UiO : Department of Chemistry
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FYS4480: Quantum mechanics for many-particle systems

Second Midterm

Ensemble of Energy Approximating Methods Performed on the Pairing Model

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1 Model

"We present a simplified Hamiltonian consisting of an unperturbed Hamiltonian and a so-called pairing interaction term. It is a model which to a large extent mimicks some central features of atomic nuclei, certain atoms and systems which exhibit superfluidity or superconductivity. To study this system, we will use a mix of many-body perturbation theory (MBPT), Hartree-Fock (HF) theory and full configuration interaction (FCI) theory. The latter will also provide us with the exact answer. When setting up the Hamiltonian matrix you will need to solve an eigenvalue problem.
We define first the Hamiltonian, with a definition of the model space and the single-particle basis.
The Hamiltonian acting in the comple Hilbert space (usually infinite dimensional) consists of an unperturbed one-body part, $\hat{H}_0$, and a perturbation $\hat{V}$.
We limit ourselves to at most two-body interactions, our Hamiltonian is then represented by the following operators

$$\hat{H} = \sum_{\alpha\beta} \langle\alpha|\, \hat{h}_0 \,|\beta\rangle\, \hat{a}^\dagger_\alpha\, \hat{a}_\beta + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle\alpha\beta|\, \hat{V} \,|\gamma\delta\rangle\, \hat{a}^\dagger_\alpha\, \hat{a}^\dagger_\beta\, \hat{a}_\delta\, \hat{a}_\gamma,$$

where $\hat{a}^\dagger_\alpha$ and $\hat{a}_\alpha$ etc. are standard fermion creation and annihilation operators, respectively, and $\alpha\beta\gamma\delta$ represent all possible single-particle quantum numbers. The full single-particle space is defined by the completeness relation $\hat{\mathbf{1}} = \sum_{\alpha=1}^{\infty} |\alpha\rangle\langle\alpha|$. In our calculations we will let the single-particle states $|\alpha\rangle$ be eigenfunctions of the one-particle operator $\hat{h}_0$. Note that the two-body part of the Hamiltonian contains anti-symmetrized matrix elements.
The above Hamiltonian acts in turn on various many-body Slater determinants constructed from the single-basis defined by the one-body operator $\hat{h}_0$. As an example, the two-particle model space $\mathscr{P}$ is defined by an operator

$$\hat{P} = \sum_{\alpha\beta=1}^{m} |\alpha\beta\rangle\langle\alpha\beta|\,,$$

where we assume that $m = \dim(\mathscr{P})$ and the full space is defined by

$$\hat{P} + \hat{Q} = \hat{\mathbf{1}},$$

with the projection operator

$$\hat{Q} = \sum_{\alpha\beta=m+1}^{\infty} |\alpha\beta\rangle\langle\alpha\beta|\,,$$

being the complement of $\hat{P}$.
Our specific model consists of N doubly-degenerate and equally spaced single-particle levels labelled by $p = 1, 2, \ldots$ and spin $\sigma = \pm 1$. These states are schematically portrayed in . The first two single-particle levels define a possible model space, indicated by the label $\mathscr{P}$. The remaining states span the excluded space $\mathscr{Q}$.
We write the Hamiltonian as

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

where

$$\hat{H}_0 = \xi \sum_{p\sigma} (p-1)\, \hat{a}^\dagger_{p\sigma}\, \hat{a}_{p\sigma}$$

and

$$\hat{V} = -\frac{1}{2} g \sum_{pq} \hat{a}^\dagger_{p+}\, \hat{a}^\dagger_{p-}\, \hat{a}_{q-}\, \hat{a}_{q+}.$$

Here, $\hat{H}_0$ is the unperturbed Hamiltonian with a spacing between successive single-particle states given by ξ, which we will set to a constant value $\xi = 1$ without loss of generality. The two-body operator $\hat{V}$ has one term only. It represents the pairing contribution and carries a constant strength g.
The indices $\sigma = \pm$ represent the two possible spin values. The interaction can only couple pairs and excites therefore only two particles at the time.
In our model we have kept both the interaction strength and the single-particle level as constants. In a realistic system like an atom or the atomic nucleus this is not the case."-This is directly copied from (Hjorth-Jensen, 2022).

1.1 Hamiltonian and commutation relations

Here we will focus on total spin $S = 0$, and therefore some simplifications are in order. We first define the pair creation and annihilation operators

$$\hat{P}_p^+ := \hat{a}_{p+}^\dagger \, \hat{a}_{p-}^\dagger,$$
$$\hat{P}_p^- := \hat{a}_{p-} \, \hat{a}_{p+},$$

and an operator, $\hat{N}_p$, that counts the number of fermions in the pth energy level,

$$\hat{N}_p = \sum_{\sigma=\pm} \hat{a}_{p\sigma}^\dagger \, \hat{a}_{p\sigma}.$$

The commutation relations between the pair creation and pair annihilation operator is

$$\begin{aligned}
\left[\hat{P}_p^+, \hat{P}_q^-\right] &= \hat{P}_p^+ \, \hat{P}_q^- - \hat{P}_q^- \, \hat{P}_p^+ \\
&= \hat{a}_{p+}^\dagger \, \hat{a}_{p-}^\dagger \, \hat{a}_{q-} \, \hat{a}_{q+} - \hat{a}_{q-} \, \hat{a}_{q+} \, \hat{a}_{p+}^\dagger \, \hat{a}_{p-}^\dagger \\
&= \hat{a}_{p+}^\dagger \, \hat{a}_{p-}^\dagger \, \hat{a}_{q-} \, \hat{a}_{q+} - \hat{a}_{q-} \left(\delta_{pq} - \hat{a}_{p+}^\dagger \, \hat{a}_{q+}\right) \hat{a}_{p-}^\dagger \\
&= \hat{a}_{p+}^\dagger \, \hat{a}_{p-}^\dagger \, \hat{a}_{q-} \, \hat{a}_{q+} - \delta_{pq} \, \hat{a}_{q-} \, \hat{a}_{p-}^\dagger - \hat{a}_{p+}^\dagger \, \hat{a}_{q-} \, \hat{a}_{q+} \, \hat{a}_{p-}^\dagger \\
&= \hat{a}_{p+}^\dagger \, \hat{a}_{p-}^\dagger \, \hat{a}_{q-} \, \hat{a}_{q+} - \delta_{pq} \, \hat{a}_{q-} \, \hat{a}_{p-}^\dagger + \hat{a}_{p+}^\dagger \, \hat{a}_{q-} \, \hat{a}_{p-}^\dagger \, \hat{a}_{q+} \\
&= \hat{a}_{p+}^\dagger \, \hat{a}_{p-}^\dagger \, \hat{a}_{q-} \, \hat{a}_{q+} - \delta_{pq} \, \hat{a}_{q-} \, \hat{a}_{p-}^\dagger + \hat{a}_{p+}^\dagger \left(\delta_{pq} - \hat{a}_{p-}^\dagger \, \hat{a}_{q-}\right) \hat{a}_{q+} \\
&= -\delta_{pq} \, \hat{a}_{q-} \, \hat{a}_{p-}^\dagger + \delta_{pq} \, \hat{a}_{p+}^\dagger \, \hat{a}_{p+} \\
&= -\hat{a}_{p-} \, \hat{a}_{p-}^\dagger + \hat{a}_{p+}^\dagger \, \hat{a}_{p+} \\
&= \delta_{pq}\left(-\left(1 - \hat{a}_{p-}^\dagger \, \hat{a}_{p-}\right) + \hat{a}_{p+}^\dagger \, \hat{a}_{p+}\right) \\
&= \delta_{pq}(\hat{N}_p - 1).
\end{aligned}$$

We have then the commutation relations between the pair creation and annihilation operators, summarized as

$$\left[\hat{P}_p^+, \hat{P}_q^-\right] = \delta_{pq}(\hat{N}_p - 1),$$
$$\left[\hat{P}_q^-, \hat{P}_p^+\right] = \delta_{pq}(1 - \hat{N}_p).$$

The commutation relations between the pair creation and annihilation operators and the counting operator, $\left[\hat{P}_p^+, \hat{N}_q\right]$ and $\left[\hat{P}_p^-, \hat{N}_q\right]$, will be very useful. The commutation relation

between the pair creation and counting operator becomes

$$\begin{aligned}
\Big[\hat{P}^+_p, \hat{N}_q\Big] &= \hat{P}^+_p\,\hat{N}_q - \hat{N}_q\,\hat{P}^+_p \\
&= \hat{a}^\dagger_{p+}\,\hat{a}^\dagger_{p-}\Big(\hat{a}^\dagger_{q+}\,\hat{a}_{q+} + \hat{a}^\dagger_{q-}\,\hat{a}_{q-}\Big) - \Big(\hat{a}^\dagger_{q+}\,\hat{a}_{q+} + \hat{a}^\dagger_{q-}\,\hat{a}_{q-}\Big)\,\hat{a}^\dagger_{p+}\,\hat{a}^\dagger_{p-} \\
&= \hat{a}^\dagger_{p+}\,\hat{a}^\dagger_{p-}\Big(\hat{a}^\dagger_{q+}\,\hat{a}_{q+} + \hat{a}^\dagger_{q-}\,\hat{a}_{q-}\Big) - \Big(\hat{a}^\dagger_{q+}\Big(\delta_{pq} - \hat{a}^\dagger_{p+}\,\hat{a}_{q+}\Big) - \hat{a}^\dagger_{q-}\,\hat{a}^\dagger_{p+}\,\hat{a}_{q-}\Big)\,\hat{a}^\dagger_{p-} \\
&= \hat{a}^\dagger_{p+}\,\hat{a}^\dagger_{p-}\Big(\hat{a}^\dagger_{q+}\,\hat{a}_{q+} + \hat{a}^\dagger_{q-}\,\hat{a}_{q-}\Big) - \delta_{pq}\,\hat{a}^\dagger_{q+}\,\hat{a}^\dagger_{p-} - \Big(\hat{a}^\dagger_{p+}\,\hat{a}^\dagger_{q+}\,\hat{a}_{q+} + \hat{a}^\dagger_{p+}\,\hat{a}^\dagger_{q-}\,\hat{a}_{q-}\Big)\,\hat{a}^\dagger_{p-} \\
&= \hat{a}^\dagger_{p+}\,\hat{a}^\dagger_{p-}\Big(\hat{a}^\dagger_{q+}\,\hat{a}_{q+} + \hat{a}^\dagger_{q-}\,\hat{a}_{q-}\Big) - \delta_{pq}\,\hat{a}^\dagger_{q+}\,\hat{a}^\dagger_{p-} - \Big(-\,\hat{a}^\dagger_{p+}\,\hat{a}^\dagger_{q+}\,\hat{a}^\dagger_{p-}\,\hat{a}_{q+} + \hat{a}^\dagger_{p+}\,\hat{a}^\dagger_{q-}\Big(\delta_{pq} - \hat{a}^\dagger_{p-}\,\hat{a}_{q-}\Big)\Big), \\
&= \hat{a}^\dagger_{p+}\,\hat{a}^\dagger_{p-}\Big(\hat{a}^\dagger_{q+}\,\hat{a}_{q+} + \hat{a}^\dagger_{q-}\,\hat{a}_{q-}\Big) - \delta_{pq}\,\hat{a}^\dagger_{q+}\,\hat{a}^\dagger_{p-} - \delta_{pq}\,\hat{a}^\dagger_{p+}\,\hat{a}^\dagger_{q-} \\
&\quad - \Big(-\,\hat{a}^\dagger_{p+}\,\hat{a}^\dagger_{q+}\,\hat{a}^\dagger_{p-}\,\hat{a}_{q+} - \hat{a}^\dagger_{p+}\,\hat{a}^\dagger_{q-}\,\hat{a}^\dagger_{p-}\,\hat{a}_{q-}\Big) \\
&= \hat{a}^\dagger_{p+}\,\hat{a}^\dagger_{p-}\Big(\hat{a}^\dagger_{q+}\,\hat{a}_{q+} + \hat{a}^\dagger_{q-}\,\hat{a}_{q-}\Big) - \delta_{pq}\,\hat{a}^\dagger_{q+}\,\hat{a}^\dagger_{p-} - \delta_{pq}\,\hat{a}^\dagger_{p+}\,\hat{a}^\dagger_{q-} \\
&\quad - \Big(\hat{a}^\dagger_{p+}\,\hat{a}^\dagger_{p-}\,\hat{a}^\dagger_{q+}\,\hat{a}_{q+} - \hat{a}^\dagger_{p+}\,\hat{a}^\dagger_{p-}\,\hat{a}^\dagger_{q-}\,\hat{a}_{q-}\Big) \\
&= \hat{a}^\dagger_{p+}\,\hat{a}^\dagger_{p-}\Big(\hat{a}^\dagger_{q+}\,\hat{a}_{q+} + \hat{a}^\dagger_{q-}\,\hat{a}_{q-}\Big) - \delta_{pq}\,\hat{a}^\dagger_{q+}\,\hat{a}^\dagger_{p-} - \delta_{pq}\,\hat{a}^\dagger_{p+}\,\hat{a}^\dagger_{q-} \\
&\quad - \hat{a}^\dagger_{p+}\,\hat{a}^\dagger_{p-}\Big(\hat{a}^\dagger_{q+}\,\hat{a}_{q+} - \hat{a}^\dagger_{q-}\,\hat{a}_{q-}\Big) \\
&= -\,\delta_{pq}\,\hat{a}^\dagger_{q+}\,\hat{a}^\dagger_{p-} - \delta_{pq}\,\hat{a}^\dagger_{p+}\,\hat{a}^\dagger_{q-} \\
&= -\,2\delta_{pq}\,\hat{P}^+_p,
\end{aligned}$$

