FYS-KJM4480 - Quantum mechanics for many-particle systems

Project 2

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November 20, 2017

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

1 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.

2 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

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

1A

1B

1C

We are supposed to show that $\hat{P}$ commutes with $\hat{S}_z$, with other words $[\hat{P}, \hat{S}_z] = 0$

$$
\begin{aligned}
[\hat{P}, \hat{S}_z] &= [\sum_p \hat{P}_p^\dagger \hat{P}_p, \frac{1}{2}\sum_{q\sigma} \sigma c_{q\sigma}^\dagger c_{q\sigma}] \\
&= \frac{1}{2}\sum_{pq\sigma} \sigma [\hat{P}_p^\dagger \hat{P}_p, c_{q\sigma}^\dagger c_{q\sigma}] \\
&= \frac{1}{2}\sum_{pq} \Big(+ (c_{p+}^\dagger c_{p-}^\dagger c_{p-} c_{p+} c_{q+}^\dagger c_{q+} - c_{q+}^\dagger c_{q+} c_{p+}^\dagger c_{p-}^\dagger c_{p-} c_{p+}) \\
&\quad - (c_{p+}^\dagger c_{p-}^\dagger c_{p-} c_{p+} c_{q-}^\dagger c_{q-} - c_{q-}^\dagger c_{q-} c_{p+}^\dagger c_{p-}^\dagger c_{p-} c_{p+})\Big) \qquad (9)
\end{aligned}
$$

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

$$c_{p+}^\dagger c_{p-}^\dagger c_{p-} c_{p+} c_{q+}^\dagger c_{q+} = \{c_{p+}^\dagger c_{p-}^\dagger c_{q+}^\dagger c_{q+} c_{p-} c_{p+}\} + \delta_{pq} c_{p+}^\dagger c_{p-}^\dagger c_{p-} c_{q+} \qquad (10)$$

$$c_{q+}^\dagger c_{q+} c_{p+}^\dagger c_{p-}^\dagger c_{p-} c_{p+} = \{c_{p+}^\dagger c_{p-}^\dagger c_{q+}^\dagger c_{q+} c_{p-} c_{p+}\} + \delta_{qp} c_{q+}^\dagger c_{p-}^\dagger c_{p-} c_{p+} \qquad (11)$$

$$c_{p+}^\dagger c_{p-}^\dagger c_{p-} c_{p+} c_{q-}^\dagger c_{q-} = \{c_{p+}^\dagger c_{p-}^\dagger c_{q-}^\dagger c_{q-} c_{p-} c_{p+}\} - \delta_{pq} c_{p+}^\dagger c_{p-}^\dagger c_{p+} c_{q-} \qquad (12)$$

$$c_{q-}^\dagger c_{q-} c_{p+}^\dagger c_{p-}^\dagger c_{p-} c_{p+} = \{c_{p+}^\dagger c_{p-}^\dagger c_{q-}^\dagger c_{q-} c_{p-} c_{p+}\} - \delta_{qp} c_{p+}^\dagger c_{q-}^\dagger c_{p+} c_{p-} \qquad (13)$$

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.

$$
\begin{aligned}
[\hat{P}, \hat{S}_z] =& \frac{1}{2}\sum_p \Big((c_{p+}^\dagger c_{p-}^\dagger c_{p-} c_{p+} + c_{p+}^\dagger c_{p-}^\dagger c_{p+} c_{p-}) - \\
& (c_{p+}^\dagger c_{p-}^\dagger c_{p-} c_{p+} + c_{p+}^\dagger c_{p-}^\dagger c_{p+} c_{p-})\Big) \qquad (14) \\
=& 0 \qquad (15)
\end{aligned}
$$

1D

$$[\hat{P}_p, \hat{P}_q^\dagger] = \hat{P}_p \hat{P}_q^\dagger - \hat{P}_q^\dagger \hat{P}_p \qquad (16)$$

