FYS-KJM4480 - Quantum mechanics for many-particle systems

Project 2

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- For the Github repository containing programs and results, follow this link: `https://github.com/evenmn/master/tree/master/FYSKJM4480/Project2`

Introduction

Superconductivity might be one of 20th century's most exciting physical discoveries, and for a long time the theory behind was a mystery. In 1957, 46 years after the first observation by Kamerlingh Onnes [REFERENCE], John Bardeen, Leon Cooper and John Robert Schrieffer came up with a quantum theory describing superconductivity on microscopic level[REFERENCE]. This theory was built on Cooper pairs, which is a pair of electrons with lower energy than the Fermi energy, i.e. there is a bounding between them. We can treat the pairs as a spinless particle, which is a boson, and this boson-like pair is the reason why the current can flow unhindered in a superconductor.

Furthermore the theory is also used in nuclear physics to describe the paring interaction between nucleons in an atomic nucleus.

This project aims to study such a pairing model, known as BCS-theory after its founders. In the first part we are working with this model independently. Then we will use Full Configuration-Interaction (FCI) to find the exact energy eigenvalues and Rayleigh-Schrodinger Perturbation Theory of third order (RSPT3) as an approximation to make the equations computer-friendly. Thereafter we repeat this using Coupled-Cluster Doubled (CCD), and finally we compare the approximations to the exact solutions.

1 Pairing model

In this project we use a slightly simplified pairing model, which we assume to be carrying a constant strength g. The Hamiltonian is therefore given by

$$\hat{H} = \hat{H}_0 + \hat{V} \tag{1}$$

with

$$\hat{H}_0 = \sum_{p\sigma} \epsilon_p c^\dagger_{p\sigma} c_{p\sigma}, \quad \epsilon_p = \xi \cdot (p-1) \tag{2}$$

and

$$\hat{V} = -\frac{1}{2} g \sum_{pq} c^\dagger_{p+} c^\dagger_{p-} c_{q-} c_{q+}. \tag{3}$$

where $\epsilon_p = \xi(p-1)$, with ξ set to 1.

We will only study systems of a even number of particles, N, and the ground-state wavefunction is then given by the Slater determinant

$$|\Phi\rangle = c^\dagger_{1+} c^\dagger_{1-} \dots c^\dagger_{N/2+} c^\dagger_{N/2-} |\Phi\rangle. \tag{4}$$

Further I will define some operators that will be useful when doing the calculations.

$$\hat{P}^\dagger_p \equiv c^\dagger_{p+} c^\dagger_{p-}, \quad \hat{P}_p \equiv c_{p-} c_{p+} \tag{5}$$

$$\hat{n}_p \equiv \sum_\sigma c^\dagger_{p\sigma} c_{p\sigma} \tag{6}$$

$$\hat{P} = \sum_p \hat{P}^\dagger_p \hat{P}_p \tag{7}$$

and finally

$$\hat{S}_z = \frac{1}{2} \sum_{p\sigma} \sigma c^\dagger_{p\sigma} c_{p\sigma}. \tag{8}$$

If $\hat{H}$, $\hat{P}$ and $\hat{S}_z$ commute, we can reduce this problem to an eigenvalue problem on the form

$$\begin{aligned}
\hat{H}|\Psi_k; S_z, P\rangle &= E_{k,S_z,P}|\Psi_k; S_z, P\rangle \\
\hat{P}|\Psi_k; S_z, P\rangle &= S_z|\Psi_k; S_z, P\rangle \\
\hat{S}_z|\Psi_k; S_z, P\rangle &= P|\Psi_k; S_z, P\rangle
\end{aligned}$$

where the eigenvalues are the energies, momentums and the spin in z-direction respectively. We need to check this:

1A

Firstly, we check if the Hamiltonian commutes with the spin-projection operator, and since $\hat{H} = \hat{H}_0 + \hat{V}$, we can split this calculation into two simpler calculations. Let us start with $[\hat{H}_0, \hat{S}_z]$:

$$\begin{aligned}
[\hat{H}_0, \hat{S}_z] &= \left[\sum_{p\sigma} \epsilon_p c^\dagger_{p\sigma} c_{p\sigma}, \frac{1}{2} \sum_{q\sigma} \sigma c^\dagger_{q\sigma} c_{q\sigma} \right] \\
&= \frac{1}{2} \sum_{pq\sigma} \epsilon_p \sigma (c^\dagger_{p\sigma} c_{p\sigma} c^\dagger_{q\sigma} c_{q\sigma} - c^\dagger_{q\sigma} c_{q\sigma} c^\dagger_{p\sigma} c_{p\sigma}) \qquad (9)
\end{aligned}$$

We use Wick's theorem on the two terms, and observe that only single contraction will contribute because of the orientation

$$c^\dagger_{p\sigma} c_{p\sigma} c^\dagger_{q\sigma} c_{q\sigma} = \{c^\dagger_{p\sigma} c^\dagger_{q\sigma} c_{p\sigma} c_{q\sigma}\} + \delta_{pq} c^\dagger_{p\sigma} c_{q\sigma} \qquad (10)$$

$$c^\dagger_{q\sigma} c_{q\sigma} c^\dagger_{p\sigma} c_{p\sigma} = \{c^\dagger_{p\sigma} c^\dagger_{q\sigma} c_{p\sigma} c_{q\sigma}\} + \delta_{qp} c^\dagger_{q\sigma} c_{p\sigma} \qquad (11)$$

The first terms (the normal-ordered products) cancel, and we obtain

$$[\hat{H}_0, \hat{S}_z] = \frac{1}{2} \sum_{pq\sigma} \epsilon_p \sigma (\delta_{pq} c^\dagger_{p\sigma} c_{q\sigma} - \delta_{qp} c^\dagger_{q\sigma} c_{p\sigma}) \qquad (12)$$

We get contribution only when $q = p$

$$[\hat{H}_0, \hat{S}_z] = \frac{1}{2} \sum_{p\sigma} \epsilon_p (c^\dagger_{p\sigma} c_{p\sigma} - c^\dagger_{p\sigma} c_{p\sigma}) = 0 \qquad (13)$$

So $\hat{H}_0$ commutes with the spin-projection operator. Further we need to work out $[\hat{V}, \hat{S}_z]$:

$$\begin{aligned}
[\hat{V}, \hat{S}_z] &= \left[-\frac{1}{2} g \sum_{pq} c^\dagger_{p+} c^\dagger_{p-} c_{q-} c_{q+}, \frac{1}{2} \sum_{r\sigma} \sigma c^\dagger_{r\sigma} c_{r\sigma} \right] \\
&= -\frac{1}{4} \sum_{pqr\sigma} \sigma (c^\dagger_{p+} c^\dagger_{p-} c_{q-} c_{q+} c^\dagger_{r\sigma} c_{r\sigma} - c^\dagger_{r\sigma} c_{r\sigma} c^\dagger_{p+} c^\dagger_{p-} c_{q-} c_{q+}) \qquad (14)
\end{aligned}$$

The fours terms written out are as follows

$$c^\dagger_{p+} c^\dagger_{p-} c_{q-} c_{q+} c^\dagger_{r+} c_{r+} = \{c^\dagger_{p+} c^\dagger_{p-} c^\dagger_{r+} c_{q-} c_{q+} c_{r+}\} + \delta_{qr} c^\dagger_{p+} c^\dagger_{p-} c_{q-} c_{r+} \qquad (15)$$

$$c^\dagger_{p+} c^\dagger_{p-} c_{q-} c_{q+} c^\dagger_{r-} c_{r-} = \{c^\dagger_{p+} c^\dagger_{p-} c^\dagger_{r-} c_{q-} c_{q+} c_{r-}\} + \delta_{qr} c^\dagger_{p+} c^\dagger_{p-} c_{r-} c_{q+} \qquad (16)$$

$$c^\dagger_{r+} c_{r+} c^\dagger_{p+} c^\dagger_{p-} c_{q-} c_{q+} = \{c^\dagger_{p+} c^\dagger_{p-} c^\dagger_{r+} c_{q-} c_{q+} c_{r+}\} + \delta_{rp} c^\dagger_{r+} c^\dagger_{p-} c_{q-} c_{q+} \qquad (17)$$

$$c^\dagger_{r-}c_{r-}c^\dagger_{p+}c^\dagger_{p-}c_{q-}c_{q+} = \{c^\dagger_{p+}c^\dagger_{p-}c^\dagger_{r-}c_{q-}c_{q+}c_{r-}\} + \delta_{rp}c^\dagger_{p+}c^\dagger_{r-}c_{q-}c_{q+} \tag{18}$$

Again the first terms cancel, and we are left with

$$[\hat{V}, \hat{S}_z] = -\frac{1}{4}g\sum_{pqr\sigma}\sigma\Big((\delta_{qr}c^\dagger_{p+}c^\dagger_{p-}c_{q-}c_{r+} + \delta_{qr}c^\dagger_{p+}c^\dagger_{p-}c_{r-}c_{q+})- \\ (\delta_{rp}c^\dagger_{r+}c^\dagger_{p-}c_{q-}c_{q+} + \delta_{rp}c^\dagger_{p+}c^\dagger_{r-}c_{q-}c_{q+})\Big) \tag{19}$$

In the first two terms we will get contributions when $r = q$, and for the two last terms we will get contributions when $r = p$. We can easily see that the two first terms become equal to the two last terms, and will cancel each other.