and using the same procedure, it is easy to find that $\Big[\hat{P}^-_p, \hat{N}_q\Big] = 2\delta_{pq}\,\hat{P}^-_p$. Summarized, we have found the commutation relations between the pair creation and annihilation operators with the counting operator to be

$$\begin{aligned}
\Big[\hat{P}^+_p, \hat{N}_q\Big] &= -\Big[\hat{N}_q, \hat{P}^+_p\Big] = -\,2\delta_{pq}\,\hat{P}^+_q, \\
\Big[\hat{P}^-_p, \hat{N}_q\Big] &= -\Big[\hat{N}_q, \hat{P}^-_p\Big] = 2\delta_{pq}\,\hat{P}^-_q.
\end{aligned}$$

We also define the spin projections

$$\begin{aligned}
\hat{S}_z &:= \frac{1}{2}\sum_{p\sigma} \sigma\,\hat{a}^\dagger_{p\sigma}\,\hat{a}_{p\sigma}, \\
\hat{S}_+ &:= \sum_p \hat{a}^\dagger_{p+}\,\hat{a}_{p-}, \\
\hat{S}_- &:= \sum_p \hat{a}^\dagger_{p-}\,\hat{a}_{p+},
\end{aligned}$$

and the total spin operator

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

Remember that in our model we only have pairs of spins, and we can therefore rewrite the Hamiltonian slightly. The unperturbed part,

$$\hat{H}_0 = \xi\sum_p \Big((p-1)\,\hat{a}^\dagger_{p+}\,\hat{a}_{p+} + (p-1)\,\hat{a}^\dagger_{p-}\,\hat{a}_{p-}\Big),$$

can stay the same. The two-body operator $\hat{V}$ can be rewritten

$$\begin{aligned}
\hat{V} &= -\frac{g}{2}\sum_{pq} \hat{a}^\dagger_{p+}\,\hat{a}^\dagger_{p-}\,\hat{a}_{q-}\,\hat{a}_{q+} \\
&= -\frac{g}{2}\sum_{pq} \hat{P}^+_p\,\hat{P}^-_q,
\end{aligned}$$

where it becomes a one-body operator in a basis of pairs. Since we know that there are no broken pairs, we can rewrite the Hamiltonian further, to be

$$\hat{H} = \hat{H}_{\text{pair}} + \hat{V},$$

where we have defined a new operator, a pairwise single-particle energy operator,

$$\hat{H}_{\text{pair}} = 2\xi \sum_p (p-1)\, \hat{P}_p^+ \, \hat{P}_p^-.$$

In this latest rewriting of the Hamiltonian, we have shifted our basis space from covering single-particle states, to coupled-particles states. The full Hamiltonian in the pairwise basis set becomes

$$\hat{H} = 2\xi \sum_p (p-1)\, \hat{N}_p^- - \frac{g}{2} \sum_{pq} \hat{P}_p^+ \, \hat{P}_q^-.$$

This Hamiltonian is not in general the same as our original Hamiltonian, as the unperturbed part of the Hamiltonian only counts the energies if the fermions come in pairs. For our model this will be equivalent, as all fermions must be paired.
Intuitively, we can see that the pair creation and annihilation operators must commute with the spin projection operators, because if we try to add two particles to a fermion state (degeneracy is two) that already contains a particle (has spin$\neq 0$), the state becomes zero. The same logic tells us that the pair annihilation operators also should commute. The idea can be illustrated as

$$\hat{P}_p^+ \, \hat{a}_{p-}^\dagger \, |0\rangle = 0,$$
$$\hat{P}_p^- \, \hat{a}_{p-}^\dagger \, |0\rangle = 0.$$

However, to be able to block-diagonalize the matrix, we need to show that the spin projection $\hat{S}_z$ and the total spin $\hat{S}^2$ commutes with the Hamiltonian,

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

Since the Hamiltonian, in this specific case, with total spin $S = 0$, can be written in terms of pair creation and annihilation operators, we only need to show that these commute with the spin operators. We start with

$$\begin{aligned}\left[\hat{P}_q^+, \hat{S}_+\right] &= \hat{a}_{q+}^\dagger \left[\hat{a}_{q-}^\dagger, \sum_p \hat{a}_{p+}^\dagger \, \hat{a}_{p-}\right] + \left[\hat{a}_{q+}^\dagger, \sum_p \hat{a}_{p+}^\dagger \, \hat{a}_{p-}\right] \hat{a}_{q-}^\dagger, \\ &= \sum_p \left(\hat{a}_{q+}^\dagger \, \hat{a}_{p+}^\dagger \left[\hat{a}_{q-}^\dagger, \hat{a}_{p-}\right] + \hat{a}_{q+}^\dagger \left[\hat{a}_{q-}^\dagger, \hat{a}_{p+}^\dagger\right] \hat{a}_{p-} + \hat{a}_{p+}^\dagger \left[\hat{a}_{q+}^\dagger, \hat{a}_{p-}\right] \hat{a}_{q-} + \left[\hat{a}_{q+}^\dagger, \hat{a}_{p+}^\dagger\right] \hat{a}_{p-} \, \hat{a}_{q-}\right)\end{aligned}$$

where the only commutator terms that does not become zero are the ones where $p = q$, and we have

$$\begin{aligned}\left[\hat{P}_q^+, \hat{S}_+\right] &= \hat{a}_{q+}^\dagger \, \hat{a}_{q+}^\dagger \left[\hat{a}_{q-}^\dagger, \hat{a}_{q-}\right] + \hat{a}_{q+}^\dagger \left[\hat{a}_{q-}^\dagger, \hat{a}_{q+}^\dagger\right] \hat{a}_{q-} + \hat{a}_{q+}^\dagger \left[\hat{a}_{q+}^\dagger, \hat{a}_{q-}\right] \hat{a}_{q-} + \left[\hat{a}_{q+}^\dagger, \hat{a}_{q+}^\dagger\right] \hat{a}_{q-} \, \hat{a}_{q-} \\ &= \hat{a}_{q+}^\dagger \, \hat{a}_{q+}^\dagger + 0 + 0 + 0 \\ &= 0.\end{aligned}$$

We calculate $\left[\hat{P}_p^+, \hat{S}_-\right]$ in a similar fashion,

$$\begin{aligned}
\left[\hat{P}_q^+, \hat{S}_-\right] =& \hat{a}_{q+}^\dagger \left[\hat{a}_{q-}^\dagger, \sum_p \hat{a}_{p-}^\dagger \hat{a}_{p+}\right] + \left[\hat{a}_{q+}^\dagger, \sum_p \hat{a}_{p-}^\dagger \hat{a}_{p+}\right] \hat{a}_{q-}^\dagger \\
=& \sum_p \left(\hat{a}_{q+}^\dagger \hat{a}_{p-}^\dagger \left[\hat{a}_{q-}^\dagger, \hat{a}_{p+}\right] + \hat{a}_{q+}^\dagger \left[\hat{a}_{q-}^\dagger, \hat{a}_{p+}^\dagger\right] \hat{a}_{p-} + \hat{a}_{p-}^\dagger \left[\hat{a}_{q+}^\dagger, \hat{a}_{p+}\right] \hat{a}_{q-}^\dagger + \left[\hat{a}_{q-}^\dagger, \hat{a}_{p-}^\dagger\right] \hat{a}_{p+} \hat{a}_{q-}\right) \\
=& \hat{a}_{q-}^\dagger \hat{a}_{q-}^\dagger \\
=& 0.
\end{aligned}$$

This means that the pair creation operator commutes with $\hat{S}_-$ and $\hat{S}_+$, and by very similar calculations we find that the pair annihilation operators also commute. We need to look at $\left[\hat{P}_q^+, \hat{S}_z\right]$ and $\left[\hat{P}_q^-, \hat{S}_z\right]$ before we revisit the Hamiltonian. The commutator between the pair creation operator and projection operator $\hat{S}_z$ becomes

$$\begin{aligned}
\left[\hat{P}_q^+, \hat{S}_z\right] =& \hat{a}_{q+}^\dagger \left[\hat{a}_{q-}^\dagger, \sum_{p\sigma} \sigma\, \hat{a}_{p\sigma}^\dagger \hat{a}_{p\sigma}\right] + \left[\hat{a}_{q+}^\dagger, \sum_{p\sigma} \sigma\, \hat{a}_{p\sigma}^\dagger \hat{a}_{p\sigma}\right] \hat{a}_{q-}^\dagger \\
=& \sum_{p\sigma} \sigma \Big(\hat{a}_{q+}^\dagger \hat{a}_{p\sigma}^\dagger \left[\hat{a}_{q-}^\dagger, \hat{a}_{p\sigma}\right] + \hat{a}_{q+}^\dagger \left[\hat{a}_{q-}^\dagger, \hat{a}_{p\sigma}^\dagger\right] \hat{a}_{p\sigma} + \hat{a}_{p\sigma}^\dagger \left[\hat{a}_{q+}^\dagger, \hat{a}_{p\sigma}\right] \hat{a}_{q-}^\dagger + \left[\hat{a}_{q+}^\dagger, \hat{a}_{p\sigma}^\dagger\right] \hat{a}_{p\sigma}\, \hat{a}_{q-}^\dagger\Big) \\
=& \sum_{p\sigma} \sigma \Big(\hat{a}_{q+}^\dagger \hat{a}_{p\sigma}^\dagger \delta_{qp}\delta_{-\sigma} + 0 + \hat{a}_{p\sigma}^\dagger \delta_{qp}\delta_{+\sigma}\, \hat{a}_{q-}^\dagger + 0\Big) \\
=& -\hat{a}_{q+}^\dagger \hat{a}_{q-}^\dagger + \hat{a}_{q+}^\dagger \hat{a}_{q-}^\dagger \\
=& 0,
\end{aligned}$$

and the commutator between the pair annihilation operator and projection operator $\hat{S}_z$ becomes

$$\begin{aligned}
\left[\hat{P}_q^-, \hat{S}_z\right] =& \sum_{p\sigma} \sigma \Big(\hat{a}_{q-} \left[\hat{a}_{q+}, \hat{a}_{p\sigma}^\dagger \hat{a}_{p\sigma}\right] + \left[\hat{a}_{q-}, \hat{a}_{p\sigma}^\dagger \hat{a}_{p\sigma}\right] \hat{a}_{q+}\Big) \\
=& \sum_{p\sigma} \sigma \Big(\hat{a}_{q-} \hat{a}_{p\sigma}^\dagger [\hat{a}_{q+}, \hat{a}_{p\sigma}] + \hat{a}_{q-} \left[\hat{a}_{q+}, \hat{a}_{p\sigma}^\dagger\right] \hat{a}_{p\sigma} + \hat{a}_{p\sigma}^\dagger [\hat{a}_{q-}, \hat{a}_{p\sigma}]\, \hat{a}_{q+} + \left[\hat{a}_{q-}, \hat{a}_{p\sigma}^\dagger\right] \hat{a}_{p\sigma}\, \hat{a}_{q+}\Big) \\
=& -\hat{a}_{q-} \hat{a}_{q+} + \hat{a}_{q-} \hat{a}_{q+} \\
=& 0.
\end{aligned}$$