Will only include terms which contribute, and we obtain

$$
\begin{aligned}
\hat{P}_p\hat{P}_q^\dagger &= \sum_{pq} c_{p-}c_{p+}c_{q+}^\dagger c_{q-}^\dagger \\
&= \{c_{q+}^\dagger c_{q-}^\dagger c_{p-}c_{p+}\} + \{c_{p-}c_{p+}c_{q+}^\dagger c_{q-}^\dagger\} + \{c_{p-}c_{p+}c_{q+}^\dagger c_{q-}^\dagger\} + \{c_{p-}c_{p+}c_{q+}^\dagger c_{q-}^\dagger\} \\
&= \{c_{q+}^\dagger c_{q-}^\dagger c_{p-}c_{p+}\} - \delta_{pq}c_{p+}c_{q+}^\dagger - \delta_{pq}c_{p-}c_{q-}^\dagger + \delta_{pq}\delta_{pq} \qquad (17)
\end{aligned}
$$

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:

$$\hat{P}_q^\dagger\hat{P}_p = \{c_{q+}^\dagger c_{q-}^\dagger c_{p-}c_{p+}\}. \qquad (18)$$

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. We set $p = q$, but not in the Dirac delta functions:

$$
\begin{aligned}
\hat{P}_p\hat{P}_q^\dagger - \hat{P}_q^\dagger\hat{P}_p &= -\delta_{pq}c_{q+}^\dagger c_{q+} - \delta_{pq}c_{q-}^\dagger c_{q-} + \delta_{pq}\delta_{qq} \\
&= \delta_{pq}(1 - c_{q+}^\dagger c_{q+} - c_{q-}^\dagger c_{q-}) \\
&= \delta_{pq}(1 - \hat{n}_q) \qquad (19)
\end{aligned}
$$

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) such that this happens. We have $N = 4$, thus

$$
\begin{aligned}
|\Phi\rangle &= c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger|-\rangle \qquad (20) \\
&= \hat{P}_1^\dagger\hat{P}_2^\dagger|-\rangle. \qquad (21)
\end{aligned}
$$

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

$$
\begin{aligned}
\hat{P} &= \sum_{p=1}^{M}\hat{P}_p^\dagger\hat{P}_p \qquad (22) \\
&= \hat{P}_1^\dagger\hat{P}_1 + \hat{P}_2^\dagger\hat{P}_2 + \hat{P}_3^\dagger\hat{P}_3 + \hat{P}_4^\dagger\hat{P}_4 \qquad (23)
\end{aligned}
$$

since $M = 4$.

$$
\begin{aligned}
\hat{P}|\Phi\rangle &= \Big(\hat{P}_1^\dagger\hat{P}_1\hat{P}_1^\dagger\hat{P}_2^\dagger + \hat{P}_2^\dagger\hat{P}_2\hat{P}_1^\dagger\hat{P}_2^\dagger + ...\Big)|-\rangle \qquad (24) \\
&= \Big(\delta_{11}\hat{P}_1^\dagger\hat{P}_2^\dagger + \delta_{22}\hat{P}_1^\dagger\hat{P}_2^\dagger\Big)|-\rangle \qquad (25) \\
&= 2|\Phi\rangle \qquad (26)
\end{aligned}
$$

where the two last terms in $\hat{P}$ do not contribute since $|\Phi\rangle$ does not contain creation operators with index 3 or 4. This computation was quite short since we could replace all operators with $\hat{P}$ which is not always the case, something we will see when calculating $\hat{S}_z|\Phi\rangle$.

$$
\begin{aligned}
\hat{S}_z =& \frac{1}{2}\sum_{p\sigma} \sigma c^\dagger_{p\sigma} c_{p\sigma} && (27)\\
=& \frac{1}{2}\Big(c^\dagger_{1+}c_{1+} - c^\dagger_{1-}c_{1-} + c^\dagger_{2+}c_{2+} - c^\dagger_{2-}c_{2-} + \\
& c^\dagger_{3+}c_{3+} - c^\dagger_{3-}c_{3-} + c^\dagger_{4+}c_{4+} - c^\dagger_{4-}c_{4-}\Big)|-\rangle && (28)
\end{aligned}
$$