1B

Secondly, we check if the Hamiltonian commutes with the counter-operator. Again we split up:

$$\begin{aligned}[\hat{H}_0, \hat{P}] &= \Big[\sum_{p\sigma}\epsilon_p c^\dagger_{p\sigma}c_{p\sigma}, \sum_q \hat{P}_q\hat{P}_q\Big] \\ &= \sum_{pq}\epsilon_p\Big[(c^\dagger_{p+}c_{p+}c^\dagger_{q+}c^\dagger_{q-}c_{q-}c_{q+} + c^\dagger_{p-}c_{p-}c^\dagger_{q+}c^\dagger_{q-}c_{q-}c_{q+}) \\ &\qquad (c^\dagger_{q+}c^\dagger_{q-}c_{q-}c_{q+}c^\dagger_{p+}c_{p+} + c^\dagger_{q+}c^\dagger_{q-}c_{q-}c_{q+}c^\dagger_{p-}c_{p-})\Big]\end{aligned}$$

We can immediately see that each term only will allow one (non-zero) contraction when Wick's theorem is used:

$$c^\dagger_{p+}c_{p+}c^\dagger_{q+}c^\dagger_{q-}c_{q-}c_{q+} = \{c^\dagger_{p+}c^\dagger_{q+}c^\dagger_{q-}c_{p+}c_{q-}c_{q+}\} + \delta_{pq}c^\dagger_{p+}c^\dagger_{q-}c_{q-}c_{q+} \tag{20}$$

$$c^\dagger_{p-}c_{p-}c^\dagger_{q+}c^\dagger_{q-}c_{q-}c_{q+} = \{c^\dagger_{p-}c^\dagger_{q+}c^\dagger_{q-}c_{p-}c_{q-}c_{q+}\} - \delta_{pq}c^\dagger_{p-}c^\dagger_{q+}c_{q-}c_{q+} \tag{21}$$

$$c_{q+}c_{q-}c^\dagger_{p+}c_{p+}c^\dagger_{q+}c^\dagger_{q-} = \{c^\dagger_{p+}c^\dagger_{q+}c^\dagger_{q-}c_{p+}c_{q-}c_{q+}\} + \delta_{qp}c^\dagger_{q+}c^\dagger_{q-}c_{q-}c_{p+} \tag{22}$$

$$c_{q+}c_{q-}c^\dagger_{p-}c_{p-}c^\dagger_{q+}c^\dagger_{q-} = \{c^\dagger_{p-}c^\dagger_{q+}c^\dagger_{q-}c_{p-}c_{q-}c_{q+}\} - \delta_{qp}c^\dagger_{q-}c^\dagger_{q+}c_{p-}c_{q+} \tag{23}$$

Recall that we sum over all possible p and qs, and for each p we will have a q which is equal. Due to the Kronecker delta, we only get contributions when this happens ($p = q$), but a watchful eye will see that the terms cancel in this case $\Rightarrow [\hat{H}_0, \hat{P}] = 0$.

1C

The last commutator we need to check is $[\hat{P}, \hat{S}_z]$:

$$
\begin{aligned}
[\hat{P}, \hat{S}_z] &= [\sum_p \hat{P}_p^\dagger \hat{P}_p, \frac{1}{2}\sum_{q\sigma} \sigma c^\dagger_{q\sigma} c_{q\sigma}] \\
&= \frac{1}{2}\sum_{pq\sigma} \sigma [\hat{P}_p^\dagger \hat{P}_p, c^\dagger_{q\sigma} c_{q\sigma}] \\
&= \frac{1}{2}\sum_{pq} \Big(+ (c^\dagger_{p+}c^\dagger_{p-}c_{p-}c_{p+}c^\dagger_{q+}c_{q+} - c^\dagger_{q+}c_{q+}c^\dagger_{p+}c^\dagger_{p-}c_{p-}c_{p+}) \\
&\quad -(c^\dagger_{p+}c^\dagger_{p-}c_{p-}c_{p+}c^\dagger_{q-}c_{q-} - c^\dagger_{q-}c_{q-}c^\dagger_{p+}c^\dagger_{p-}c_{p-}c_{p+})\Big)
\end{aligned} \tag{24}
$$

We get four terms, which will be worked out separately:

$$c^\dagger_{p+}c^\dagger_{p-}c_{p-}c_{p+}c^\dagger_{q+}c_{q+} = \{c^\dagger_{p+}c^\dagger_{p-}c^\dagger_{q+}c_{q+}c_{p-}c_{p+}\} + \delta_{pq}c^\dagger_{p+}c^\dagger_{p-}c_{p-}c_{q+} \tag{25}$$

$$c^\dagger_{q+}c_{q+}c^\dagger_{p+}c^\dagger_{p-}c_{p-}c_{p+} = \{c^\dagger_{p+}c^\dagger_{p-}c^\dagger_{q+}c_{q+}c_{p-}c_{p+}\} + \delta_{qp}c^\dagger_{q+}c^\dagger_{p-}c_{p-}c_{p+} \tag{26}$$

$$c^\dagger_{p+}c^\dagger_{p-}c_{p-}c_{p+}c^\dagger_{q-}c_{q-} = \{c^\dagger_{p+}c^\dagger_{p-}c^\dagger_{q-}c_{q-}c_{p-}c_{p+}\} - \delta_{pq}c^\dagger_{p+}c^\dagger_{p-}c_{p+}c_{q-} \tag{27}$$

$$c^\dagger_{q-}c_{q-}c^\dagger_{p+}c^\dagger_{p-}c_{p-}c_{p+} = \{c^\dagger_{p+}c^\dagger_{p-}c^\dagger_{q-}c_{q-}c_{p-}c_{p+}\} - \delta_{qp}c^\dagger_{p+}c^\dagger_{q-}c_{p+}c_{p-} \tag{28}$$

Observe that the first terms cancel, and we are left with terms of δ_{pq} and δ_{qp}. Those will contribute if and only if $p = q$, which happens exactly once since both p and q runs over all possible states.

$$
\begin{aligned}
[\hat{P}, \hat{S}_z] &= \frac{1}{2}\sum_p \Big((c^\dagger_{p+}c^\dagger_{p-}c_{p-}c_{p+} + c^\dagger_{p+}c^\dagger_{p-}c_{p+}c_{p-}) - \\
&\qquad (c^\dagger_{p+}c^\dagger_{p-}c_{p-}c_{p+} + c^\dagger_{p+}c^\dagger_{p-}c_{p+}c_{p-})\Big) \\
&= 0
\end{aligned} \tag{29}
$$

1D

$$[\hat{P}_p, \hat{P}_q^\dagger] = \hat{P}_p\hat{P}_q^\dagger - \hat{P}_q^\dagger\hat{P}_p \tag{30}$$

Will only include terms which contribute, and we obtain

$$
\begin{aligned}
\hat{P}_p\hat{P}_q^\dagger &= c_{p-}c_{p+}c^\dagger_{q+}c^\dagger_{q-} \\
&= \{c^\dagger_{q+}c^\dagger_{q-}c_{p-}c_{p+}\} + c_{p-}c_{p+}c^\dagger_{q+}c^\dagger_{q-} + c_{p-}c_{p+}c^\dagger_{q+}c^\dagger_{q-} + c_{p-}c_{p+}c^\dagger_{q+}c^\dagger_{q-} \\
&= \{c^\dagger_{q+}c^\dagger_{q-}c_{p-}c_{p+}\} - \delta_{pq}c_{p+}c^\dagger_{q+} - \delta_{pq}c_{p-}c^\dagger_{q-} + \delta_{pq}\delta_{pq}
\end{aligned} \tag{31}
$$

due to Wick's theorem. Several terms vanish since a delta function of operators of opposite spin does not contribute, i.e. $\delta_{p+q-} = 0$. Calculating $\hat{P}_q^\dagger \hat{P}_p$ is a simple task:

$$\hat{P}_q^\dagger \hat{P}_p = \{c_{q+}^\dagger c_{q-}^\dagger c_{p-} c_{p+}\}. \tag{32}$$

Furthermore we will omit the spin in delta functions, because it does not affect the delta function as long as the spin is equally directed. As always the deltas δ_{pq} contribute if and only if $p = q$, so we can set $q = p$ in the operators after the first delta in each term:

$$\begin{aligned}\hat{P}_p \hat{P}_q^\dagger - \hat{P}_q^\dagger \hat{P}_p &= -\delta_{pq} c_{q+}^\dagger c_{q+} - \delta_{pq} c_{q-}^\dagger c_{q-} + \delta_{pq}\delta_{qq} \\ &= \delta_{pq}(1 - c_{q+}^\dagger c_{q+} - c_{q-}^\dagger c_{q-}) \\ &= \delta_{pq}(1 - \hat{n}_q)\end{aligned} \tag{33}$$

