger for large g. This is even easier to see for the difference plot:

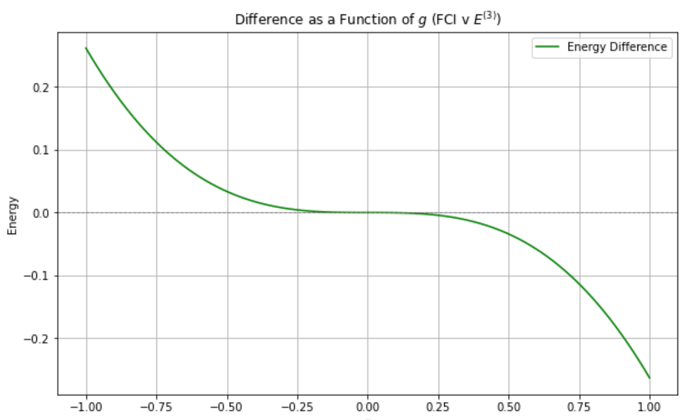

Figure 8: Difference between FCI and $E^{(3)}$

We see a characteristic $-x^3$ shape for the difference. Of our non-linear methods, this is by far the biggest error we've seen until now.

Problem 6

We designate a operator $\chi^{(1)}$, which is the first order wave operator, defined as:

$$\chi^{(1)}|\Phi_0\rangle = \sum_p \sum_q |\Phi_p^\sigma\rangle \frac{\langle \Phi_{pq}^{\sigma_p \sigma_q}|\hat{V}|\Phi_0\rangle}{E^{(0)} - E_{p\sigma}^{(0)}} \delta(\sigma_p, \sigma_q)$$

which is (as shown by the Kronecker delta) only valid for states where the the spins are opposite. The second order contributions are simply written as:

$$E^{(2)} = \sum_p \frac{\langle \Phi_0|\hat{V}|\Phi_p\rangle\langle \Phi_p|\hat{V}|\Phi_0\rangle}{\langle \Phi_p|\hat{H}_0|\Phi_p\rangle - \langle \Phi_0|\hat{V}|\Phi_0\rangle}$$

from which we get:

$$E^{(2)} = \sum_{ia} \frac{\langle i_+ i_-|\hat{V}|a_+ a_-\rangle_{AS}\langle a_+ a_-|\hat{V}|i_+ i_-\rangle_{AS}}{2\epsilon_a - 2\epsilon_i}$$

I am not entirely sure about what to do from here in regards to comparing our results with those of problem 3), so this has been left out.

Problem 7

We can immediately off the bat disregard *1p1h* as they are not paired, thus not fitting with our Hamiltonian.
We have then the *2p2h* diagrams. It is hard to make out exactly what contributes, as they all look *very* much alike. As such, I am going to be guessing for these. We note that $5, 6$ and $14, 15$ are the only diagrams mirrored along the y-axis, for lack of a better term. Therefore, we choose these.
For *3p3h*, I believe can again disregard these as they are incompatible with our Hamiltonian, though I am not certain.
For *4p4h*, we have first the most obvious ones, 36 and 37. We secondly have the unlinked diagrams 33 and 41. According to the linked diagram, we can disregard the contributions of 33 and 41, as their contributions are typically a product of lower-order diagrams (that is to say that they factorize into products of lower-order diagrams).
Because of this, we only need to look at a total of six diagrams, $5_2, 6_2, 14_2, 15_2, 36_4$ and 37_4, the subscript indicating which series of diagrams they belong to.
From here, we try the same approach as we did in problem 5, but we note that as all these are symmetric, we only need to calculate three, then change the indices to get it's opposite. We have:

$$(5) \quad \frac{1}{128}\sum_{acik} \frac{g^4}{(i-a)(k-a)(k-c)} \rightarrow (6) \quad \frac{1}{128}\sum_{acik} \frac{g^4}{(i-a)(i-c)(k-c)}$$

$$(14) \quad \frac{1}{128}\sum_{acei} \frac{g^4}{(i-a)(i-c)(i-e)} \rightarrow (15) \quad \frac{1}{64}\sum_{acei} \frac{g^4}{(i-a)(i-a)(m-a)}$$

$$(36) \quad \frac{1}{128}\sum_{acik} \frac{g^4}{(i-a)(i+k-a-c)(i-c)} \rightarrow (37) \quad \frac{1}{128}\sum_{acik} \frac{g^4}{(i-a)(i+k-a-c)(k-a)}$$

Summing this is tedious and ultimately a very pointless exercise (just know that the procedure is the same as in the latter half of 5)), so we leave it to Python, and find the following plot when varying g:

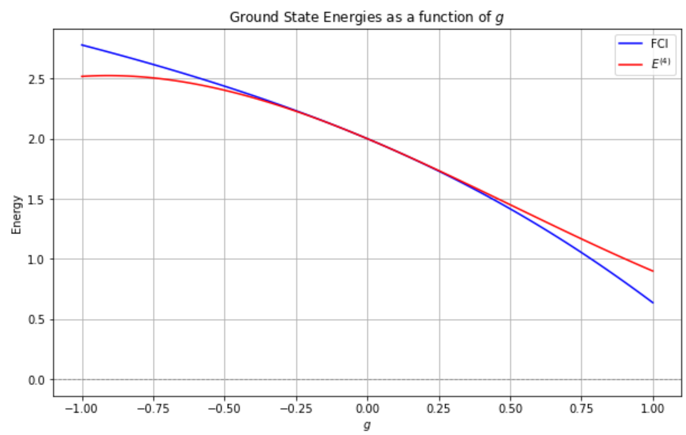

Figure 9: Difference between FCI and $E^{(4)}$

which is a (albeit small) change from $E^{(3)}$. This is quite hard to see, so we (instead of looking at the usual difference between FCI and whatever method we're studying) look at the absolute difference between the differences. That is to say, we first look at the difference between $E^{(3)}$ and FCI, then ditto for $E^{(4)}$. We then compare those differences to each other, which is:

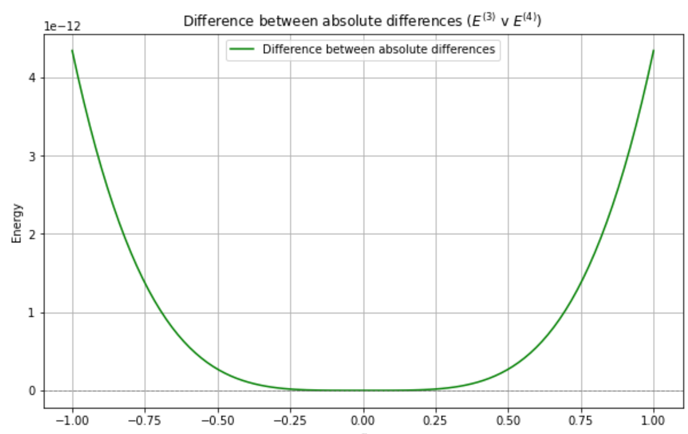

Figure 10: Absolute difference between $E^{(3)}$ and $E^{(4)}$

This result is not entirely unexpected. After all, increasing the order of our energy corrections is not necessarily a guarantee that it will perform better (or worse) than previously.

Lastly, we decide to look all the methods discussed in this midterm in one final plot, as a 'summary' of our work: We see here that, ultimately, the margin between *most* of the methods are very

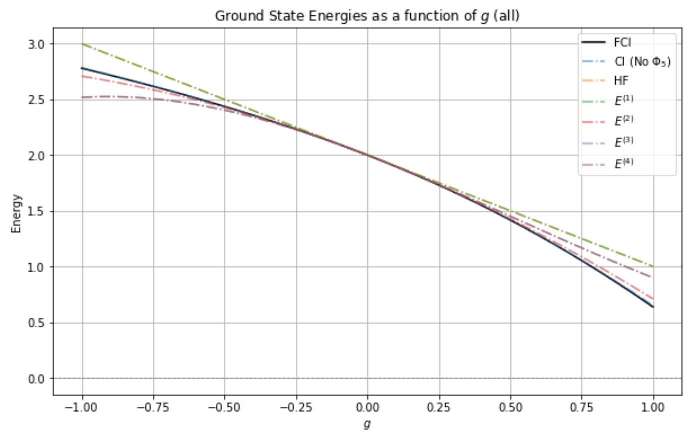

Figure 11: All the methods discussed in this midterm on one single plot

small to non-existent for any g in the $\{-0.5, 0.5\}$ range. We can further study this by blowing up our plot: which as we can see, further emphasizes the margins of many of our studied methods.

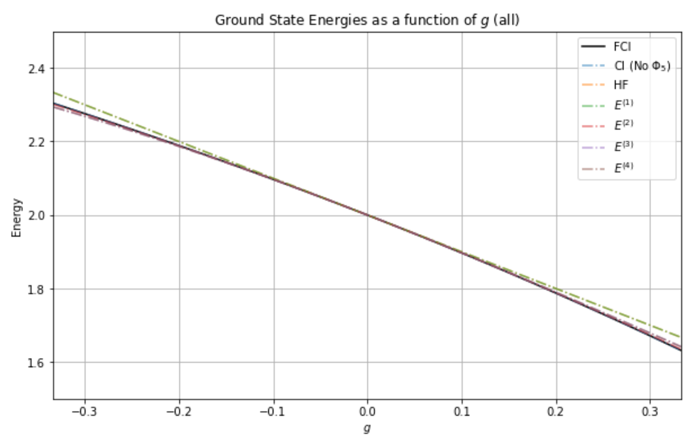

Figure 12: A zoomed in version of Figure 11