$$
\begin{aligned}
\hat{S}_z|\Phi\rangle =& \frac{1}{2}\Big(c^\dagger_{1+}c_{1+}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-} - c^\dagger_{1-}c_{1-}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-} \\
& + c^\dagger_{2+}c_{2+}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-} - c^\dagger_{2-}c_{2-}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-}\Big)|-\rangle && (29)\\
=& \frac{1}{2}\Big(c^\dagger_{1+}c_{1+}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-} - c^\dagger_{1-}c_{1-}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-} \\
& + c^\dagger_{2+}c_{2+}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-} - c^\dagger_{2-}c_{2-}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-}\Big)|-\rangle && (30)\\
=& \frac{1}{2}\Big(\delta_{1+1+}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-} - \delta_{1-1-}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-} \\
& + \delta_{2+2+}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-} - \delta_{2-2-}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-}\Big)|-\rangle && (31)\\
=& \frac{1}{2}(1-1+1-1)|\Phi\rangle && (32)\\
=& 0|\Phi\rangle && (33)
\end{aligned}
$$

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

$$
n_M = \sum_{m=1}^{M-1} (M - m). \tag{34}
$$

1G

Need to figure out this

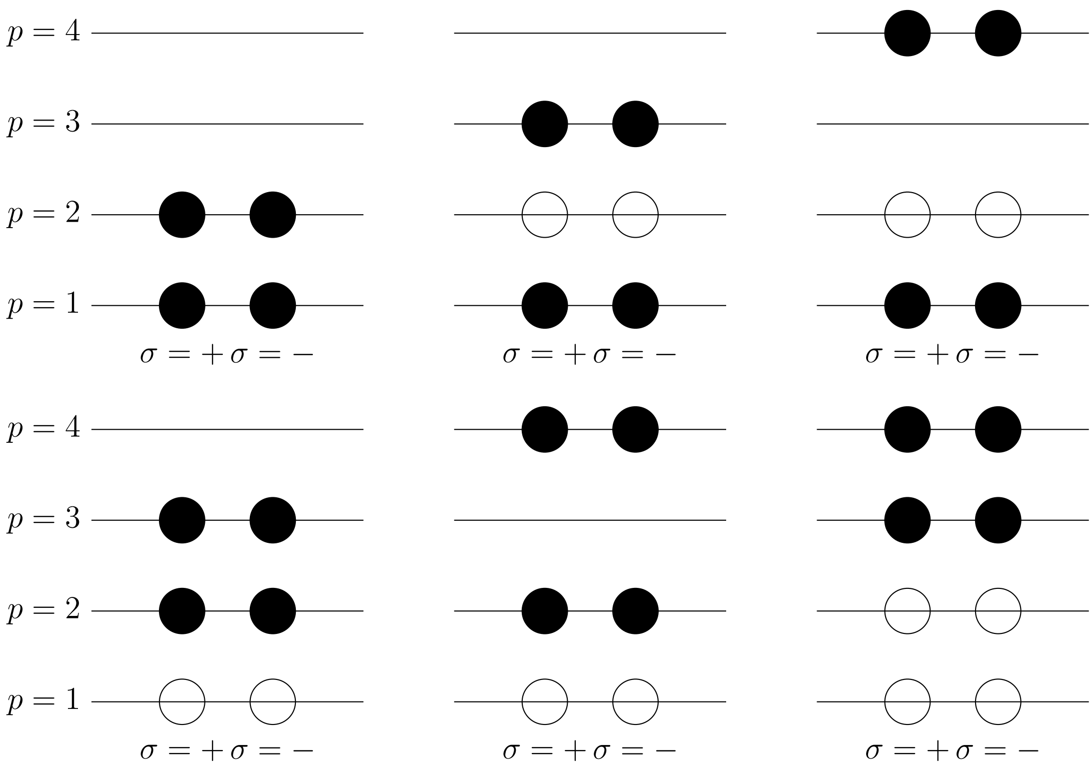

Figure 1: Need good caption here.