1E

A fundamental property of the annihilation operator states that a such operator acting on the vacuum state becomes zero. This property will be used multiple times henceforce to get rid of terms, and the approach will often be to move the annihilation operator(s) all the way to the right such that this happens. We have $N = 4$, thus

$$|\Phi\rangle = c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger |-\rangle \tag{34}$$

$$= \hat{P}_1^\dagger \hat{P}_2^\dagger |-\rangle. \tag{35}$$

M is the number of states, with p as the index

$$\hat{P} = \sum_{p=1}^{M} \hat{P}_p^\dagger \hat{P}_p \tag{36}$$

$$= \hat{P}_1^\dagger \hat{P}_1 + \hat{P}_2^\dagger \hat{P}_2 + \hat{P}_3^\dagger \hat{P}_3 + \hat{P}_4^\dagger \hat{P}_4 \tag{37}$$

since $M = 4$.

$$\hat{P}|\Phi\rangle = \sum_p \hat{P}_p^\dagger \hat{P}_p \hat{P}_1^\dagger \hat{P}_2^\dagger |-\rangle \tag{38}$$

The result obtained in exercise 1D will not be used to move $\hat{P}_p$ (the only operator containing annihilation operators) to the right.

$$\begin{aligned}\hat{P}|\Phi\rangle &= \sum_p \hat{P}_p^\dagger \Big(\hat{P}_1^\dagger \hat{P}_p + \delta_{p1}(1 - \hat{n}_1)\Big) \hat{P}_2^\dagger |-\rangle \\ &= \sum_p \hat{P}_p^\dagger \hat{P}_1^\dagger \hat{P}_p \hat{P}_2^\dagger |-\rangle + \sum_p \delta_{p1} \hat{P}_p^\dagger \hat{P}_2^\dagger |-\rangle + \sum_p \delta_{p1} \hat{P}_p^\dagger \hat{n}_1 \hat{P}_2^\dagger |-\rangle\end{aligned}$$

The last term vanishes because the number operator is hermitian, and can therefore be moved to the right. The second term becomes $|\Phi\rangle$ since the delta "requires" $p = 1$. We are left with the first term to work out, and again we use equation (33):

$$
\begin{aligned}
\sum_p \hat{P}_p^\dagger \hat{P}_1^\dagger \hat{P}_p \hat{P}_2^\dagger |-\rangle &= \sum_p \hat{P}_p^\dagger \hat{P}_1^\dagger \hat{P}_2^\dagger \hat{P}_p |-\rangle + \sum_p \hat{P}_p^\dagger \hat{P}_1^\dagger \delta_{p2}(1-\hat{n}_2)|-\rangle \\
&= \sum_p \delta_{p2} \hat{P}_p^\dagger \hat{P}_1^\dagger |-\rangle + \sum_p \hat{P}_p^\dagger \hat{P}_1^\dagger \hat{n}_2 |-\rangle \\
&= \hat{P}_2^\dagger \hat{P}_1^\dagger |-\rangle = |\Phi\rangle
\end{aligned}
$$

On line number one the first term vanished because an annihilation operator acted on the vacuum state and on the second line the last term vanished since it contained a number operator. In total we then have:

$$
\hat{P}|\Phi\rangle = |\Phi\rangle + |\Phi\rangle = 2|\Phi\rangle \tag{39}
$$

The calculations above are pretty well-commented, but since the same operations are repeating, I do not consider that much comments as necessary in the coming calculations. For the $\hat{P}|\Phi\rangle$ calculation we were lucky since we could use pair creation and pair annihilation operators and could use the result from 1D. This is not always the case, something we will see when calculating $\hat{S}_z|\Phi\rangle$.

$$
\hat{S}_z = \frac{1}{2} \sum_{p\sigma} \sigma c_{p\sigma}^\dagger c_{p\sigma} \tag{40}
$$

$$
\begin{aligned}
&= \frac{1}{2}\Big(c_{1+}^\dagger c_{1+} - c_{1-}^\dagger c_{1-} + c_{2+}^\dagger c_{2+} - c_{2-}^\dagger c_{2-} + \\
&\quad c_{3+}^\dagger c_{3+} - c_{3-}^\dagger c_{3-} + c_{4+}^\dagger c_{4+} - c_{4-}^\dagger c_{4-} \Big)|-\rangle
\end{aligned} \tag{41}
$$

$$
\begin{aligned}
\hat{S}_z|\Phi\rangle &= \frac{1}{2}\Big(c^\dagger_{1+}c_{1+}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-} - c^\dagger_{1-}c_{1-}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-} \\
&\quad + c^\dagger_{2+}c_{2+}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-} - c^\dagger_{2-}c_{2-}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-}\Big)|-\rangle \qquad (42) \\
&= \frac{1}{2}\Big(c^\dagger_{1+}c_{1+}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-} - c^\dagger_{1-}c_{1-}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-} \\
&\quad + c^\dagger_{2+}c_{2+}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-} - c^\dagger_{2-}c_{2-}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-}\Big)|-\rangle \qquad (43) \\
&= \frac{1}{2}\Big(\delta_{1+1+}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-} - \delta_{1-1-}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-} \\
&\quad + \delta_{2+2+}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-} - \delta_{2-2-}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-}\Big)|-\rangle \qquad (44) \\
&= \frac{1}{2}(1-1+1-1)|\Phi\rangle \qquad (45) \\
&= 0|\Phi\rangle \qquad (46)
\end{aligned}
$$

PS: I know this was a tedious approach, and perhaps it would be better to not write out the sum

1F

Observe that $|1\bar{1}2\bar{2}\rangle = |\Phi\rangle$.

From figure (1) one can observe that the dimension of the subspace for $M = 4$ is $3+2+1 = 6$, which is the number of possible states. We can easily imagine that for $M = 2$ we would get 1 state, with $M = 5$ we would get $4+3+2+1 = 10$ states and so on. Thus the dimension of the subspace for an arbitrary M is given by the arithmetic series

$$n_M = \sum_{m=1}^{M-1}(M-m). \qquad (47)$$

1G

Need to figure out this

1H

$$\hat{H} = \hat{H}_0 + \hat{V} \qquad (48)$$

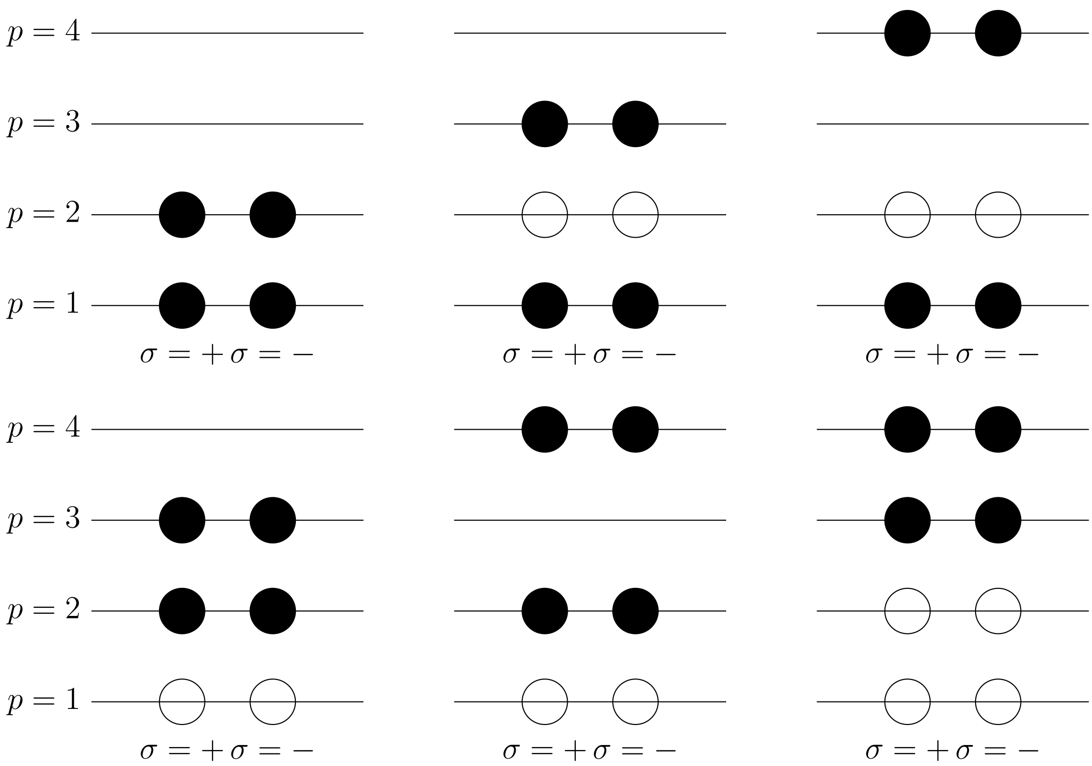

Figure 1: Need good caption here.