The spin projection operators and the pair creation and annihilation operators all commute,

$$\left[\hat{P}_q^+, \hat{S}_\pm\right] = \left[\hat{P}_q^-, \hat{S}_\pm\right] = \left[\hat{P}_q^\pm, \hat{S}_z\right] = 0.$$

The commutation relation between the Hamiltonian and the spin projection can be rewritten as

$$\begin{aligned}
[\hat{H}, \hat{S}_z] =& \left[2\xi \sum_p (p-1)\, \hat{P}_p^+ \hat{P}_p^- - \frac{g}{2} \sum_{pq} \hat{P}_p^+ \hat{P}_q^-, \hat{S}_z\right] \\
=& 2\xi \sum_p (p-1) \left[\hat{P}_p^+ \hat{P}_p^-, \hat{S}_z\right] - \frac{g}{2} \sum_{pq} \left[\hat{P}_p^+ \hat{P}_q^-, \hat{S}_z\right] \\
=& 2\xi \sum_p (p-1) \Big(\hat{P}_p^+ \left[\hat{P}_q^-, \hat{S}_z\right] + \left[\hat{P}_p^+, \hat{S}_z\right] \hat{P}_q^-\Big) - \frac{g}{2} \sum_{pq} \Big(\hat{P}_p^+ \left[\hat{P}_q^-, \hat{S}_z\right] + \left[\hat{P}_p^+, \hat{S}_z\right] \hat{P}_q^-\Big)
\end{aligned}$$

and we know that $\left[\hat{P}_p^\pm, \hat{S}_z\right] = 0$, which tells us that the Hamiltonian and the spin projection operator, $\hat{S}_z$, in fact commute.

The commutation relation between the total spin operator and the Hamiltonian can be written as

$$\begin{aligned}
\Big[\hat{H},\hat{S}^2\Big] =& \Big[2\xi\sum_p (p-1)\,\hat{P}_p^+\,\hat{P}_p^- - \frac{g}{2}\sum_{pq}\hat{P}_p^+\,\hat{P}_q^-, \hat{S}_z^2 + \frac{1}{2}(\hat{S}_+\,\hat{S}_- + \hat{S}_-\,\hat{S}_+)\Big] \\
=& 2\xi\sum_p (p-1)\Big(\Big[\hat{P}_p^+\,\hat{P}_p^-,\hat{S}_z^2\Big] + \frac{1}{2}\Big[\hat{P}_p^+\,\hat{P}_p^-,\hat{S}_+\,\hat{S}_-\Big] + \frac{1}{2}\Big[\hat{P}_p^+\,\hat{P}_p^-,\hat{S}_-\,\hat{S}_+\Big]\Big) \\
&- \frac{g}{2}\sum_{pq}\Big(\Big[\hat{P}_p^+\,\hat{P}_q^-,\hat{S}_z^2\Big] + \frac{1}{2}\Big[\hat{P}_p^+\,\hat{P}_q^-,\hat{S}_+\,\hat{S}_-\Big] + \frac{1}{2}\Big[\hat{P}_p^+\,\hat{P}_q^-,\hat{S}_-\,\hat{S}_+\Big]\Big) \\
=& 2\xi\sum_p (p-1)\Big(\hat{P}_p^+\,\hat{S}_z\Big[\hat{P}_p^-,\hat{S}_z\Big] + \hat{P}_p^+\Big[\hat{P}_p^-,\hat{S}_z\Big]\,\hat{S}_z + \Big[\hat{P}_p^+,\hat{S}_z\Big]\,\hat{P}_p^-\,\hat{S}_z + \hat{S}_z\Big[\hat{P}_p^+,\hat{S}_z\Big]\,\hat{P}_p^-\Big) \\
&+ \xi\sum_p (p-1)\Big(\hat{P}_p^+\,\hat{S}_+\Big[\hat{P}_p^-,\hat{S}_-\Big] + \hat{P}_p^+\Big[\hat{P}_p^-,\hat{S}_+\Big]\,\hat{S}_- + \Big[\hat{P}_p^+,\hat{S}_+\Big]\,\hat{P}_p^-\,\hat{S}_- + \hat{S}_+\Big[\hat{P}_p^+,\hat{S}_-\Big]\,\hat{P}_p^-\Big) \\
&+ \xi\sum_p (p-1)\Big(\hat{P}_p^+\,\hat{S}_-\Big[\hat{P}_p^-,\hat{S}_+\Big] + \hat{P}_p^+\Big[\hat{P}_p^-,\hat{S}_-\Big]\,\hat{S}_+ + \Big[\hat{P}_p^+,\hat{S}_-\Big]\,\hat{P}_p^-\,\hat{S}_+ + \hat{S}_-\Big[\hat{P}_p^+,\hat{S}_+\Big]\,\hat{P}_p^-\Big) \\
&- \frac{g}{2}\sum_{pq}\Big(\hat{P}_p^+\,\hat{S}_z\Big[\hat{P}_q^-,\hat{S}_z\Big] + \hat{P}_p^+\Big[\hat{P}_q^-,\hat{S}_z\Big]\,\hat{S}_z + \Big[\hat{P}_p^+,\hat{S}_z\Big]\,\hat{P}_q^-\,\hat{S}_z + \hat{S}_z\Big[\hat{P}_p^+,\hat{S}_z\Big]\,\hat{P}_q^-\Big) \\
&- \frac{g}{4}\sum_{pq}\Big(\hat{P}_p^+\,\hat{S}_+\Big[\hat{P}_q^-,\hat{S}_-\Big] + \hat{P}_p^+\Big[\hat{P}_q^-,\hat{S}_+\Big]\,\hat{S}_- + \Big[\hat{P}_p^+,\hat{S}_+\Big]\,\hat{P}_q^-\,\hat{S}_- + \hat{S}_+\Big[\hat{P}_p^+,\hat{S}_-\Big]\,\hat{P}_q^-\Big) \\
&- \frac{g}{4}\sum_{pq}\Big(\hat{P}_p^+\,\hat{S}_-\Big[\hat{P}_q^-,\hat{S}_+\Big] + \hat{P}_p^+\Big[\hat{P}_q^-,\hat{S}_-\Big]\,\hat{S}_+ + \Big[\hat{P}_p^+,\hat{S}_-\Big]\,\hat{P}_q^-\,\hat{S}_+ + \hat{S}_-\Big[\hat{P}_p^+,\hat{S}_+\Big]\,\hat{P}_q^-\Big),
\end{aligned}$$

where all commutation relations in this expression becomes 0, and we have

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

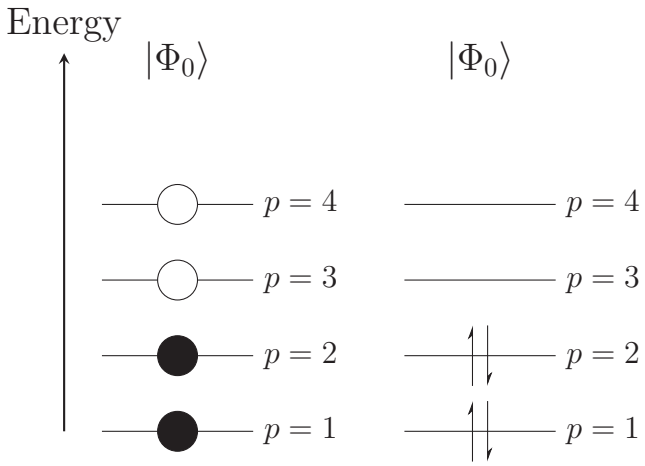


Figure 1.1: *Schematic drawing of our anzats for the ground state in our model, with two representations; the pair representation to the left and spin representation to the right. As we will only deal with paired configurations, we will use the left one henceforth. The space is truncated to only include* $p \in \{1,2,3,4\}$.

The commutator between two pair creation or annihilation operators become

$$\begin{aligned}
\Big[\hat{P}_p^+,\hat{P}_p^+\Big] &= \hat{a}_{p+}^\dagger\,\hat{a}_{p-}^\dagger\,\hat{a}_{p+}^\dagger\,\hat{a}_{p-}^\dagger - \hat{a}_{p+}^\dagger\,\hat{a}_{p-}^\dagger\,\hat{a}_{p+}^\dagger\,\hat{a}_{p-}^\dagger \\
&= 0,
\end{aligned}$$

and

$$\begin{aligned}\left[\hat{P}_p^-, \hat{P}_p^-\right] &= \hat{a}_{p-}\,\hat{a}_{p+}\,\hat{a}_{p-}\,\hat{a}_{p+} - \hat{a}_{p-}\,\hat{a}_{p+}\,\hat{a}_{p-}\,\hat{a}_{p+} \\ &= 0.\end{aligned}$$

1.1.1 Extra task, commutator between pair of creation and annihilation operators with the Hamiltonian

My commutation relations between the Hamiltonian and the pair of creation and annihilation operators are

$$\begin{aligned}\left[\hat{P}_p^+\,\hat{P}_p^-, \hat{H}_0\right] &= 0, \\ \left[\hat{P}_p^+\,\hat{P}_p^-, \hat{V}\right] &= -\frac{g}{2}\sum_{qr}\left[\hat{P}_p^+\,\hat{P}_p^-, \hat{P}_q^+\,\hat{P}_r^-\right] \\ &= \sum_q \hat{P}_p^+\,\hat{P}_q^- - \hat{P}_q^+\,\hat{P}_p^- \neq 0,\end{aligned}$$

and the commutation relation between the product of the pair creation and annihilation operators and the Hamiltonian is

$$\left[\hat{P}_p^+\,\hat{P}_p^-, \hat{H}\right] = \sum_q \hat{P}_p^+\,\hat{P}_q^- - \hat{P}_q^+\,\hat{P}_p^- \neq 0.$$

1.2 The Hamiltonian Matrix

We first start by listing all possible states in our model space, shown in Figure 1.2. Since all possible states can be represented by pair creation and annihilation operators, I will use that representation forward. The ground state $|\Psi_0\rangle = \hat{P}_2^+\,\hat{P}_1^+\,|0\rangle$ is simply filling the holestates given in Figure 1.2. This will be our new Fermi vacuum. All possible particle-hole states can be listed as

$$\begin{aligned}\left|\Psi_2^3\right\rangle &= \hat{P}_3^+\,\hat{P}_1^+\,|0\rangle = \hat{P}_3^+\,\hat{P}_2^-\,|\Psi_0\rangle\,, \\ \left|\Psi_2^4\right\rangle &= \hat{P}_4^+\,\hat{P}_1^+\,|0\rangle = \hat{P}_4^+\,\hat{P}_2^-\,|\Psi_0\rangle\,, \\ \left|\Psi_1^3\right\rangle &= \hat{P}_3^+\,\hat{P}_2^+\,|0\rangle = \hat{P}_3^+\,\hat{P}_1^-\,|\Psi_0\rangle\,, \\ \left|\Psi_1^4\right\rangle &= \hat{P}_4^+\,\hat{P}_2^+\,|0\rangle = \hat{P}_4^+\,\hat{P}_1^-\,|\Psi_0\rangle\,, \\ \left|\Psi_{12}^{34}\right\rangle &= \hat{P}_4^+\,\hat{P}_3^+\,|0\rangle = \hat{P}_4^+\,\hat{P}_3^+\,\hat{P}_2^-\,\hat{P}_1^-\,|\Psi_0\rangle\,.\end{aligned}$$