1H

$$\hat{H} = \hat{H}_0 + \hat{V} \tag{35}$$

We use equation ... and ..., and get

$$\begin{aligned}
\hat{V} &= -\frac{1}{2} g \sum_{pq} c^\dagger_{p+} c^\dagger_{p-} c_{q-} c_{q+} \\
&= -\frac{1}{2} g \sum_{p}^{M} c^\dagger_{p+} c^\dagger_{p-} \sum_{q}^{M} c_{q-} c_{q+} \\
&= -\frac{1}{2} g \left(\sum_{p=1}^{4} \hat{P}^\dagger_p \right) \left(\sum_{q=1}^{4} \hat{P}_q \right)
\end{aligned} \tag{36}$$

Similarly we get

$$\begin{aligned}
\hat{H}_0 &= \sum_{p\sigma} \varepsilon_p c^\dagger_{p\sigma} c_{p\sigma} \\
&= \sum_{p} (p-1) \sum_{\sigma} c^\dagger_{p\sigma} c_{p\sigma} \\
&= \sum_{p} (p-1) \hat{n}_p .
\end{aligned} \tag{37}$$

Thus we end up with

$$\hat{H} = \sum_{p} (p-1) \hat{n}_p - \frac{1}{2} g \left(\sum_{p=1}^{4} \hat{P}^\dagger_p \right) \left(\sum_{q=1}^{4} \hat{P}_q \right) \tag{38}$$

3 Configuration-Interaction (CI)

2A

$$\sum_{s} \hat{P}_s |p\bar{p}q\bar{q}\rangle = \sum_{s} \hat{P}_s \hat{P}^\dagger_p \hat{P}^\dagger_q |-\rangle \tag{39}$$

We use the result from exercise 1D (equation(19)) twice, and get

$$\begin{aligned}
\hat{P}_s \hat{P}^\dagger_p \hat{P}^\dagger_q =& \hat{P}^\dagger_p \hat{P}_s \hat{P}^\dagger_q + \delta_{sp}(1-\hat{n}_p)\hat{P}^\dagger_q \\
=& \hat{P}^\dagger_p \hat{P}^\dagger_q \hat{P}_s + \hat{P}^\dagger_p \delta_{sq}(1-\hat{n}_q) + \delta_{sp}(1-\hat{n}_p)\hat{P}^\dagger_q
\end{aligned} \tag{40}$$

Then insert back into equation (39):

$$
\begin{aligned}
&\sum_s (\hat{P}_p^\dagger \hat{P}_q^\dagger \hat{P}_s + \hat{P}_p^\dagger \delta_{sq}(1-\hat{n}_q) + \delta_{sp}(1-\hat{n}_p)\hat{P}_q^\dagger)|-\rangle \\
&= \sum_s (\hat{P}_p^\dagger \delta_{sq}(1-\hat{n}_q) + \delta_{sp}(1-\hat{n}_p)\hat{P}_q^\dagger)|-\rangle \\
&= \sum_s (\delta_{sq}\hat{P}_p^\dagger - \delta_{sq}\hat{P}_p^\dagger \hat{n}_q + \delta_{sp}\hat{P}_q^\dagger - \delta_{sp}\hat{n}_p\hat{P}_q^\dagger)|-\rangle \\
&= \sum_s (\delta_{sp}\hat{P}_p^\dagger + \delta_{sq}\hat{P}_q^\dagger)|-\rangle \\
&= (\hat{P}_p^\dagger + \hat{P}_q^\dagger)|-\rangle \\
&= |p\bar{p}\rangle + |q\bar{q}\rangle
\end{aligned}
\tag{41}
$$

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

$$
\langle p'\bar{p}'q'\bar{q}|\hat{H}|p\bar{p}q\bar{q}\rangle = \langle p'\bar{p}'q'\bar{q}|\hat{H}_0|p\bar{p}q\bar{q}\rangle + \langle p'\bar{p}'q'\bar{q}|\hat{V}|p\bar{p}q\bar{q}\rangle \tag{42}
$$