We use equation (2) and (3), and get

$$
\begin{aligned}
\hat{V} &= -\frac{1}{2}g\sum_{pq} c^\dagger_{p+}c^\dagger_{p-}c_{q-}c_{q+} \\
&= -\frac{1}{2}g\sum_{p}^{M} c^\dagger_{p+}c^\dagger_{p-}\sum_{q}^{M} c_{q-}c_{q+} \\
&= -\frac{1}{2}g\Bigg(\sum_{p=1}^{4}\hat{P}^\dagger_p\Bigg)\Bigg(\sum_{q=1}^{4}\hat{P}_q\Bigg) \qquad (49)
\end{aligned}
$$

Similarly we get

$$
\begin{aligned}
\hat{H}_0 &= \sum_{p\sigma}\varepsilon_p c^\dagger_{p\sigma}c_{p\sigma} \\
&= \sum_{p}(p-1)\sum_{\sigma} c^\dagger_{p\sigma}c_{p\sigma} \\
&= \sum_{p}(p-1)\hat{n}_p. \qquad (50)
\end{aligned}
$$

Thus we end up with

$$
\hat{H} = \sum_{p}(p-1)\hat{n}_p - \frac{1}{2}g\Bigg(\sum_{p=1}^{4}\hat{P}^\dagger_p\Bigg)\Bigg(\sum_{q=1}^{4}\hat{P}_q\Bigg) \qquad (51)
$$

2 Configuration-Interaction (CI)

2A

$$
\sum_{s}\hat{P}_s|p\bar{p}q\bar{q}\rangle = \sum_{s}\hat{P}_s\hat{P}^\dagger_p\hat{P}^\dagger_q|-\rangle \qquad (52)
$$

We use the result from exercise 1D (equation(33)) twice, and get

$$
\begin{aligned}
\hat{P}_s\hat{P}^\dagger_p\hat{P}^\dagger_q =& \hat{P}^\dagger_p\hat{P}_s\hat{P}^\dagger_q + \delta_{sp}(1-\hat{n}_p)\hat{P}^\dagger_q \\
=& \hat{P}^\dagger_p\hat{P}^\dagger_q\hat{P}_s + \hat{P}^\dagger_p\delta_{sq}(1-\hat{n}_q) + \delta_{sp}(1-\hat{n}_p)\hat{P}^\dagger_q \qquad (53)
\end{aligned}
$$

Then insert back into equation (52):

$$\begin{aligned}
&\sum_s (\hat{P}_p^\dagger \hat{P}_q^\dagger \hat{P}_s + \hat{P}_p^\dagger \delta_{sq}(1-\hat{n}_q) + \delta_{sp}(1-\hat{n}_p)\hat{P}_q^\dagger)|-\rangle \\
&= \sum_s (\hat{P}_p^\dagger \delta_{sq}(1-\hat{n}_q) + \delta_{sp}(1-\hat{n}_p)\hat{P}_q^\dagger)|-\rangle \\
&= \sum_s (\delta_{sq}\hat{P}_p^\dagger - \delta_{sq}\hat{P}_p^\dagger \hat{n}_q + \delta_{sp}\hat{P}_q^\dagger - \delta_{sp}\hat{n}_p\hat{P}_q^\dagger)|-\rangle \\
&= \sum_s (\delta_{sp}\hat{P}_p^\dagger + \delta_{sq}\hat{P}_q^\dagger)|-\rangle \\
&= (\hat{P}_p^\dagger + \hat{P}_q^\dagger)|-\rangle \\
&= |p\bar{p}\rangle + |q\bar{q}\rangle
\end{aligned} \tag{54}$$

Firstly the first term vanishes, since an annihilation operator acts on the vacuum. Also when $\hat{n}_p$ acts on vacuum the term dies, and since this operator is hermitian, it can always be moved to the vacuum. Further we will find the Hamiltonian matrix

$$\langle p'\bar{p}'q'\bar{q}|\hat{H}|p\bar{p}q\bar{q}\rangle = \langle p'\bar{p}'q'\bar{q}|\hat{H}_0|p\bar{p}q\bar{q}\rangle + \langle p'\bar{p}'q'\bar{q}|\hat{V}|p\bar{p}q\bar{q}\rangle \tag{55}$$

I will start with the first one:

$$\hat{H}_0|p\bar{p}q\bar{q}\rangle = \sum_{r\sigma} \epsilon_r c_{r\sigma}^\dagger c_{r\sigma} c_{p+}^\dagger c_{p-}^\dagger c_{q+}^\dagger c_{q-}^\dagger |-\rangle \tag{56}$$

Wick's theorem is used to calculate this, and since it requires normal ordering, the vacuum state will kill all strings including an annihilation operator. In this case we therefore get four terms which come from single contraction. We will get delta functions, which only contribute when both indexes are equal, so for instance if we get δ_{rp} we need to set $r = p$ since r runs over all possible states.

$$\begin{aligned}
\hat{H}_0|p\bar{p}q\bar{q}\rangle &= \sum_{r\sigma} \epsilon_r \{c^\dagger_{r\sigma} c^\dagger_{p+} c^\dagger_{p-} c^\dagger_{q+} c^\dagger_{q-} c_{r\sigma}\}|-\rangle \\
&\quad + \sum_{r\sigma} \epsilon_r \delta_{r\sigma p+} c^\dagger_{r\sigma} c^\dagger_{p-} c^\dagger_{q+} c^\dagger_{q-}|-\rangle \\
&\quad - \sum_{r\sigma} \epsilon_r \delta_{r\sigma p-} c^\dagger_{r\sigma} c^\dagger_{p+} c^\dagger_{q+} c^\dagger_{q-}|-\rangle \\
&\quad + \sum_{r\sigma} \epsilon_r \delta_{r\sigma q+} c^\dagger_{r\sigma} c^\dagger_{p+} c^\dagger_{p-} c^\dagger_{q-}|-\rangle \\
&\quad - \sum_{r\sigma} \epsilon_r \delta_{r\sigma q-} c^\dagger_{r\sigma} c^\dagger_{p+} c^\dagger_{p-} c^\dagger_{q+}|-\rangle \qquad (57) \\
&= (\epsilon_p c^\dagger_{p+} c^\dagger_{p-} c^\dagger_{q+} c^\dagger_{q-} - \epsilon_p c^\dagger_{p-} c^\dagger_{p+} c^\dagger_{q+} c^\dagger_{q-} \\
&\quad + \epsilon_q c^\dagger_{q+} c^\dagger_{p+} c^\dagger_{p-} c^\dagger_{q-} - \epsilon_q c^\dagger_{q-} c^\dagger_{p+} c^\dagger_{p-} c^\dagger_{q+})|-\rangle \qquad (58) \\
&= (\epsilon_p c^\dagger_{p+} c^\dagger_{p-} c^\dagger_{q+} c^\dagger_{q-} + \epsilon_p c^\dagger_{p+} c^\dagger_{p-} c^\dagger_{q+} c^\dagger_{q-} \\
&\quad + \epsilon_q c^\dagger_{p+} c^\dagger_{p-} c^\dagger_{q+} c^\dagger_{q-} + \epsilon_q c^\dagger_{p+} c^\dagger_{p-} c^\dagger_{q+} c^\dagger_{q-})|-\rangle \qquad (59) \\
&= 2(\epsilon_p + \epsilon_q)(\hat{P}^\dagger_p \hat{P}^\dagger_p)|-\rangle \qquad (60) \\
&= 2(2 - p - q)|p\bar{p}q\bar{q}\rangle \qquad (61)
\end{aligned}$$

where $\xi = 1$ is assumed. We then get

$$\langle p'\bar{p}'q'\bar{q}'|\hat{H}_0|p\bar{p}q\bar{q}\rangle = 2(2-p-q)\langle p'\bar{p}'q'\bar{q}'|p\bar{p}q\bar{q}\rangle \qquad (62)$$

So we still need to calculate the braket (Puh)

$$\langle p'\bar{p}'q'\bar{q}'|p\bar{p}q\bar{q}\rangle = \langle -|\hat{P}_{p'}\hat{P}_{q'}\hat{P}^\dagger_p\hat{P}^\dagger_q|-\rangle \qquad (63)$$

Again we will try to move the annihilation operator all the way to the right, such that it acts on the vacuum. The result from exercise 1D will be applied several times.

$$\begin{aligned}
\hat{P}_{p'}\hat{P}_{q'}\hat{P}^\dagger_p\hat{P}^\dagger_q &= \hat{P}_{p'}\hat{P}^\dagger_p\hat{P}_{q'}\hat{P}^\dagger_q + \delta_{q'p}\hat{P}_{p'}(1-\hat{n}_p)\hat{P}^\dagger_q \qquad (64) \\
&= \hat{P}_{p'}\hat{P}^\dagger_p\hat{P}_{q'}\hat{P}^\dagger_q + \delta_{q'p}\hat{P}_{p'}\hat{P}^\dagger_q + \delta_{q'p}\hat{P}_{p'}\hat{n}_p\hat{P}^\dagger_q \qquad (65)
\end{aligned}$$