A schematic drawing of the states are displayed in Figure 1.3. The Hamiltonian matrix becomes

$$\begin{pmatrix}
\langle\Psi_0|\,\hat{H}\,|\Psi_0\rangle & \langle\Psi_0|\,\hat{H}\,|\Psi_2^3\rangle & \langle\Psi_0|\,\hat{H}\,|\Psi_2^4\rangle & \langle\Psi_0|\,\hat{H}\,|\Psi_1^3\rangle & \langle\Psi_0|\,\hat{H}\,|\Psi_1^4\rangle & \langle\Psi_0|\,\hat{H}\,|\Psi_{12}^{34}\rangle \\
\langle\Psi_2^3|\,\hat{H}\,|\Psi_0\rangle & \langle\Psi_2^3|\,\hat{H}\,|\Psi_2^3\rangle & \langle\Psi_2^3|\,\hat{H}\,|\Psi_2^4\rangle & \langle\Psi_2^3|\,\hat{H}\,|\Psi_1^3\rangle & \langle\Psi_2^3|\,\hat{H}\,|\Psi_1^4\rangle & \langle\Psi_2^3|\,\hat{H}\,|\Psi_{12}^{34}\rangle \\
\langle\Psi_2^4|\,\hat{H}\,|\Psi_0\rangle & \langle\Psi_2^4|\,\hat{H}\,|\Psi_2^3\rangle & \langle\Psi_2^4|\,\hat{H}\,|\Psi_2^4\rangle & \langle\Psi_2^4|\,\hat{H}\,|\Psi_1^3\rangle & \langle\Psi_2^4|\,\hat{H}\,|\Psi_1^4\rangle & \langle\Psi_2^4|\,\hat{H}\,|\Psi_{12}^{34}\rangle \\
\langle\Psi_1^3|\,\hat{H}\,|\Psi_0\rangle & \langle\Psi_1^3|\,\hat{H}\,|\Psi_2^3\rangle & \langle\Psi_1^3|\,\hat{H}\,|\Psi_2^4\rangle & \langle\Psi_1^3|\,\hat{H}\,|\Psi_1^3\rangle & \langle\Psi_1^3|\,\hat{H}\,|\Psi_1^4\rangle & \langle\Psi_1^3|\,\hat{H}\,|\Psi_{12}^{34}\rangle \\
\langle\Psi_1^4|\,\hat{H}\,|\Psi_0\rangle & \langle\Psi_1^4|\,\hat{H}\,|\Psi_2^3\rangle & \langle\Psi_1^4|\,\hat{H}\,|\Psi_2^4\rangle & \langle\Psi_1^4|\,\hat{H}\,|\Psi_1^3\rangle & \langle\Psi_1^4|\,\hat{H}\,|\Psi_1^4\rangle & \langle\Psi_1^4|\,\hat{H}\,|\Psi_{12}^{34}\rangle \\
\langle\Psi_{12}^{34}|\,\hat{H}\,|\Psi_0\rangle & \langle\Psi_{12}^{34}|\,\hat{H}\,|\Psi_2^3\rangle & \langle\Psi_{12}^{34}|\,\hat{H}\,|\Psi_2^4\rangle & \langle\Psi_{12}^{34}|\,\hat{H}\,|\Psi_1^3\rangle & \langle\Psi_{12}^{34}|\,\hat{H}\,|\Psi_1^4\rangle & \langle\Psi_{12}^{34}|\,\hat{H}\,|\Psi_{12}^{34}\rangle
\end{pmatrix}, \tag{1.1}$$

which is

$$\begin{pmatrix} 2\xi - g & -\frac{g}{2} & -\frac{g}{2} & -\frac{g}{2} & -\frac{g}{2} & 0 \\ -\frac{g}{2} & 4\xi - g & -\frac{g}{2} & -\frac{g}{2} & 0 & -\frac{g}{2} \\ -\frac{g}{2} & -\frac{g}{2} & 6\xi - g & 0 & -\frac{g}{2} & -\frac{g}{2} \\ -\frac{g}{2} & -\frac{g}{2} & 0 & 6\xi - g & -\frac{g}{2} & -\frac{g}{2} \\ -\frac{g}{2} & 0 & -\frac{g}{2} & -\frac{g}{2} & 8\xi - g & -\frac{g}{2} \\ 0 & -\frac{g}{2} & -\frac{g}{2} & -\frac{g}{2} & -\frac{g}{2} & 10\xi - g \end{pmatrix}.$$

Diagonalizing this matrix will yield the best approximation to the many-body energy levels of all methods in subsequent sections in this paper. Figure 1.4 displays the energy levels given from diagonalization, for the range of $g \in [-\xi, \xi]$.

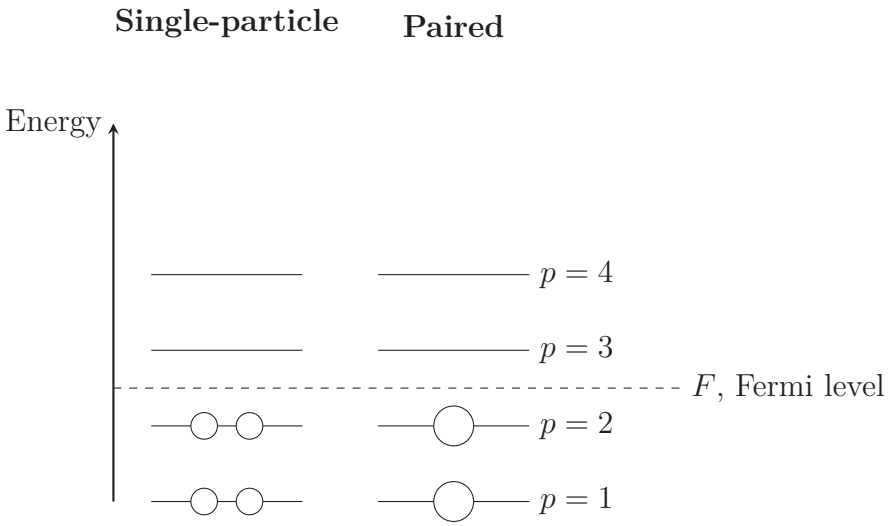


Figure 1.2: *Schematic drawing of our state space in the single-particle basis (left) and the paired basis (right). The white circles indicate hole states. We have truncated the space to only include* $p \in \{1, 2, 3, 4\}$.

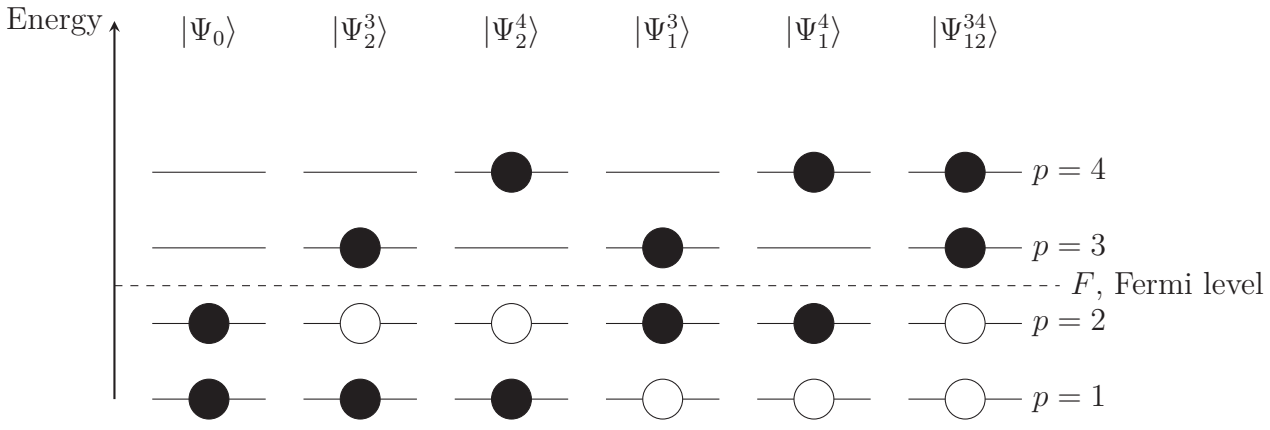


Figure 1.3: *Schematic drawing of the possible states in the paired basis. The white circles indicate possible hole states, given four fermions in our ground state. The dashed line indicates the Fermi level. The space has been truncated to only include* $p \in \{1, 2, 3, 4\}$.

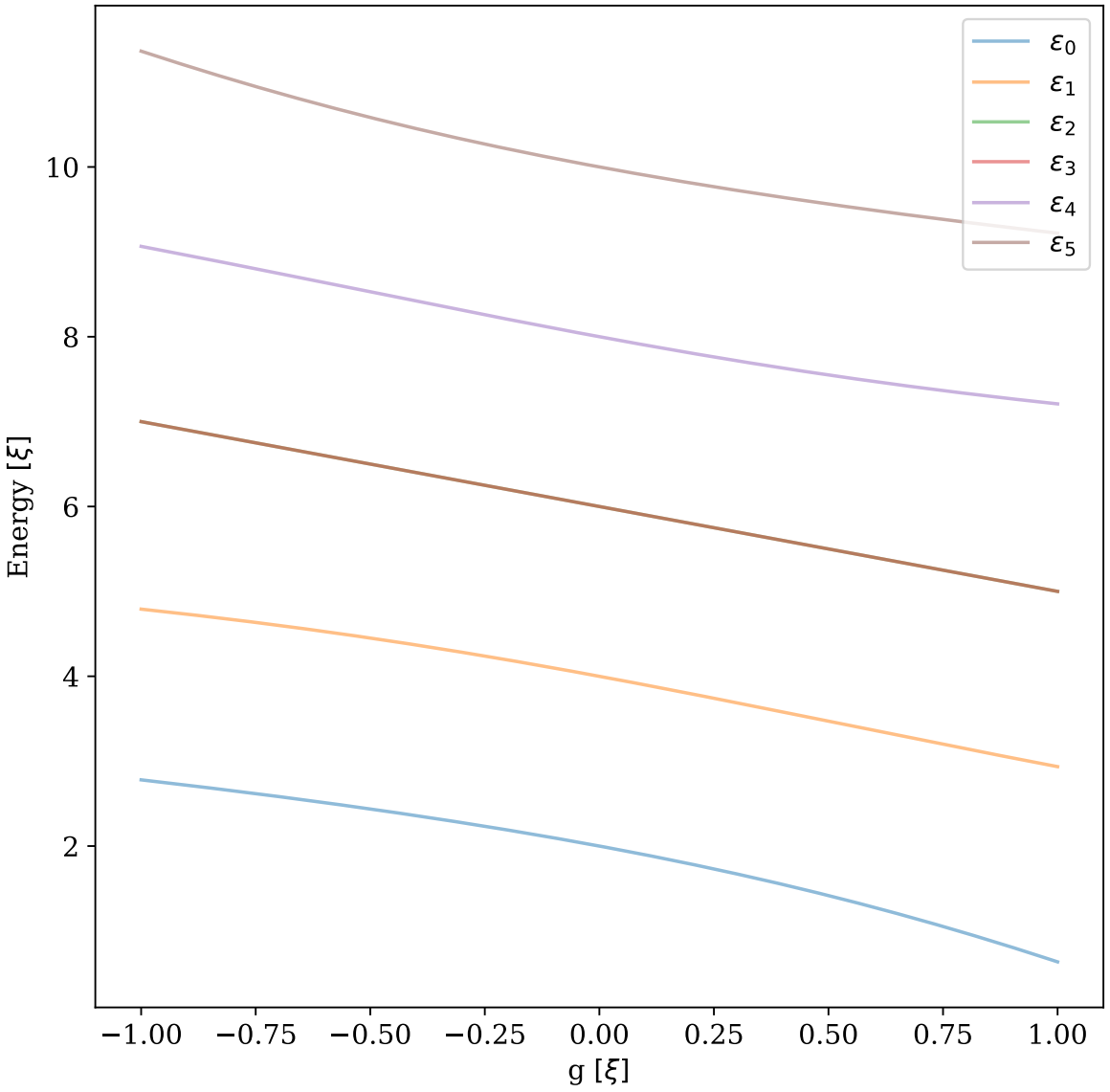


Figure 1.4: *Yielded energies of the full diagonalization of the Hamiltonian matrix in Equation 1.1. The ϵ_is representing the energies of the states are sorted in ascending order, and the curve labeled ϵ_0 indicates the ground state. Notice also the degeneracy in two of the excited states.*