I will start with the first one:

$$
\hat{H}_0|p\bar{p}q\bar{q}\rangle = \sum_{r\sigma} \epsilon_r c_{r\sigma}^\dagger c_{r\sigma} c_{p+}^\dagger c_{p-}^\dagger c_{q+}^\dagger c_{q-}^\dagger|-\rangle \tag{43}
$$

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.

$$\begin{aligned}\hat{H}_0|p\bar{p}q\bar{q}\rangle =&\sum_{r\sigma}\epsilon_r\{c^\dagger_{r\sigma}c^\dagger_{p+}c^\dagger_{p-}c^\dagger_{q+}c^\dagger_{q-}c_{r\sigma}\}|-\rangle \\ &+\sum_{r\sigma}\epsilon_r\delta_{r\sigma p+}c^\dagger_{r\sigma}c^\dagger_{p-}c^\dagger_{q+}c^\dagger_{q-}|-\rangle \\ &-\sum_{r\sigma}\epsilon_r\delta_{r\sigma p-}c^\dagger_{r\sigma}c^\dagger_{p+}c^\dagger_{q+}c^\dagger_{q-}|-\rangle \\ &+\sum_{r\sigma}\epsilon_r\delta_{r\sigma q+}c^\dagger_{r\sigma}c^\dagger_{p+}c^\dagger_{p-}c^\dagger_{q-}|-\rangle \\ &-\sum_{r\sigma}\epsilon_r\delta_{r\sigma q-}c^\dagger_{r\sigma}c^\dagger_{p+}c^\dagger_{p-}c^\dagger_{q+}|-\rangle \qquad (44)\\ =&(\epsilon_p c^\dagger_{p+}c^\dagger_{p-}c^\dagger_{q+}c^\dagger_{q-}-\epsilon_p c^\dagger_{p-}c^\dagger_{p+}c^\dagger_{q+}c^\dagger_{q-} \\ &+\epsilon_q c^\dagger_{q+}c^\dagger_{p+}c^\dagger_{p-}c^\dagger_{q-}-\epsilon_q c^\dagger_{q-}c^\dagger_{p+}c^\dagger_{p-}c^\dagger_{q+})|-\rangle \qquad (45)\\ =&(\epsilon_p c^\dagger_{p+}c^\dagger_{p-}c^\dagger_{q+}c^\dagger_{q-}+\epsilon_p c^\dagger_{p+}c^\dagger_{p-}c^\dagger_{q+}c^\dagger_{q-} \\ &+\epsilon_q c^\dagger_{p+}c^\dagger_{p-}c^\dagger_{q+}c^\dagger_{q-}+\epsilon_q c^\dagger_{p+}c^\dagger_{p-}c^\dagger_{q+}c^\dagger_{q-})|-\rangle \qquad (46)\\ =&2(\epsilon_p+\epsilon_q)(\hat{P}^\dagger_p\hat{P}^\dagger_p)|-\rangle \qquad (47)\\ =&2(2-p-q)|p\bar{p}q\bar{q}\rangle \qquad (48)\end{aligned}$$

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

$$\langle p'\bar{p}'q'\bar{q}'|\hat{H}_0|p\bar{p}q\bar{q}\rangle = 2(2-p-q)\langle p'\bar{p}'q'\bar{q}'|p\bar{p}q\bar{q}\rangle \qquad (49)$$

So we still need to calculate the braket (Puh)

$$\langle p'\bar{p}'q'\bar{q}'|p\bar{p}q\bar{q}\rangle = \langle -|\hat{P}_{p'}\hat{P}_{q'}\hat{P}^\dagger_p\hat{P}^\dagger_q|-\rangle \qquad (50)$$

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.

$$\begin{aligned}\hat{P}_{p'}\hat{P}_{q'}\hat{P}^\dagger_p\hat{P}^\dagger_q &= \hat{P}_{p'}\hat{P}^\dagger_p\hat{P}_{q'}\hat{P}^\dagger_q+\delta_{q'p}\hat{P}_{p'}(1-\hat{n}_p)\hat{P}^\dagger_q \qquad (51)\\ &= \hat{P}_{p'}\hat{P}^\dagger_p\hat{P}_{q'}\hat{P}^\dagger_q+\delta_{q'p}\hat{P}_{p'}\hat{P}^\dagger_q+\delta_{q'p}\hat{P}_{p'}\hat{n}_p\hat{P}^\dagger_q \qquad (52)\end{aligned}$$