Since $\hat{n}_p$ is hermitian, we can move it to the right in the last term, and the term will vanish when it acts on the vacuumstate. From now on I will stop commenting that annihilators are killed by the vacuum. The second term becomes

$$\begin{aligned}
\delta_{q'p}\hat{P}_{p'}\hat{P}^\dagger_q &= \delta_{q'p}\hat{P}^\dagger_q\hat{P}_{p'} + \delta_{q'p}\delta_{p'q} + \delta_{q'p}\delta_{p'q}\hat{n}_q \qquad (66) \\
&= \delta_{q'p}\delta_{p'q} \qquad (67)
\end{aligned}$$

while the first term is slightly more complicated. We need to switch the two latter operators to get the annihilation operator acting in vacuum:

$$\hat{P}_{p'}\hat{P}_p^\dagger\hat{P}_{q'}\hat{P}_q^\dagger = \hat{P}_{p'}\hat{P}_p^\dagger\hat{P}_q^\dagger\hat{P}_{q'} + \delta_{q'q}\hat{P}_{p'}\hat{P}_p^\dagger(1-\hat{n}_q) \tag{68}$$
$$= \delta_{q'q}\hat{P}_{p'}\hat{P}_p^\dagger \tag{69}$$
$$= \delta_{q'q}\delta_{p'p} - \delta_{q'q}\delta_{p'p}\hat{n}_q + \delta_{q'q}\hat{P}_p^\dagger\hat{P}_{p'} \tag{70}$$
$$= \delta_{q'q}\delta_{p'p} \tag{71}$$

So we obtain

$$\langle p'\bar{p}'q'\bar{q}'|p\bar{p}q\bar{q}\rangle = \delta_{q'p}\delta_{p'q} + \delta_{q'q}\delta_{p'p} \tag{72}$$

and

$$\langle p'\bar{p}'q'\bar{q}'|\hat{H}_0|p\bar{p}q\bar{q}\rangle = 2(2-p-q)(\delta_{q'p}\delta_{p'q} + \delta_{q'q}\delta_{p'p}). \tag{73}$$

One term done, one to go. Fortunately the potential term is much easier to calculate:

$$\langle p'\bar{p}'q'\bar{q}|\hat{V}|p\bar{p}q\bar{q}\rangle = -\frac{1}{2}g\langle p'\bar{p}'q'\bar{q}|(\sum_r \hat{P}_r^\dagger)(\sum_s \hat{P}_s)|p\bar{p}q\bar{q}\rangle \tag{74}$$

In the beginning of this exercise we proved that $\sum_s \hat{P}_s|p\bar{p}q\bar{q}\rangle = |p\bar{p}q\bar{q}\rangle$. Similarly one can prove the corresponding complex conjugate

$$\langle p'\bar{p}'q'\bar{q}'|\sum_r \hat{P}_r^\dagger = \langle p'\bar{p}'| + \langle q'\bar{q}'| \tag{75}$$

With this in mind, we can rewrite the potential braket into four small brakets

$$\langle p'\bar{p}'q'\bar{q}|\hat{V}|p\bar{p}q\bar{q}\rangle = -\frac{1}{2}g(\langle p'\bar{p}'|p\bar{p}\rangle + \langle p'\bar{p}'|q\bar{q}\rangle + \langle q'\bar{q}'|p\bar{p}\rangle + \langle q'\bar{q}'|q\bar{q}\rangle) \tag{76}$$

where the first one is

$$\langle p'\bar{p}'|p\bar{p}\rangle = \langle -|\hat{P}_{p'}\hat{P}_p^\dagger|-\rangle = \langle -|\hat{P}_p^\dagger\hat{P}_{p'} + \delta_{p'p}(1-\hat{n}_p)|-\rangle = \delta_{p'p} \tag{77}$$

and similar for the other three. We can finally write out the matrix element expression

$$\langle p'\bar{p}'q'\bar{q}|\hat{H}|p\bar{p}q\bar{q}\rangle = 2(2-p-q)(\delta_{q'p}\delta_{p'q} + \delta_{q'q}\delta_{p'p}) - \frac{1}{2}g(\delta_{p'p} + \delta_{p'q} + \delta_{q'p} + \delta_{q'q}) \tag{78}$$

Observe that the first term from $\hat{H}_0$ will never contribute since Pauli's exclusion principle restricts $q > p$ (and $q' > p'$). $\hat{H}_0$ will therefore only make contributions on the diagonal when we form a matrix based on Full Configuration-Interactions. It is also worth to notice that there will not be any contribution if all the indexes are different.

2B

In our case we get a matrix on the form

$$\begin{pmatrix} H_{12}^{12} & H_{12}^{13} & H_{12}^{14} & H_{12}^{23} & H_{12}^{24} & H_{12}^{34} \\ H_{13}^{12} & H_{13}^{13} & H_{13}^{14} & H_{13}^{23} & H_{13}^{24} & H_{13}^{34} \\ H_{14}^{12} & H_{14}^{13} & H_{14}^{14} & H_{14}^{23} & H_{14}^{24} & H_{14}^{34} \\ H_{23}^{12} & H_{23}^{13} & H_{23}^{14} & H_{23}^{23} & H_{23}^{24} & H_{23}^{34} \\ H_{24}^{12} & H_{24}^{13} & H_{24}^{14} & H_{24}^{23} & H_{24}^{24} & H_{24}^{34} \\ H_{34}^{12} & H_{34}^{13} & H_{34}^{14} & H_{34}^{23} & H_{34}^{24} & H_{34}^{34} \end{pmatrix} \tag{79}$$

where

$$H_{12}^{34} = \langle 12|\hat{H}|34\rangle = 2(2-3-4)(0+0) - \frac{1}{2}g(0+0+0+0) = 0 \tag{80}$$

etc.. Calculate all elements, and get

$$\langle p'\bar{p}'q'\bar{q}|\hat{H}|p\bar{p}q\bar{q}\rangle = \begin{pmatrix} -2-g & -1/2g & -1/2g & -1/2g & -1/2g & 0 \\ -1/2g & -4-g & -1/2g & -1/2g & 0 & -1/2g \\ -1/2g & -1/2g & -6-g & 0 & -1/2g & -1/2g \\ -1/2g & -1/2g & 0 & -6-g & -1/2g & -1/2g \\ -1/2g & 0 & -1/2g & -1/2g & -8-g & -1/2g \\ 0 & -1/2g & -1/2g & -1/2g & -1/2g & -10-g \end{pmatrix}. \tag{81}$$

The eigenvalues of the Hamiltonian are the diagonal elements after diagonalization, and we find them using the numpy package in Python (see Appendix A). The eigenvalues as a function of g are plotted in figure (**??**).

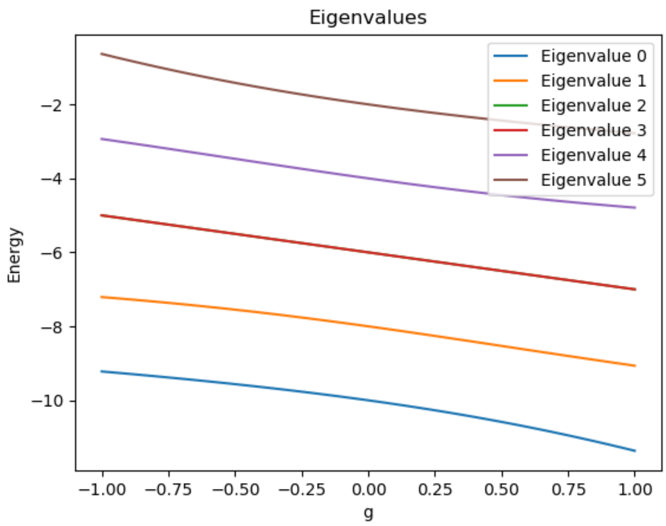

Figure 2: NEED CAPTION

We can only spot 5 eigenvalue lines, even though we know it should be 6 and the legend tells us there is 6 eigenvalues. The reason is obvious, eigenvalue 3 and 4 are the same, and we have a degeneracy.