1.3 An Approximation to the Ground State Energy using only 2p2h Excitations.

Our first approximation to the FCI calculation given our basis set (Figure 1.4), is to neglect the the 4p4h possible excitation in the original basis. This would correspond to what is called CID (configuration interaction doubles) in our original basis. Alternatively, we can use the pairwise basis set, and we can label this CIS (configuration interaction singles), where the 4p4h from the original basis becomes a 2p2h to be ommitted. To avoid confusion I will refer to this as a CID calculation for now. The matrix to be diagonalized is simply the Hamiltonian matrix from Equation 1.1, but the last column and row has been removed,

becoming

$$\begin{pmatrix} 2\xi - g & -\frac{g}{2} & -\frac{g}{2} & -\frac{g}{2} & \\ -\frac{g}{2} & 4\xi - g & -\frac{g}{2} & -\frac{g}{2} & 0 \\ -\frac{g}{2} & -\frac{g}{2} & 6\xi - g & 0 & -\frac{g}{2} \\ -\frac{g}{2} & -\frac{g}{2} & 0 & 6\xi - g & -\frac{g}{2} \\ -\frac{g}{2} & 0 & -\frac{g}{2} & -\frac{g}{2} & 8\xi - g \end{pmatrix}. \tag{1.2}$$

The resulting energy levels of the diagonalization for the same range of $g(\in [-\xi, \xi])$ are displayed in **??**. This is very close to the FCI calculation, which is expected, since we only removed a single row and column. The difference in the ground state energies between the two methods are displayed in Figure 1.6, showing that the difference is not symmetric with respect to g. I therefore deduce that for positive values of g the omitted contribution to the energy is a larger part of the true ground state compared with the negative values of g.

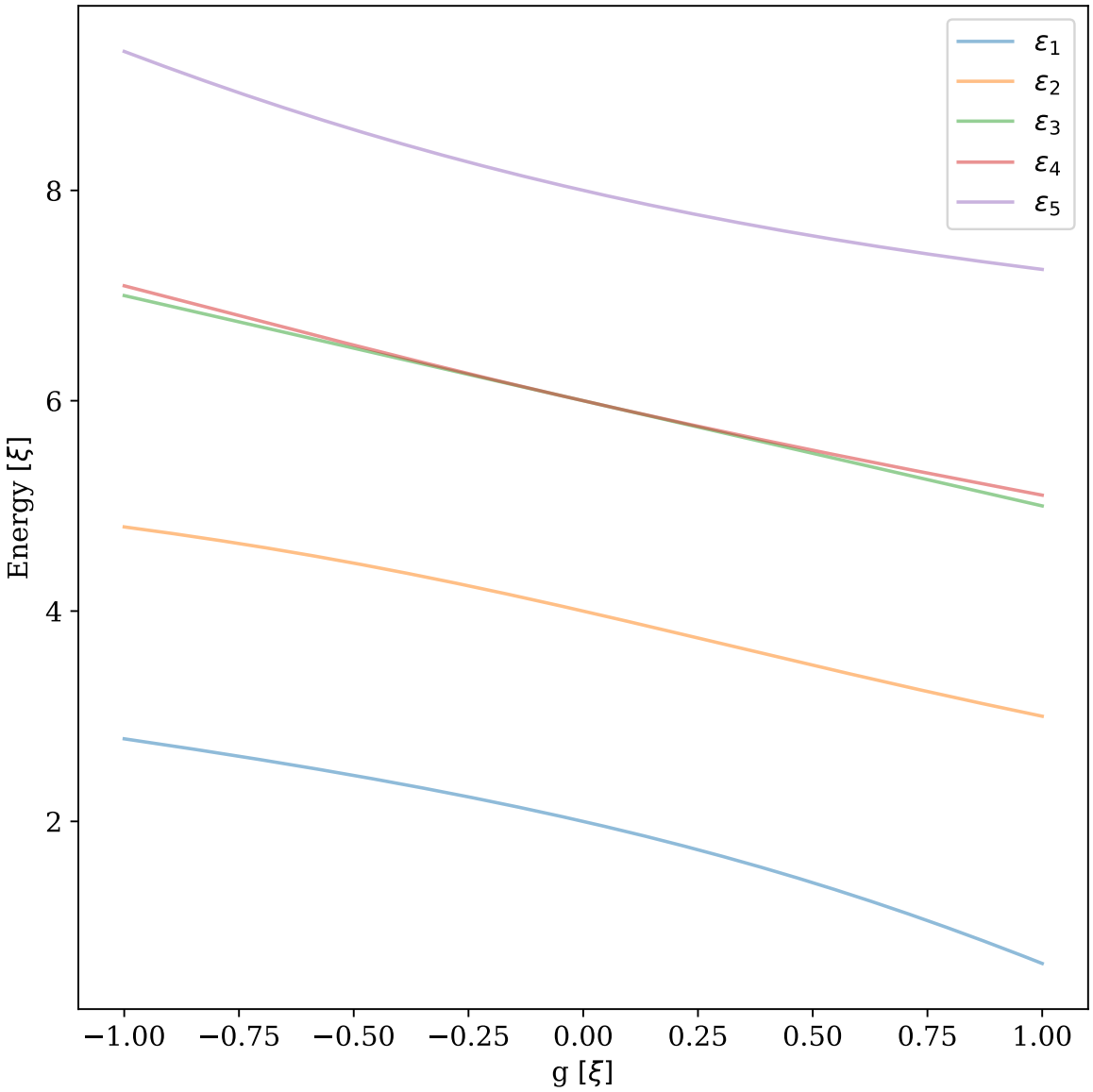


Figure 1.5: *Energy levels of the many-body state using the CID approximation. The degeneracy between the two energy levels in the FCI has been lost for all $g \neq 0$.*

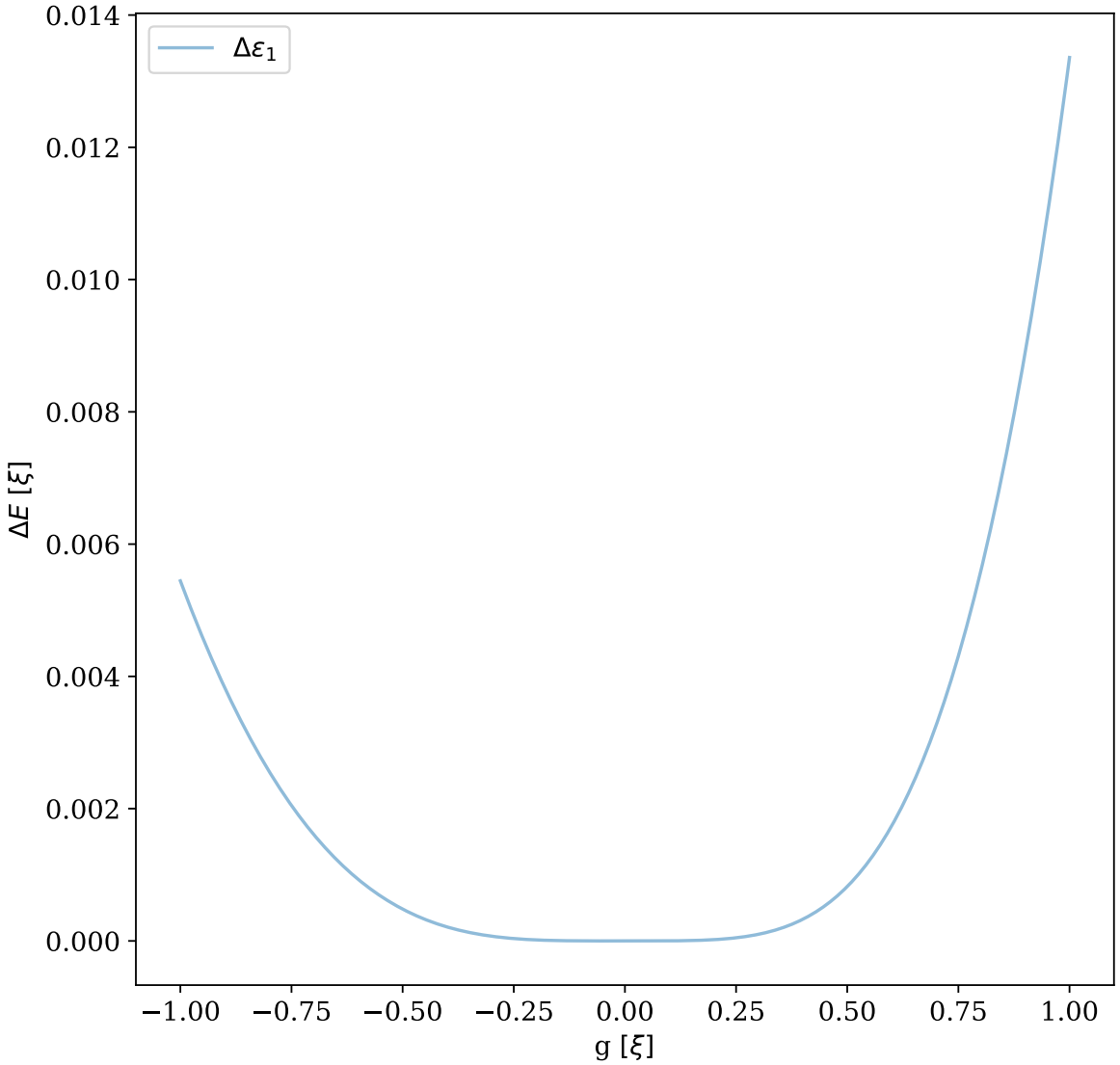


Figure 1.6: *Comparison of ground state energies of the FCI calculation and the CID approximation.*

1.4 Normal-Ordered Hamiltonians and Hartree-Fock

To be able to perform calculations using Wick's theorem, we need to normal-order the Hamiltonian with respect to a new Fermi vacuum. In our case this vacuum becomes the ground state ansatz, $|\Psi_0\rangle$, and we denote all single-particle (and pair) states with indices $i, j, k, \ldots$. The one-body term can be normal-ordered with respect to this new Fermi vacuum, and becomes

$$\hat{a}_p^\dagger \hat{a}_q = \delta_{pq<F} + \left\{\hat{a}_p^\dagger \hat{a}_q\right\}.$$

The normal-ordered two-body term becomes

$$\begin{aligned}\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r =& \left\{\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r\right\} + \delta_{qs<F}\left\{\hat{a}_p^\dagger \hat{a}_r\right\} + \delta_{pr<F}\left\{\hat{a}_q^\dagger \hat{a}_s\right\} \\ &- \delta_{qr<F}\left\{\hat{a}_p^\dagger \hat{a}_s\right\} - \delta_{ps<F}\left\{\hat{a}_q^\dagger \hat{a}_r\right\} + \delta_{pr}\delta_{qs} + \delta_{ps}\delta_{qr} \\ =& \left\{\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r\right\} + 4\delta_{rs<F}\left\{\hat{a}_p^\dagger \hat{a}_q\right\} + 2\delta_{pr}\delta_{qs}.\end{aligned}$$

In the calculations below, these relations are used (to save space).