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

$$\begin{aligned}\delta_{q'p}\hat{P}_{p'}\hat{P}^\dagger_q &= \delta_{q'p}\hat{P}^\dagger_q\hat{P}_{p'}+\delta_{q'p}\delta_{p'q}+\delta_{q'p}\delta_{p'q}\hat{n}_q \qquad (53)\\ &= \delta_{q'p}\delta_{p'q} \qquad (54)\end{aligned}$$

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

$$\hat{P}_{p'}\hat{P}_p^\dagger\hat{P}_{q'}\hat{P}_q^\dagger = \hat{P}_{p'}\hat{P}_p^\dagger\hat{P}_q^\dagger\hat{P}_{q'} + \delta_{q'q}\hat{P}_{p'}\hat{P}_p^\dagger(1-\hat{n}_q) \tag{55}$$

$$= \delta_{q'q}\hat{P}_{p'}\hat{P}_p^\dagger \tag{56}$$

$$= \delta_{q'q}\delta_{p'p} - \delta_{q'q}\delta_{p'p}\hat{n}_q + \delta_{q'q}\hat{P}_p^\dagger\hat{P}_{p'} \tag{57}$$

$$= \delta_{q'q}\delta_{p'p} \tag{58}$$

So we obtain

$$\langle p'\bar{p}'q'\bar{q}'|p\bar{p}q\bar{q}\rangle = \delta_{q'p}\delta_{p'q} + \delta_{q'q}\delta_{p'p} \tag{59}$$

and

$$\langle p'\bar{p}'q'\bar{q}'|\hat{H}_0|p\bar{p}q\bar{q}\rangle = 2(2-p-q)(\delta_{q'p}\delta_{p'q} + \delta_{q'q}\delta_{p'p}). \tag{60}$$

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

$$\langle p'\bar{p}'q'\bar{q}|\hat{V}|p\bar{p}q\bar{q}\rangle = -\frac{1}{2}g\langle p'\bar{p}'q'\bar{q}|(\sum_r \hat{P}_r^\dagger)(\sum_s \hat{P}_s)|p\bar{p}q\bar{q}\rangle \tag{61}$$

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

$$\langle p'\bar{p}'q'\bar{q}'|\sum_r \hat{P}_r^\dagger = \langle p'\bar{p}'| + \langle q'\bar{q}'| \tag{62}$$

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

$$\langle p'\bar{p}'q'\bar{q}|\hat{V}|p\bar{p}q\bar{q}\rangle = -\frac{1}{2}g(\langle p'\bar{p}'|p\bar{p}\rangle + \langle p'\bar{p}'|q\bar{q}\rangle + \langle q'\bar{q}'|p\bar{p}\rangle + \langle q'\bar{q}'|q\bar{q}\rangle) \tag{63}$$

where the first one is

$$\langle p'\bar{p}'|p\bar{p}\rangle = \langle -|\hat{P}_{p'}\hat{P}_p^\dagger|-\rangle = \langle -|\hat{P}_p^\dagger\hat{P}_{p'} + \delta_{p'p}(1-\hat{n}_p)|-\rangle = \delta_{p'p} \tag{64}$$

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

$$\langle p'\bar{p}'q'\bar{q}|\hat{H}|p\bar{p}q\bar{q}\rangle = 2(2-p-q)(\delta_{q'p}\delta_{p'q} + \delta_{q'q}\delta_{p'p}) - \frac{1}{2}g(\delta_{p'p} + \delta_{p'q} + \delta_{q'p} + \delta_{q'q}) \tag{65}$$

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.