Need probability plot as well

2C

The single excited determinants ($|\Phi_i^a\rangle$) will not contribute to the exact eigefunction since we require $p = \bar{p}$, i.e two particles with opposite spin shall always lay on the same level. We will work with Configuration-Interaction Doubles (CID), but have in mind that it is the same as CConfiguration-Interaction Singles-Doubles (CISD). In general the doubly excited determinants can be written

$$|\Phi_{ij}^{ab}\rangle = c_a^\dagger c_b^\dagger c_i c_j |\Phi\rangle \tag{82}$$

In our case the first unoccupied index a has positive spin, while the second has negative spin. Since they both will lay on the same level, the second index is denoted with a bar, which implies negative spin. Similarly the second occupied index has negative spin, so we have

$$|\Phi_{i\bar{i}}^{a\bar{a}}\rangle = c_{a+}^\dagger c_{a-}^\dagger c_{i+} c_{i-} |\Phi\rangle = \hat{P}_a^\dagger \hat{P}_i |\Phi\rangle \tag{83}$$

The CISD space is given by

$$\hat{H}_{CISD} = \begin{pmatrix} E_{SCF} & 0 & \hat{H}_{OD} \\ 0 & \hat{H}_{SS} & \hat{H}_{SD} \\ \hat{H}_{D0} & \hat{H}_{DS} & \hat{H}_{DD} \end{pmatrix} \tag{84}$$

Since CID now corresponds to CISD, we get

$$\hat{H}_{CID} = \begin{pmatrix} H_{12}^{12} & 0 & H_{12}^{34} \\ 0 & H_{13}^{13} & H_{13}^{34} \\ H_{34}^{12} & H_{34}^{13} & H_{34}^{34} \end{pmatrix} = \begin{pmatrix} -2-g & 0 & 0 \\ 0 & -4-g & -1/2g \\ 0 & -1/2g & -10-g \end{pmatrix} \tag{85}$$

Where all the matrix elements have been calculating in a earlier exercise. We can see that we only pick 7 elements out of 36, and we miss 29 FCI basis functions. In figure (3) we ground-state energy from FCI is plotted together with the CID ground-state energy, and we see that the FCI energy is bending as function of g, while the CID energy is linear. They are the same at $g = 0$.

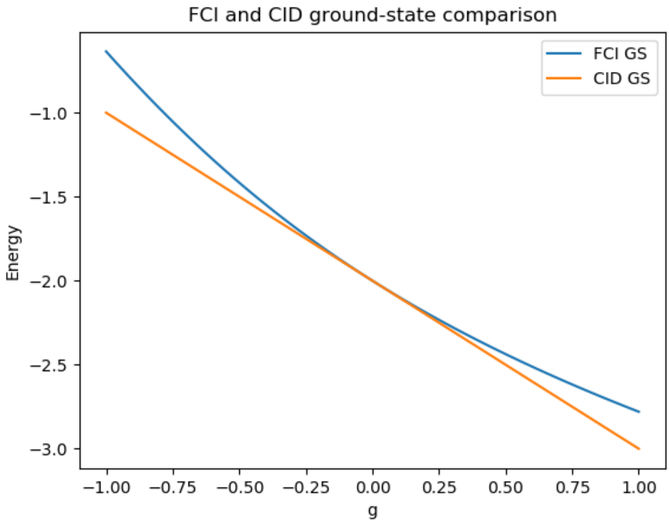

Figure 3: The FCI and CID ground-state (GS) energies as functions of g

2D

The non-degenerate Rayleigh-Schrodinger Perturbation Theory (RSPT) energy is given by

$$E^{(n)} = \langle\Phi|\hat{V}|\Psi^{(n-1)}\rangle \tag{86}$$

with

$$|\Psi^{(n)}\rangle = \hat{R}\Big[\hat{V}|\Phi^{(n-1)}\rangle - \sum_{j=1}^{n-1}|\Psi^{(j)}\rangle\Big]. \tag{87}$$

The first order energy correction becomes

$$E^{(1)} = \langle\Phi|\hat{V}|\Psi^{(0)}\rangle = \langle\Phi|\hat{V}|\Phi\rangle. \tag{88}$$

We also calculate $|\Psi^{(1)}\rangle$, which we will need for higher order energy expressions.

$$|\Psi^{(1)}\rangle = \hat{R}\Big[\hat{V}|\Psi^{(0)}\rangle - \sum_{j=1}^{0}E^{(1-j)}|\Psi^{(j)}\rangle\Big] = \hat{R}\hat{V}|\Phi\rangle \tag{89}$$

We then obtain the following for the second order correction:

$$E^{(2)} = \langle\Phi|\hat{V}|\Psi^{(1)}\rangle = \langle\Phi|\hat{V}\hat{R}\hat{V}|\Phi\rangle \tag{90}$$

and

$$|\Psi^{(2)}\rangle = \hat{R}\Big[\hat{V}\hat{R}\hat{V}|\Phi\rangle - E^{(1)}|\Psi^{(1)}\rangle\Big] = \hat{R}\Big[\hat{V} - \langle\Phi|\hat{V}|\Phi\rangle\Big]\hat{R}\hat{V}|\Phi\rangle. \tag{91}$$

Finally we can compute the third order correction energy:

$$E^{(3)} = \langle\Phi|\hat{V}\hat{R}\hat{V}\hat{R}\hat{V}|\Phi\rangle - \langle\Phi|\hat{V}|\Phi\rangle\langle\Phi|\hat{V}\hat{R}\hat{R}\hat{V}|\Phi\rangle \tag{92}$$

We can see that the first term follows a certain pattern for increasing order corrections, and is considered as the leading term. The second term is smaller, and in rough estimates it is normal to omit it.

2E

We are now going to compute the ground state energy to third order in Rayleigh-Schrodinger perturbation theory

$$E_{RSPT3} = E^{(0)} + gE^{(1)} + g^2E^{(2)} + g^3E^{(3)}. \tag{93}$$

There are two way to do this: We could use second quantization and many-body perturbation theory (MBPT) or we could use basic PT on matrix form.

3 Coupled-Cluster (CC)

3A

The general CCD wavefunction is as following

$$|\Psi_{CID}\rangle = \exp(\hat{T})|\Phi\rangle = (1 + \hat{T} + \frac{1}{2}\hat{T}^2)|\Phi\rangle \tag{94}$$

Because our system contains of only four particles, higher order terms do not appear.

3B

$$|\Psi_{CID}\rangle = (1 + \hat{C}_2)|\phi\rangle = (1 + \hat{T})|\Phi\rangle \tag{95}$$

$$|\Psi_{CCD}\rangle = |\Psi_{CID}\rangle + (1/2\hat{T}^2)|\Phi\rangle \tag{96}$$

3C

$$\langle\Phi|\hat{H}(1 + \hat{T})|\Phi\rangle = \langle\Phi|\hat{H}|\Phi\rangle + \langle\Phi|\hat{H}\hat{T}|\Phi\rangle \tag{97}$$

The first term is already calculated, and we found it to be $(2(\epsilon_p+\epsilon_q)-g)(\delta_{p'p}+\delta_{p'q}+\delta_{q'p}+\delta_{q'q})$. In this case we deal with the reference wave function, such that $p' = p$ and $q' = q$. We then obtain

$$\langle\Phi|\hat{H}|\Phi\rangle = 2\epsilon_p + 2\epsilon_q - g \tag{98}$$

Furthermore we work out the second term. Recall that a is an unoccupied index, i is occupied and $p, , rq$ and s are arbitrary indexes. Because of $\hat{H}$ we can immediately see that the term again can be split up in two new terms:

$$\begin{aligned}\langle\Phi|\hat{H}|\Phi\rangle = \langle p'\bar{p}'q'\bar{q}'|(\sum_r (r-1)\hat{n}_r)(\sum_{ia} t_i^a \hat{P}_a^\dagger \hat{P}_i)|p\bar{p}q\bar{q}\rangle \\ +\langle p'\bar{p}'q'\bar{q}'| - \frac{1}{2}g(\sum_r \hat{P}_r^\dagger)(\sum_s \hat{P}_s)(\sum_{ia} t_i^a \hat{P}_a^\dagger \hat{P}_i)|p\bar{p}q\bar{q}\rangle\end{aligned} \tag{99}$$

We first examine the first of these terms:

$$\langle p'\bar{p}'q'\bar{q}'|(\sum_r (r-1)\hat{n}_r)(\sum_{ia} t_i^a \hat{P}_a^\dagger \hat{P}_i)|p\bar{p}q\bar{q}\rangle = \sum_{ria} \epsilon_r \langle -|\hat{P}_p \hat{P}_p^\dagger (\sum_\sigma c_{r\sigma}^\dagger c_{r\sigma})\hat{P}_a^\dagger \hat{P}_i|-\rangle$$

We could calculate this, but instead I will argue why it becomes zero. The rightmost operator is an annihilation operator, which means that it never will be contracted in a non-zero term. If we use Wick's theorem on the operators, we then will have an annihilation operator in every term, and since we need to leave them on normal order, we will always have an annihilation operator acting on the vacuum which is zero by definition.