General Hamiltonian

The general Hamiltonian can be written as

$$\hat{H} = \sum_{pq} \langle p| \hat{h}_0 |q\rangle \, \hat{a}_p^\dagger \, \hat{a}_q + \frac{1}{4} \sum_{pqrs} \langle pq| \hat{v} |rs\rangle_{AS} \, \hat{a}_p^\dagger \, \hat{a}_q^\dagger \, \hat{a}_s \, \hat{a}_r.$$

The normal-ordered general Hamiltonian becomes

$$\begin{aligned}\hat{H} =& \sum_{i<F} \langle i| \hat{h}_0 |i\rangle + \sum_{pq} \langle p| \hat{h}_0 |q\rangle \left\{\hat{a}_p^\dagger \, \hat{a}_q\right\} \\ &+ \frac{1}{4} \sum_{pqrs} \langle pq| \hat{v} |rs\rangle_{AS} \left\{\hat{a}_p^\dagger \, \hat{a}_q^\dagger \, \hat{a}_s \, \hat{a}_r\right\} + \sum_{i<F,pq} \langle pi| \hat{v} |qi\rangle_{AS} \left\{\hat{a}_p^\dagger \, \hat{a}_q\right\} + \frac{1}{2} \sum_{ij<F} \langle ij| \hat{v} |ij\rangle_{AS} \\ =& E_0^{\text{ref}} + \hat{F}_N + \hat{V}_N,\end{aligned}$$

where we have defined E_0^{ref}, $\hat{F}_N$ and $\hat{V}_N$ as:

$$\begin{aligned}E_0^{\text{ref}} :=& \sum_{i<F} \langle i| \hat{h}_0 |i\rangle + \frac{1}{2} \sum_{ij<F} \langle ij| \hat{v} |ij\rangle_{AS}, \\ \hat{F}_N :=& \sum_{pq} \langle p| \hat{h}_0 |q\rangle \, \hat{a}_p^\dagger \, \hat{a}_q + \sum_{i<F} \langle pi| \hat{v} |qi\rangle_{AS} \, \hat{a}_p^\dagger \, \hat{a}_q, \\ \hat{V}_N :=& \frac{1}{4} \sum_{pqrs} \langle pq| \hat{v} |rs\rangle_{AS} \, \hat{a}_p^\dagger \, \hat{a}_q^\dagger \, \hat{a}_s \, \hat{a}_r.\end{aligned}$$

Using single-particle formalism

The Hamiltonian for our system in single-particle formalism is

$$\hat{H} = \xi \sum_{p\sigma} (p-1) \, \hat{a}_{p\sigma}^\dagger \, \hat{a}_{p\sigma} - \frac{g}{2} \sum_{pq} \hat{a}_{p+}^\dagger \, \hat{a}_{p-}^\dagger \, \hat{a}_{q-} \, \hat{a}_{q+},$$

alternatively written as

$$\hat{H} = \sum_{p\sigma} \langle p\sigma| \hat{h}_0 |p\sigma\rangle \, \hat{a}_{p\sigma}^\dagger \, \hat{a}_{p\sigma} + \sum_{pq} \langle p+p-| \hat{v} |q+q-\rangle_{AS} \, \hat{a}_{p+}^\dagger \, \hat{a}_{p-}^\dagger \, \hat{a}_{q+} \, \hat{a}_{q-},$$

and we identify the matrix elements $\langle p\sigma| \hat{h}_0 |p\sigma\rangle = \xi(p-1)$ and $\langle p+p-| \hat{v} |q+q-\rangle_{AS} = -g/2$. A normal-ordered Hamiltonian with respect to a Fermi vacuum is defined as the Hamiltonian on the system subtracting the reference energy (the energy of the ground state ansatz, $|\Psi_0\rangle$). We will rewrite the Hamiltonian in this normal-order to reflect the particle-hole formalism to be able to use Wick's theorem. The Hamiltonian can be rewritten as

$$\hat{H} = \hat{H}_N + E_0^{\text{ref}},$$

where $\hat{H}_N$ is the part of the Hamiltonian that will yield zero on our Fermi vacuum, and E_0^{ref} is the energy of this Fermi vacuum. The Fermi vacuum energy can be written as

$$\begin{aligned}E_0^{\text{ref}} =& \sum_{i\sigma} \langle i\sigma| \hat{h}_0 |i\sigma\rangle + \sum_{ij} \langle i+i-| \hat{v} |j+j-\rangle_{AS} \, \delta_{ij} \\ =& \sum_{i\sigma} \langle i\sigma| \hat{h}_0 |i\sigma\rangle + \sum_{i} \langle i+i-| \hat{v} |i+i-\rangle_{AS} \\ =& \sum_{i\sigma} \xi(i-1) + \sum_{i} \left(-\frac{g}{2}\right),\end{aligned}$$

and the $\hat{H}_N$ is

$$\hat{H}_N = \sum_{p\sigma} \langle p\sigma | \hat{h}_0 | p\sigma \rangle \left\{ \hat{a}^\dagger_{p\sigma} \hat{a}_{p\sigma} \right\} + \sum_{pq} \langle p+p- | \hat{v} | q+q- \rangle_{AS} \left\{ \hat{a}^\dagger_{p+} \hat{a}^\dagger_{p-} \hat{a}_{q-} \hat{a}_{q+} \right\},$$

where we indicate that the operators within the $\{\}$ are normal-ordered with respect to the Fermi vacuum. The normal-ordered Hamiltonian written out is

$$\begin{aligned}\hat{H} = &\sum_{p\sigma} \langle p\sigma | \hat{h}_0 | p\sigma \rangle \left\{ \hat{a}^\dagger_{p\sigma} \hat{a}_{p\sigma} \right\} + \sum_{pq} \langle p+p- | \hat{v} | q+q- \rangle_{AS} \left\{ \hat{a}^\dagger_{p+} \hat{a}^\dagger_{p-} \hat{a}_{q-} \hat{a}_{q+} \right\} \\ &+ \sum_{i\sigma} \langle i\sigma | \hat{h}_0 | i\sigma \rangle + \sum_{i} \langle i+i- | \hat{v} | i+i- \rangle_{AS}.\end{aligned}$$

Using pair-of-particles formalism

The Hamiltonian for our system in our paired states basis is

$$\hat{H} = 2\xi \sum_p \hat{P}^+_p \hat{P}^-_p - \frac{g}{2} \sum_{pq} \hat{P}^+_p \hat{P}^-_q,$$

and normal-ordering with respect to the Fermi vacuum, given in pair state basis as

$$|\Psi_0\rangle = \hat{P}^+_2 \hat{P}^+_1 |0\rangle,$$

gives

$$\hat{H} = 2\xi \sum_i (i-1) + 2\xi \sum_p \left\{ \hat{P}^+_p \hat{P}^-_q \right\} - \sum_i \frac{g}{2} - \frac{g}{2} \sum_{pq} \left\{ \hat{P}^+_p \hat{P}^-_q \right\}$$

Functional minimization

The most general way to define the Hartree-Fock method is, in my mind, simply the minimization of the energy functional given a trial state $|\Phi\rangle$, using the method of setting the first order variation in the energy to zero,

$$\delta E = 0.$$

We define the energy functional as

$$E[\Phi] = \langle \Phi | \hat{H} | \Phi \rangle.$$

Then we vary the trial state by an arbitrary amount

$$|\Phi\rangle \leftarrow |\Phi\rangle + \delta |\Phi\rangle,$$

which in turn will yield a variation in the energy functional, which we can write as a Taylor expansion on the form

$$E[\Phi + \delta\Phi] = E[\Phi] + \delta E + \ldots,$$

and we set the first variation, δE, to be zero. The first variation can be written as

$$\delta E = \langle \delta\Phi | \hat{H} | \Phi \rangle + \langle \Phi | \hat{H} | \delta\Phi \rangle.$$

We need our trial states to be properly normalized, so we have a constraint that can be written as

$$\langle \Phi | \Phi \rangle = 1,$$

and we express this problem as a Lagrangian. We set the Lagrangian multiplier to be the energy, and the Lagrangian is

$$\mathscr{L}[\Phi] = \langle\Phi|\,\hat{H}\,|\Phi\rangle - E(\langle\Phi|\Phi\rangle - 1)$$

The first variation in the Lagrangian also needs to be zero,

$$\delta\mathscr{L} = \delta E - E\,\langle\delta\Phi|\Phi\rangle - E\,\langle\Phi|\delta\Phi\rangle = 0.$$

To be able to do this, we need variational parameters in our trial state. For these purposes we say that the trial state is a linear expansion of states, $|\phi\rangle$,

$$|\Phi\rangle = \sum_i^N c_i\,|\phi_i\rangle\,,$$

where N is the number of particles and c_i is the weight coefficient determining how much of the state $|\phi_i\rangle$ the trial state contains. We write the variation in the trial state as a variation in the coefficients of the linear expansion,

$$\delta\,|\Phi\rangle = \sum_i^N \delta c_i\,|\phi_i\rangle\,.$$

We now define the Hamiltonian matrix, $\mathbf{H}$, to have the elements

$$H_{ij} = \langle\phi_i|\,\hat{H}\,|\phi_j\rangle\,,$$

and we write the variation in the Lagrangian as

$$\delta\mathscr{L} = \sum_{ij}^N \delta c_i^* c_j H_{ij} - E\sum_{ij}^N \delta c_i^* c_j\,\langle\phi_i|\phi_j\rangle + \sum_{ij}^N c_i^*\delta c_j H_{ij} - E\sum_{ij}^N c_i^*\delta c_j\,\langle\phi_i|\phi_j\rangle\,.$$

We can treat the coefficients c_i and c_i^* as independent. We can then factor out one of them, and we have an pseudo (pseudo because the $\langle\phi_i|\phi_j\rangle$ does not necessarily need to be δ_{ij}) eigenvalue equation within the square brackets,

$$\delta c_i^*\left[\sum_j c_j H_{ij} - E c_j\,\langle\phi_i|\phi_j\rangle\right] = 0.$$

We now define the general overlap matrix, $\mathbf{S}$, with elements

$$S_{ij} = \langle\phi_i|\phi_j\rangle\,,$$

and we can write the minimization of the energy functional with respect to the first variation as

$$\mathbf{Hc} = E\mathbf{Sc},$$

where $\mathbf{c}$ is the vector containing the coefficients of the trial state with the lowest energy under these conditions, $\left|\hat{\Phi}\right\rangle$.