2B

In our case we get a matrix on the form

$$\begin{pmatrix} H_{12}^{12} & H_{12}^{13} & H_{12}^{14} & H_{12}^{23} & H_{12}^{24} & H_{12}^{34} \\ H_{13}^{12} & H_{13}^{13} & H_{13}^{14} & H_{13}^{23} & H_{13}^{24} & H_{13}^{34} \\ H_{14}^{12} & H_{14}^{13} & H_{14}^{14} & H_{14}^{23} & H_{14}^{24} & H_{14}^{34} \\ H_{23}^{12} & H_{23}^{13} & H_{23}^{14} & H_{23}^{23} & H_{23}^{24} & H_{23}^{34} \\ H_{24}^{12} & H_{24}^{13} & H_{24}^{14} & H_{24}^{23} & H_{24}^{24} & H_{24}^{34} \\ H_{34}^{12} & H_{34}^{13} & H_{34}^{14} & H_{34}^{23} & H_{34}^{24} & H_{34}^{34} \end{pmatrix} \tag{66}$$

where

$$H_{12}^{34} = \langle 12|\hat{H}|34\rangle = 2(2-3-4)(0+0) - \frac{1}{2}g(0+0+0+0) = 0 \tag{67}$$

etc.. Calculate all elements, and get

$$\langle p'\bar{p}'q'\bar{q}|\hat{H}|p\bar{p}q\bar{q}\rangle = \begin{pmatrix} -2-g & -1/2g & -1/2g & -1/2g & -1/2g & 0 \\ -1/2g & -4-g & -1/2g & -1/2g & 0 & -1/2g \\ -1/2g & -1/2g & -6-g & 0 & -1/2g & -1/2g \\ -1/2g & -1/2g & 0 & -6-g & -1/2g & -1/2g \\ -1/2g & 0 & -1/2g & -1/2g & -8-g & -1/2g \\ 0 & -1/2g & -1/2g & -1/2g & -1/2g & -10-g \end{pmatrix}. \tag{68}$$

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 (2).

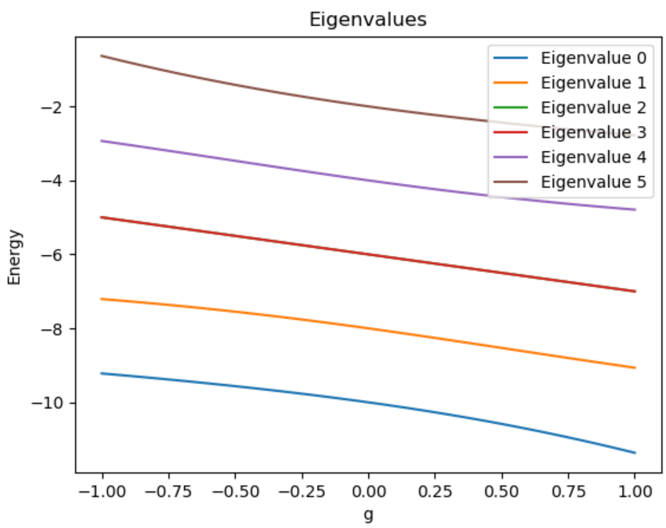

Figure 2: NEED CAPTION

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

2D

2E

4 Coupled-Cluster (CC)

3A

Just write down the expressions

3B

...

3C

$$\langle\Phi|\hat{H}(1+\hat{T})|\Phi\rangle = \langle\Phi|\hat{H}|\Phi\rangle + \langle\Phi|\hat{H}\hat{T}|\Phi\rangle \tag{69}$$

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

$$\langle\Phi|\hat{H}|\Phi\rangle = 2\epsilon_p + 2\epsilon_q \tag{70}$$

Furthermore the second term

5 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:

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


g_list = np.linspace(-1, 1, 100)
eigenvalues = []

for g in g_list:
    M = 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.append((np.linalg.eigh(M)[0]))

for k in range(M.shape[0]):
    new_list = []
    for i in range(len(eigenvalues)):
        new_list.append(eigenvalues[i][k])
    plt.plot(g_list, new_list, label='Eigenvalue {}'.format
        ↪ (k))
plt.legend(loc='best')
plt.title('Eigenvalues')
plt.xlabel('g')
plt.ylabel('Energy')
plt.savefig('eigenvalues.png')
plt.show()
```