Further we need to calculate the second term.

$$\begin{aligned}\langle p'\bar{p}'q'\bar{q}'| - \frac{1}{2}g(\sum_r \hat{P}_r^\dagger)(\sum_s \hat{P}_s)(\sum_{ia} t_i^a \hat{P}_a^\dagger \hat{P}_i)|p\bar{p}q\bar{q}\rangle \\ = -\frac{1}{2}g\sum_{rsia} t_i^a \langle -|\hat{P}_{p'}\hat{P}_{q'}\hat{P}_r^\dagger \hat{P}_s \hat{P}_a^\dagger \hat{P}_i \hat{P}_p^\dagger \hat{P}_q^\dagger|-\rangle\end{aligned} \tag{100}$$

We will now use Wick's theorem on the operators. On the same basis as for the first term, only terms without annihilation operators will contribute. There are several possible fully contracted terms, but we need to keep in mind that if an arbitrary operator has contracted to say an occupied index, it can only be contracted to occupied indexes. The fully contracted term is therefore

$$\begin{aligned}\{\hat{P}_{p'}\hat{P}_{q'}\hat{P}_r^\dagger \hat{P}_s \hat{P}_a^\dagger \hat{P}_i \hat{P}_p^\dagger \hat{P}_q^\dagger\}_{fc} &= c_{p'-}c_{p'+}c_{q'-}c_{q'+}c_{r+}^\dagger c_{r-}^\dagger c_{s-}c_{s+}c_{a+}^\dagger c_{a-}^\dagger c_{i-}c_{i+}c_{p+}^\dagger c_{p-}^\dagger c_{q+}^\dagger c_{q-}^\dagger \\ &= \delta_{p'r}\delta_{p'r}\delta_{q'a}\delta_{q'a}\delta_{sq}\delta_{sq}\delta_{ip}\delta_{ip}\end{aligned}$$

Again the sum runs over all possible indexes, i.e, at one point we will have $p' = i$, $q' = a$, $s = q$ and $r = p$, and we get contribution. After some argumentation, we obtain

$$E_{CCD} = 2\epsilon_1 + 2\epsilon_2 - g - \frac{1}{2}g\sum_{ia} t_i^a \tag{101}$$

3D

The normal ordered Fock operator is given by

$$\{\hat{F}\} = \hat{H}_0^{(1qp)} + \hat{V}^{(1qp)} \tag{102}$$

where $(1qp)$ indicates one quasi particle. If we apply Wick's theorem on $\hat{H}_0$, we get

$$\begin{aligned}
\hat{H}_0 &= \sum_{p\sigma} \epsilon_{p\sigma}^{\dagger} c_{p\sigma} \\
&= \sum_{p\sigma} \epsilon_p \{c_{p\sigma}^{\dagger} c_{p\sigma}\} + \sum_{p\sigma} \epsilon_p c_{p\sigma}^{\dagger} c_{p\sigma} \\
&= \sum_{i\sigma} \epsilon_i \{c_{i\sigma}^{\dagger} c_{i\sigma}\} + \sum_{i\sigma} \epsilon_i c_{i\sigma}^{\dagger} c_{i\sigma} + \sum_{a\sigma} \epsilon_a \{c_{a\sigma}^{\dagger} c_{a\sigma}\} + \sum_{a\sigma} \epsilon_a c_{a\sigma}^{\dagger} c_{a\sigma} \\
&= \sum_{i\sigma} \epsilon_i \{c_{i\sigma}^{\dagger} c_{i\sigma}\} + \sum_{i} \epsilon_i + \sum_{a\sigma} \epsilon_a \{c_{a\sigma}^{\dagger} c_{a\sigma}\} \\
&= \sum_{p\sigma} \epsilon_p \{c_{p\sigma}^{\dagger} c_{p\sigma}\} + \sum_{i} \epsilon_i
\end{aligned} \tag{103}$$

where the first term corresponds to one quasi particle and the second corresponds to zero quasi particles. For the potential operator I will only calculate the $(1qp)$ part, which is the terms we get from Wick's theorem with one contraction.

$$\begin{aligned}
\hat{V}^{(1qp)} &= -\frac{1}{2} g \sum_{pq} (c_{p+}^{\dagger} c_{p-}^{\dagger} c_{q-} c_{q+} + c_{p+}^{\dagger} c_{p-}^{\dagger} c_{q-} c_{q+}) \\
&= -\frac{1}{2} g \sum_{pq} (c_{i+}^{\dagger} c_{i-}^{\dagger} c_{j-} c_{j+} + c_{i+}^{\dagger} c_{i-}^{\dagger} c_{j-} c_{j+}) \\
&= -\frac{1}{2} g \sum_{ij} (\delta_{ij} c_{i-}^{\dagger} c_{j-} + \delta_{ij} c_{i+}^{\dagger} c_{j+}) \\
&= -\frac{1}{2} g \sum_{i\sigma} c_{i\sigma}^{\dagger} c_{i\sigma}
\end{aligned} \tag{104}$$

where we observed that all the unoccupied operators became zero since $c_p^\dagger c_q = b_p^\dagger b_q = 0$. We then use the definition of the Fock operator:

$$
\begin{aligned}
\hat{F}_N &= \hat{H}_0^{(1qp)} + \hat{V}^{(1qp)} \\
&= \sum_{i\sigma} \epsilon_i \{c_{i\sigma}^\dagger c_{i\sigma}\} + \sum_{a\sigma} \epsilon_a \{c_{a\sigma}^\dagger c_{a\sigma}\} - \frac{1}{2} g \sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma} \\
&= \sum_{i\sigma} (\epsilon_i - \frac{1}{2} g) \{c_{i\sigma}^\dagger c_{i\sigma}\} + \sum_{a\sigma} \epsilon_a \{c_{a+}^\dagger c_{a\sigma}\} \\
&= \sum_{p\sigma} f_p \{c_{p\sigma}^\dagger c_{p\sigma}\}
\end{aligned}
\tag{105}
$$

with $f_i = \epsilon_i - \frac{1}{2} g$ and $f_a = \epsilon_a$.

Our Baker-Campbell-Hausdorff (BCH) exponential expansion $e^{\hat{T}}$ has two terms, implying that the amplitude equation can be written as a polynomial of order no higher than $5 \Rightarrow 2$ nested commutators.

The CCD amplitude equations are in general given by

$$
F_{ij}^{ab}(t) = \langle \Phi_{ij}^{ab} | \{\hat{H}_N e^{\hat{T}}\}_c | \Phi \rangle = 0 \tag{106}
$$

The $\{...\}_c$ notation is only used around two (or more) operators, and indicates that the term contains *at least* one contraction between both operators. It is frequently used when we have a large number of terms with contraction between two certain operators, so we can replace all those terms with a $\{...\}_c$ notation. The amplitude equations simplify to

$$
\langle \Phi_{i\bar{i}}^{a\bar{a}} | \{\hat{F}_N \hat{T}\}_c | \Phi \rangle + \langle \Phi_{i\bar{i}}^{a\bar{a}} | \{\hat{V}_N (1 + \hat{T} + \frac{1}{2} \hat{T}^2)\}_c | \Phi \rangle = 0 \tag{107}
$$

because...

3E

We will now work the terms out one by one:

First term

$$
\langle \Phi_{i\bar{i}}^{a\bar{a}} | \{\hat{F}_N \hat{T}\}_c | \Phi \rangle = \sum_{jbp\sigma} f_p t_j^b \langle \Phi | c_{i+}^\dagger c_{i-}^\dagger c_{a-} c_{a+} \{c_{p\sigma}^\dagger c_{p\sigma} c_{b+}^\dagger c_{b-}^\dagger c_{j-} c_{j+}\}_c | \Phi \rangle \tag{108}
$$

We apply generalized Wick's theorem on the operator string, and we are only interested in the fully contracted terms. We need to take care of the connection restriction

$$
\begin{aligned}
c^\dagger_{i+}c^\dagger_{i-}c_{a-}c_{a+}\{c^\dagger_{p\sigma}c_{p\sigma}c^\dagger_{b+}c^\dagger_{b-}c_{j-}c_{j+}\}_c &= c^\dagger_{i+}c^\dagger_{i-}c_{a-}c_{a+}c^\dagger_{p+}c_{p+}c^\dagger_{b+}c^\dagger_{b-}c_{j-}c_{j+} \\
&\quad + c^\dagger_{i+}c^\dagger_{i-}c_{a-}c_{a+}c^\dagger_{p+}c_{p+}c^\dagger_{b+}c^\dagger_{b-}c_{j-}c_{j+} \\
&\quad + c^\dagger_{i+}c^\dagger_{i-}c_{a-}c_{a+}c^\dagger_{p-}c_{p-}c^\dagger_{b+}c^\dagger_{b-}c_{j-}c_{j+} \\
&\quad + c^\dagger_{i+}c^\dagger_{i-}c_{a-}c_{a+}c^\dagger_{p-}c_{p-}c^\dagger_{b+}c^\dagger_{b-}c_{j-}c_{j+} \\
&= \delta_{ij}\delta_{ij}\delta_{ab}\delta_{ap}\delta_{pb} - \delta_{ip}\delta_{ij}\delta_{ab}\delta_{ab}\delta_{pj} \\
&\quad + \delta_{ij}\delta_{ij}\delta_{ap}\delta_{ab}\delta_{pb} - \delta_{ip}\delta_{ij}\delta_{ab}\delta_{ab}\delta_{pj}
\end{aligned}
$$

We insert back into the bracket, and get

$$
\langle\Phi^{a\bar{a}}_{i\bar{i}}|\{\hat{F}_N\hat{T}\}_c|\Phi\rangle = f_a t^a_i - f_i t^a_i + f_a t^a_i - f_i t^a_i = 2(f_a - f_i)t^a_i \tag{109}
$$