Non-Canonical Hartree-Fock

Say we have an orthonormal basis, $\{\phi\} = \{\phi_1, \phi_2, \ldots, \phi_n\}$, where n is the number of basis functions. Again we want to minimize the energy functional, $E_0[|\Phi\rangle]$, where $|\Phi\rangle$ is our state being the Slater determinant all filled orbitals, $|\Phi\rangle = |\phi_1\phi_2\ldots\phi_N\rangle$, where N is the number of particles, and where we have assumed that the basis of orbitals are ordered in increasing single-particle energy order. This will be our ground state energy ansatz in the $\{\phi\}$ basis. We again have the constraints that, for all orbitals, we need them to be orthonormal,

$$\langle\phi_i|\phi_j\rangle = \delta_{ij}.$$

This leads us back to the familiar Lagrangian,

$$\mathscr{L}[\{\phi\}] = E_0[\{\phi\}] - \sum_{ij}^{N} \epsilon_{ji} \langle\phi_i|\phi_j\rangle ,$$

where $E_0[\{\phi\}]$ is the energy expectation value of the ground state ansatz, and the ϵ_{ij} constitutes a set of Lagrangian multipliers, that have the property

$$\epsilon_{ji} = \epsilon_{ij}^*,$$

because $\langle\phi_i|\phi_j\rangle = \langle j|i\rangle^*$ and $\mathscr{L}$ is real. If we now add an arbitrary infinitesimal variation in the **basis functions**,

$$\phi \leftarrow \phi + \delta\phi,$$

and again we set the first variation in the Lagrangian to be 0, as

$$\begin{aligned}
\delta\mathscr{L} =& \delta E_0 - \sum_{ij}^{N} \epsilon_{ji}[\langle\delta\phi_i|\phi_j\rangle + \langle\phi_i|\delta\phi_j\rangle] \\
=& \sum_i \langle\delta\phi_i|\,\hat{h}_0\,|\phi_i\rangle + \sum_i \langle\phi_i|\,\hat{h}_0\,|\delta\phi_i\rangle \\
&+ \frac{1}{4}\sum_i^N\sum_j^N [\langle\delta\phi_i\phi_j|\,\hat{v}\,|\phi_i\phi_j\rangle + \langle\phi_i\delta\phi_j|\,\hat{v}\,|\phi_i\phi_j\rangle + \langle\phi_i\phi_j|\,\hat{v}\,|\delta\phi_i\phi_j\rangle + \langle\phi_i\phi_j|\,\hat{v}\,|\phi_i\delta\phi_j\rangle] \\
&- \frac{1}{4}\sum_i^N\sum_j^N [\langle\delta\phi_i\phi_j|\,\hat{v}\,|\phi_j\phi_i\rangle + \langle\phi_i\delta\phi_j|\,\hat{v}\,|\phi_j\phi_i\rangle + \langle\phi_i\phi_j|\,\hat{v}\,|\delta\phi_j\phi_i\rangle + \langle\phi_i\phi_j|\,\hat{v}\,|\phi_j\delta\phi_i\rangle] \\
&- \sum_{ij}^{N} \epsilon_{ji}[\langle\delta\phi_i|\phi_j\rangle + \langle\phi_i|\delta\phi_j\rangle] \\
*=& \sum_i^N \langle\delta\phi_i|\,\hat{h}_0\,|\phi_i\rangle + \frac{1}{2}\sum_{ij}^N \langle\delta\phi_i\phi_j|\,\hat{v}\,|\phi_i\phi_j\rangle_{AS} \\
&- \sum_{ij}^{N} \epsilon_{ji}\langle\delta\phi_i|\phi_j\rangle \\
**=& \sum_i^N \delta\phi_i^* \left[\hat{h}_0\,|\phi_i\rangle + \frac{1}{2}\sum_j (\langle\cdot\phi_j|\,\hat{v}\,|\cdot\phi_j\rangle\,|\phi_i\rangle - \langle\cdot\phi_j|\,\hat{v}\,|\phi_j\cdot\rangle\,|\phi_i\rangle) - \sum_j^N \epsilon_{ij}\,|\phi_j\rangle\right] \\
=& 0.
\end{aligned}$$

The jump in $(*)$ is done by realising we sum over dummy indices, and we can choose to solve for the complex conjugate ϕs only, ignoring the rest of the terms. The notation used in $(**)$

is a trick Øyvind showed me, where we set the matrix elements empty using a dot notation, highlighting that the part of the equation within the square brackets should operate on a state. Let's rewrite it further, bringing forth what is called the Fock operator, which can be written

$$\begin{aligned}\hat{f}\,|\phi_k\rangle &= \hat{h}_0\,|\phi_k\rangle + \frac{1}{2}\sum_j^N [\langle\cdot\phi_j|\,\hat{v}\,|\cdot\phi_j\rangle\,|\phi_k\rangle - \langle\cdot\phi_j|\,\hat{v}\,|\phi_j\cdot\rangle\,|\phi_k\rangle] \\ &= \hat{h}_0\,|\phi_k\rangle + \frac{1}{2}\sum_j^N [\hat{J}_j\,|\phi_k\rangle - \hat{K}_j\,|\phi_k\rangle],\end{aligned}$$

where we have identified the direct interaction operator, $\hat{J}_l$, and the exhange interaction operator, $\hat{K}_l$. We know that the term within the square brackets needs to be zero for the first variation in the Lagrangian to generally be zero. We recognize that the first two terms withing these brackets to be the Fock operator, and we can write

$$\hat{f}\,|\phi_k\rangle - \sum_j^N \epsilon_{ij}\,|\phi_j\rangle = 0, \tag{1.3}$$

which is referred to as the non-canonical Hartree-Fock equation.

Canonical Hartree-Fock

The canonical Hartree-Fock applies a unitary transformation, which is a transformation that preserves the inner product of the basis set, on the basis set such that Equation 1.3 becomes an eigenvalue equation in the transformed basis. We have the original basis $\{\phi\}$, which is denoted with the latin alphabet indices $|i\rangle$, and we transform it to a new basis $\{\psi\}$, denoted with the greek alphabet indices $|\lambda\rangle$, using

$$|\lambda\rangle = \sum_i C_{\lambda i}\,|i\rangle\,,$$

where $c_{\lambda i}$ is the ith element on row λ of the unitary transformation matrix, $\mathbf{C}$. We want the transformed basis that satisfies

$$\hat{f}\,|\lambda\rangle = \epsilon_\lambda\,|\lambda\rangle\,, \tag{1.4}$$

where ϵ_λ is the single-particle energy in the new basis. This is the canonical Hartree-Fock equation. We can rewrite the Fock operator in the new basis as

$$\hat{f} = \hat{h}_0 + \sum_j^N \sum_\gamma^n \sum_\delta^n C^*_{\gamma j} C_{\delta_j} [\langle\cdot j|\,\hat{v}\,|\cdot j\rangle - \langle\cdot j|\,\hat{v}\,|j\cdot\rangle],$$

where n is the number of basis functions in both basises (the transformation matrix needs to be square, or it could not possibly be unitary). We define a new operator, $\hat{h}^{\text{HF}}_{\alpha\beta}$ which is simply a matrix element, where the Fock operator has acted on the state $\langle\alpha|$ and $|\beta\rangle$ as

$$\hat{h}^{\text{HF}}_{\alpha\beta} = \langle\alpha|\,\hat{f}\,|\beta\rangle\,,$$

and we call the resulting matrix of these operations on all states in the basis, $\alpha, \beta \in [\text{span}(\{\psi\})]$, the Hartree-Fock matrix. Equation 1.4 is only true when the Hartree-Fock matrix is diagonal. We can start with an initial guess for the coefficients (that need to satisfy orthonormality in the new basis) and update our matrix by repeatingly diagonalizing it, yielding new coefficients. This stops when the updated single-particle energies is arbitralily (user choice) close to the calculated single-particle energies from the previous iteration.

Hamiltonian in different bases

Canonical Hartree-Fock

The Hamiltonian in the canonical HF basis can be generally written as

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

where all off-diagonal elements in $\hat{F}_N$ is zero, as the basis is diagonal in the Fock operator, yielding

$$\hat{H} = E_0^{\text{ref}} + \sum_{pq} \langle p| \hat{f} |q\rangle \delta_{pq} + \frac{1}{4} \sum_{pqrs} \langle pq| \hat{v} |rs\rangle \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r.$$

The corresponding diagrams are displayed in Figure 1.7.

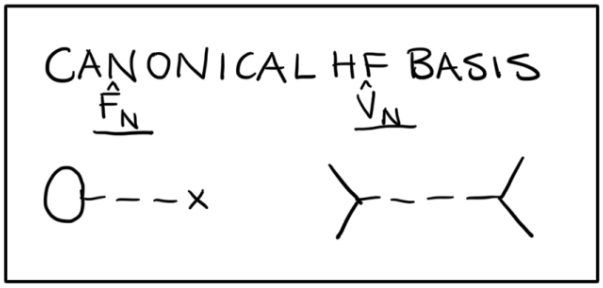


Figure 1.7: *The Hamiltonian in the canonical Hartree-Fock basis. The two-body interaction is represented by a simple two-body interaction operator.*

Non-canonical Hartree-Fock

The Hamiltonian in the non-canonical HF basis is generally written as

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

and now we have we have block off-diagonal elements in the Fock operator, where the blocks containing the off-diagonal elements are given by all hole-hole interactions and all particle-particle interactions, and the Hamiltonian can be written as

$$\begin{aligned}\hat{H} =& E_0^{\text{ref}} + \sum_{i \neq j < F} \langle i| \hat{f} |j\rangle \hat{a}_i^\dagger \hat{a}_i + \sum_{a \neq b > F} \langle a| \hat{f} |b\rangle \hat{a}_a^\dagger \hat{a}_b \\ &+ \sum_{pq} \langle p| \hat{f} |q\rangle \delta_{pq} + \frac{1}{4} \sum_{pqrs} \langle pq| \hat{v} |rs\rangle_{AS} \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r.\end{aligned}$$

The corresponding diagrams are shown in Figure 1.8

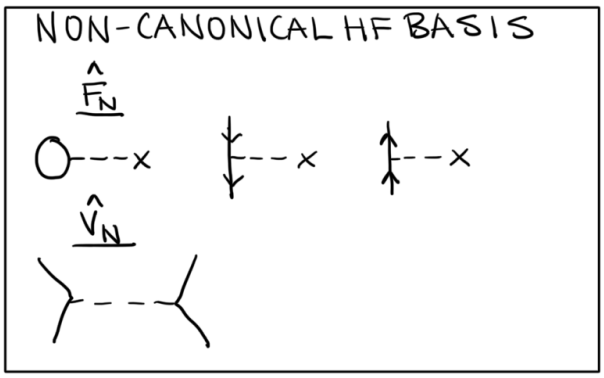


Figure 1.8: *The Hamiltonian in the non-canonical Hartree-Fock basis. The two-body interaction is represented by a simple two-body interaction operator.*

General case

In a general basis, the Hamiltonian becomes

$$\hat{H} = E_0^{\text{ref}} + \sum_{pq} \langle p| \hat{f} |q\rangle \, \hat{a}_p^\dagger \, \hat{a}_q + \frac{1}{4} \sum_{pqrs} \langle pq| \hat{v} |rs\rangle_{AS} \, \hat{a}_p^\dagger \, \hat{a}_q^\dagger \, \hat{a}_s \, \hat{a}_r,$$

and the diagrams are shown in Figure 1.9.

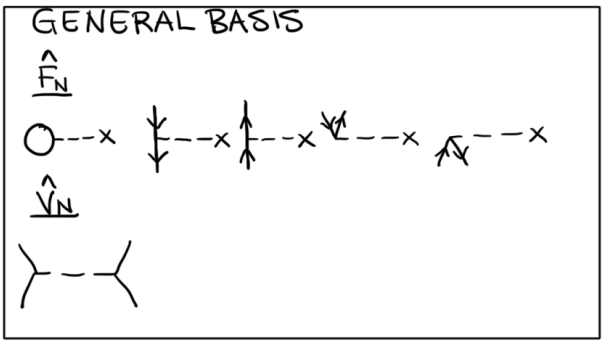


Figure 1.9: *The Hamiltonian in a general basis. The two-body interaction is represented by a simple two-body interaction operator.*

1.5 Hartree-Fock calculations

Figure 1.10 displays the Hartree-Fock energies for the ground state as a function of the interaction strength. The Hartree-Fock approximation gives a linear decay with increasing interaction strength. The first Hartree-Fock matrix to diagonalize is

$$H^{\text{HF}} = \begin{pmatrix} -\frac{g}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{g}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{g}{2}+\xi & 0 & 0 & 0 & 0 & \\ 0 & 0 & 0 & -\frac{g}{2}+\xi & 0 & 0 & 0 & \\ 0 & 0 & 0 & 0 & 2\xi & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2\xi & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3\xi & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3\xi \end{pmatrix},$$

which is diagonal. Our basis is the Hartree-Fock basis, and thus the Hartree-Fock approximation to the ground state energy becomes a linear function of the interaction strength, g. We see that this approximation fails pretty badly for strongly interacting systems, as only looking at the first variation in the energy does not take into account the higher order terms. Figure 1.10 shows that approximation holds quite well for g values close to zero, but not far away.