Second term

$$
\langle\Phi^{a\bar{a}}_{i\bar{i}}|\hat{V}_N|\Phi\rangle = -\frac{1}{2}\sum_{pq}\langle\Phi|c^\dagger_{i+}c^\dagger_{i-}\{c_{a-}c_{a+}c^\dagger_{p+}c^\dagger_{p-}c_{q-}c_{q+}\}_c|\Phi\rangle \tag{110}
$$

We apply generalized Wick's theorem on the operator string, and we are only interested in the fully contracted terms. In general we should keep in mind that the Hamiltonian fraction is connected, but it will not make any difference for this specific string.

$$
\begin{aligned}
c^\dagger_{i+}c^\dagger_{i-}c_{a-}c_{a+}c^\dagger_{p+}c^\dagger_{p-}c_{q-}c_{q+} &= c^\dagger_{i+}c^\dagger_{i-}c_{a-}c_{a+}c^\dagger_{p+}c^\dagger_{p-}c_{q-}c_{q+} \\
&= \delta_{iq}\delta_{iq}\delta_{ap}\delta_{ap}
\end{aligned} \tag{111}
$$

There is only one non-zero fully contraction

$$
\begin{aligned}
\langle\Phi^{a\bar{a}}_{i\bar{i}}|\hat{V}_N|\Phi\rangle &= -\frac{1}{2}g\sum_{pq}\delta_{iq}\delta_{iq}\delta_{ap}\delta_{ap}\langle\Phi|\Phi\rangle \\
&= -\frac{1}{2}g
\end{aligned} \tag{112}
$$

Third term

$$
\langle\Phi^{a\bar{a}}_{i\bar{i}}|\{\hat{V}_N\hat{T}\}_c|\Phi\rangle = -\frac{1}{2}g\sum_{pqjb}t^b_j\langle\Phi|c^\dagger_{i+}c^\dagger_{i-}c_{a-}c_{a+}\{c^\dagger_{p+}c^\dagger_{p-}c_{q-}c_{q+}c^\dagger_{b+}c^\dagger_{b-}c_{j-}c_{j+}\}_c|\Phi\rangle
$$

We apply generalized Wick's theorem on the operator string, and are only interested in the fully contracted terms:

$$
\begin{aligned}
&(c^\dagger_{i+}c^\dagger_{i-}c_{a-}c_{a+}c^\dagger_{p+}c^\dagger_{p-}c_{q-}c_{q+}c^\dagger_{b+}c^\dagger_{b-}c_{j-}c_{j+})_{fc} \\
&= c^\dagger_{i+}c^\dagger_{i-}c_{a-}c_{a+}c^\dagger_{p+}c^\dagger_{p-}c_{q-}c_{q+}c^\dagger_{b+}c^\dagger_{b-}c_{j-}c_{j+} + c^\dagger_{i+}c^\dagger_{i-}c_{a-}c_{a+}c^\dagger_{p+}c^\dagger_{p-}c_{q-}c_{q+}c^\dagger_{b+}c^\dagger_{b-}c_{j-}c_{j+} \\
&= \delta_{ij}\delta_{ij}\delta_{ap}\delta_{ap}\delta_{qb}\delta_{qb} + \delta_{iq}\delta_{iq}\delta_{ab}\delta_{ab}\delta_{pj}\delta_{pj}
\end{aligned}
\tag{113}
$$

We get contribution from the first term when $j = i$, $p = a$ and $q = b$, and from the second when $q = i$, $b = a$ and $p = j$. Since i and a are fixed, b and j are respectively the only "free" parameters, which we need to sum over. We obtain

$$
\begin{aligned}
\langle \Phi^{a\bar{a}}_{i\bar{i}} | \{\hat{V}_N \hat{T}\}_c | \Phi \rangle &= -\frac{1}{2} g \left(\sum_b t^b_i \delta_{ii}\delta_{ii}\delta_{aa}\delta_{aa}\delta_{bb}\delta_{bb} + \sum_j t^a_j \delta_{ii}\delta_{ii}\delta_{aa}\delta_{aa}\delta_{jj}\delta_{jj} \right) \\
&= -\frac{1}{2} g \left(\sum_b t^b_i + \sum_j t^a_j \right)
\end{aligned}
\tag{114}
$$

Fourth term

we end up with

$$
F^a_i(t) \equiv 2(f_a - f_i)t^a_i - \frac{1}{2} g \left(1 + \sum_b t^b_i + \sum_j t^a_j + t^3_1 t^4_2 + t^4_1 t^3_2 - t^a_i \sum_{bj} t^b_j \right) = 0 \tag{115}
$$

which is the CCD amplitude equations.

3F

Let us play with equation (115):

$$
2(f_i - f_a)t^a_i = -\frac{1}{2} g \left(1 + \sum_b t^b_i + \sum_j t^a_j + t^3_1 t^4_2 + t^4_1 t^3_2 - t^a_i \sum_{bj} t^b_j \right) \tag{116}
$$

Notice that the terms on the left-hand side are switched. Now we add σt^a_i on both sides, where σ is a shift parameter which we later will use to stabilize the CCD energy solution.

$$
[2(f_i - f_a) + \sigma] t^a_i = \sigma t^a_i - \frac{1}{2} g \left(1 + \sum_b t^b_i + \sum_j t^a_j + t^3_1 t^4_2 + t^4_1 t^3_2 - t^a_i \sum_{bj} t^b_j \right) \tag{117}
$$

$$
t^a_i = [2(f_i - f_a) + \sigma]^{-1} \left(\sigma t^a_i - \frac{1}{2} g \left(1 + \sum_b t^b_i + \sum_j t^a_j + t^3_1 t^4_2 + t^4_1 t^3_2 - t^a_i \sum_{bj} t^b_j \right) \right) \tag{118}
$$

4 Appendices

Appendix A

...There are in general two ways to do this: We could find the eigenvalues symbolic and insert g afterwards, or we could find the eigenvalues of each matrix inserted g. Surprisingly I found the latter to be faster, and decided to do it that way. The Python implementation looks like this:

```
import numpy as np
import matplotlib.pyplot as plt


g_list = np.linspace(-1, 1, 100)          # 100 g values

# --- Full Configuration-Interaction (FCI) ---
eigenvalues_FCI = []                       # Going to be a
    ↪ nested list (matrix)
                                           # with eigenvalues
                                               ↪ for each g

for g in g_list:
    M_FCI = np.matrix([[-2 - g, -0.5 * g, -0.5 * g, -0.5 *
        ↪ g, -0.5 * g, 0], \
                        [-0.5 * g, -4 - g, -0.5 * g, -0.5 *
                            ↪ g, 0, -0.5 * g], \
                        [-0.5 * g, -0.5 * g, -6 - g, 0, -0.5
                            ↪ * g, -0.5 * g], \
                        [-0.5 * g, -0.5 * g, 0, -6 - g, -0.5
                            ↪ * g, -0.5 * g], \
                        [-0.5 * g, 0, -0.5 * g, -0.5 * g, -8
                            ↪ - g, -0.5 * g], \
                        [0, -0.5 * g, -0.5 * g, -0.5 * g,
                            ↪ -0.5 * g, -10 - g]])

    eigenvalues_FCI.append((np.linalg.eigh(M_FCI)[0]))

for k in range(M_FCI.shape[0]):            # M_FCI.shape[0] is
    ↪  length(col1(M_FCI))
    new_list_FCI = []
    for i in range(len(eigenvalues_FCI)):
        new_list_FCI.append(eigenvalues_FCI[i][k])
    plt.plot(g_list, new_list_FCI, label='Eigenvalue {}'.
        ↪ format(k))
```

```python
plt.legend(loc='best')
plt.title('Eigenvalues')
plt.xlabel('g')
plt.ylabel('Energy')
plt.savefig('eigenvalues_FCI.png')
plt.show()

# --- Configuration-Interaction Doubles (CID) ---
eigenvalues_CID = []                                    # Going to be a
    ↪ nested list (matrix)
                                                        # with eigenvalues
                                                            ↪ for each g

for g in g_list:
    M_CID = np.matrix([[-2-g, 0, 0], [0, -4-g, -0.5*g], [0,
        ↪ -0.5*g, -10-g]])

    eigenvalues_CID.append((np.linalg.eigh(M_CID)[0]))

for k in range(M_CID.shape[0]):                         # M_CID.shape[0] is
    ↪ length(col1(M_CID))
    new_list_CID = []
    for i in range(len(eigenvalues_CID)):
        new_list_CID.append(eigenvalues_CID[i][k])
    plt.plot(g_list, new_list_CID, label='Eigenvalue {}'.
        ↪ format(k))
plt.legend(loc='best')
plt.title('Eigenvalues')
plt.xlabel('g')
plt.ylabel('Energy')
plt.savefig('eigenvalues_CID.png')
plt.show()

# --- Comparison of ground-state energy ---

plt.plot(g_list, new_list_FCI, label='FCI GS')
plt.plot(g_list, new_list_CID, label='CID GS')
plt.title('FCI and CID ground-state comparison')
plt.xlabel('g')
plt.ylabel('Energy')
plt.savefig('groundstate_comparison.png')
plt.legend(loc='best')
plt.show()
```