In this case the canonical and non-canonical Hartree-Fock basis sets are the same, as the original basis is a Hartree-Fock basis. More rigorously discussed later on, the Hartree-Fock basis is a basis where all 1p1h contributions are removed, and many of the contributions to Rayleigh-Schrödinger perturbation theory (RSPT) become zero. The only terms that survive, are those displayed in Figure 1.11 and Figure 1.12 of all possible terms up to the third degree. The Hartree-Fock energy computed here corresponds to a first order approximation in the RSPT approximation.

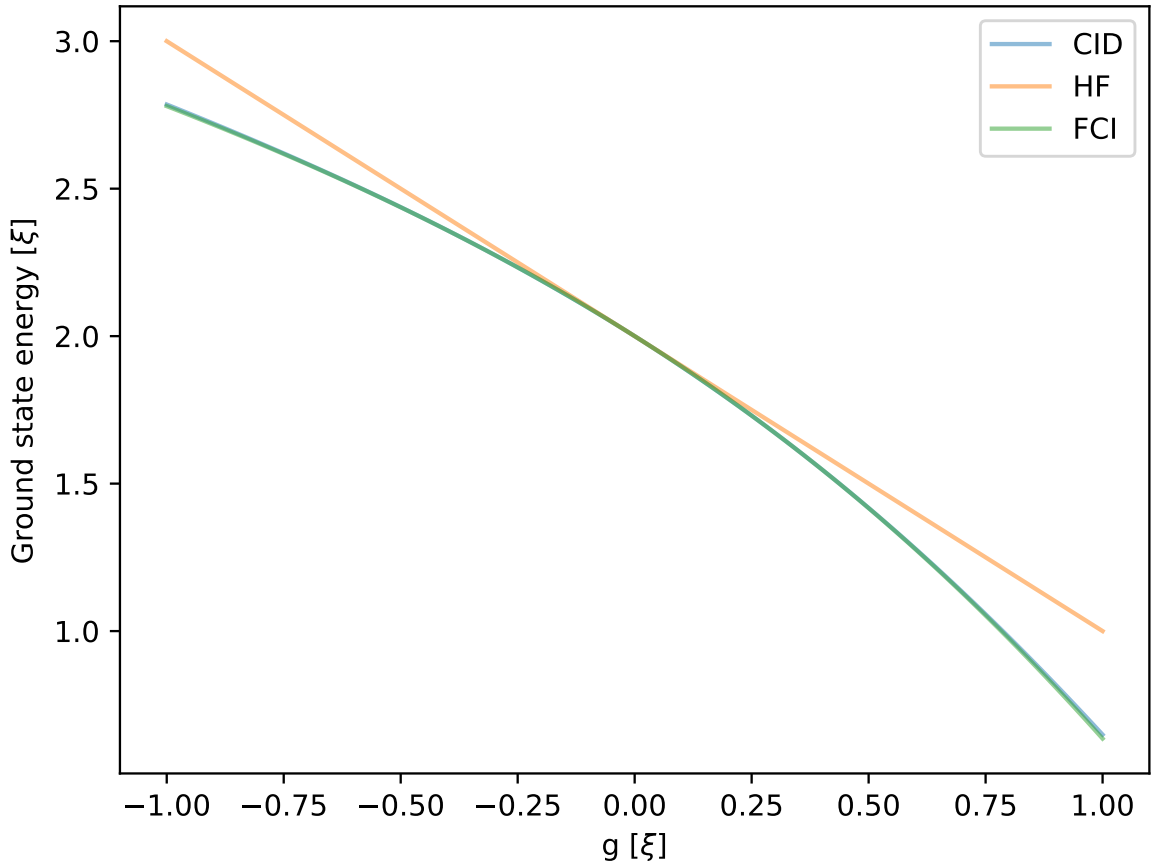


Figure 1.10: *Hartree-Fock energies compared with the CID approximation and the FCI calculation, for all interaction strength values* $g \in [-\xi, \xi]$.

1.6 Rayleigh-Schrödinger Perturbation Theory

1.6.1 Short Overview of Many-Body Perturbation Theory

We start with the Schrödinger equation (SE)

$$\hat{H} |\Psi\rangle = E |\Psi\rangle ,$$

and say the Hamiltonian can be divided into a one-body part, $\hat{H}_0$, and a interaction piece, $\hat{V}$, we write the SE as

$$(\hat{H}_0 + \hat{V})\,|\Psi\rangle = E\,|\Psi\rangle\,.$$

We have a basis, $\{\phi\}$, and a ground state ansatz for the wavefunction in that basis, $|\Phi_0\rangle$. We then make a projection operator that projects all excited states of the system in that basis out, $\hat{Q}$, in mathematical terms it will be

$$\hat{Q} = \sum_{i\neq 0} |\Phi_i\rangle\,\langle\Phi_i|\,.$$

We can rewrite our true state as

$$|\Psi\rangle = |\Phi_0\rangle + |\delta\Phi_0\rangle\,,$$

and assuming intermediate normalization,

$$\begin{aligned}\langle\Phi_0|\Psi\rangle &= \langle\Phi_0|\Phi_0\rangle + \langle\Phi_0|\,\langle\delta\Phi_0| \\ &= 1 + 0 = 1,\end{aligned}$$

where we see that we change $|\Phi\rangle$ in directions that is orthonormal to $|\Phi_0\rangle$, which corresponds to the space $\hat{Q}$ projects into, we can multiply both sides of the SE from the left with $\langle\Phi_0|$ and get

$$\begin{aligned}\langle\Phi_0|\,(\hat{H}_0 + \hat{V})\,|\Psi\rangle &= \langle\Phi_0|\,\hat{H}_0\,|\Psi\rangle + \langle\Phi_0|\,\hat{V}\,|\Psi\rangle \\ &= E_0^{(0)} + \langle\Phi_0|\,\hat{V}\,|\Psi\rangle \\ &= E_0^{(0)} + \Delta E,\end{aligned}$$

where we have exploited the hermiticity of $\hat{H}_0$ in $\langle\Phi_0|\,\hat{H}_0\,|\Psi\rangle$ so that it equals $E_0\,\langle\Phi_0|\Psi\rangle$. The resolvent operator, $\hat{R}_0(\zeta)$, is given as

$$\hat{R}_0(\zeta) = \frac{\hat{Q}}{\zeta + \hat{H}_0},$$

which is found by solving for the inverse of $\hat{Q}(\zeta - \hat{H}_0)\,\hat{Q}$. The state $|\Psi\rangle$ can be written out as a series (if the series converges) as

$$|\Psi\rangle = \sum_{m=0}^{\infty} \{\hat{R}_0(\zeta)(\hat{V} - E - \zeta)\}^m\,|\Phi_0\rangle\,.$$

Many-body perturbation theory exploits this expression for the true ground state to a specific degree, to find the approximate energy of the state. In Rayleigh-Schrödinger perturbation theory, $\zeta = \hat{H}_0$.
The energy to the nth order of the system can then be found to be

$$E_0^{(n)} = E_0^{(0)} + E_0^{(1)} + \cdots + E_0^{(n)},$$

where $E_0^{(k)}$ for all k is the contribution of the k-th order. The zeroth order contribution is $\langle\Phi_0|\,\hat{H}_0\,|\Phi_0\rangle$, and the first order contribution is

$$E_0^{(1)} = \langle\Phi_0|\,\hat{V}\,|\Phi_0\rangle\,.$$

1.6.2 Second-order contributions

Figure 1.11 displays the diagrammatic form of the second-order contribution in the many-body perturbation approximation. The second-order contribution, $E^{(2)}$, can be written as

$$E^{(2)} = \langle \Phi_0 | \hat{V} \hat{R} \hat{V} | \Phi_0 \rangle ,$$

where $|\Phi_0\rangle$ is an ansatz for the ground state with basis functions that are diagonal with respect to $\hat{H}_0$ and $\hat{R}_0$ is the resolvent, defined generally as

$$\hat{R}_0(\zeta) = \frac{\hat{Q}}{\zeta - \hat{H}_0},$$

where $\hat{Q}$ is the wave operator, projecting out the sum of all excited states of our $|\Phi_0\rangle$,

$$\hat{Q} = \sum_{p \neq 0} |\Phi_p\rangle \langle \Phi_p| ,$$

and ζ, in Rayleigh-Schrödinger perturbation theory, becomes the eigenvalue of $\hat{H}_0$ acting on the state $|\Phi_p\rangle$. With our small basis, we can write this sum out as

$$\begin{aligned}\hat{Q} = &\sum_{a>F,i<F} |\Phi_i^a\rangle \langle \Phi_i^a| + \sum_{ab>F,ij<F} \left|\Phi_{ij}^{ab}\right\rangle \left\langle \Phi_{ij}^{ab}\right| \\ &+ \sum_{abc>F,ijk<F} \left|\Phi_{ijk}^{abc}\right\rangle \left\langle \Phi_{ijk}^{abc}\right| + \sum_{abcd>F,ijkl<F} \left|\Phi_{ijkl}^{abcd}\right\rangle \left\langle \Phi_{ijkl}^{abcd}\right| ,\end{aligned}$$

and recognizing that only paired excitations are allowed, we can write $\hat{Q}$ as

$$\begin{aligned}\hat{Q} &= \sum_{a>F,i<F} \left|\Phi_{i+i-}^{a+a-}\right\rangle \left\langle \Phi_{i+i-}^{a+a-}\right| + \sum_{ab>F,ij<F} \left|\Phi_{i+i-j+-}^{a+a-b+b-}\right\rangle \\ &= \left|\Phi_{1+1-}^{3+3-}\right\rangle \left\langle \Phi_{1+1-}^{3+3-}\right| + \left|\Phi_{1+1-}^{4+4-}\right\rangle \left\langle \Phi_{1+1-}^{4+4-}\right| \\ &\quad + \left|\Phi_{2+2-}^{3+3-}\right\rangle \left\langle \Phi_{2+2-}^{3+3-}\right| + \left|\Phi_{2+2-}^{4+4-}\right\rangle \left\langle \Phi_{2+2-}^{4+4-}\right| \\ &\quad + \left|\Phi_{1+1-2+2-}^{3+3-4+4-}\right\rangle \left\langle \Phi_{1+1-2+2-}^{3+3-4+4-}\right| .\end{aligned}$$

The contribution to the second order correction of the energy

$$E^{(2)} = \sum_{p \neq 0} \frac{\langle \Phi_0 | \hat{V} | \Phi_p \rangle \langle \Phi_p | \hat{V} | \Phi_0 \rangle}{\langle \Phi_p | \hat{H}_0 | \Phi_p \rangle - \langle \Phi_0 | \hat{V} | \Phi_0 \rangle},$$

and since our interaction operator is of the two-body type, we cannot get a contribution from the 4p4h-excitation, but we get interactions of the type, $\langle \Phi_0 | \hat{V} \left| \Phi_{i+i-}^{a+a-} \right\rangle$, where

$$\begin{aligned}\langle \Phi_0 | \hat{V} \left| \Phi_{i+i-}^{a+a-} \right\rangle &= \langle i+i- | \hat{v} | a+a- \rangle_{AS} , \\ \left\langle \Phi_{i+i-}^{a+a-} \right| \hat{V} | \Phi_0 \rangle &= \langle a+a- | \hat{v} | i+i- \rangle_{AS} ,\end{aligned}$$

and the second order contribution can be written as

$$E^{(2)} = \sum_{i<F,a>F} \frac{\langle i+i- | \hat{v} | a+a- \rangle_{AS} \langle a+a- | \hat{v} | i+i- \rangle_{AS}}{2\epsilon_a - 2\epsilon_i},$$

where ϵ_p is the eigenvalue of $\hat{H}_0$ of one particle occupying state $|p\rangle$ ($\xi(p-1)$). The second-order correction term to the energy only gets contributions of this kind, and its diagrammatic form is given in Figure 1.11.

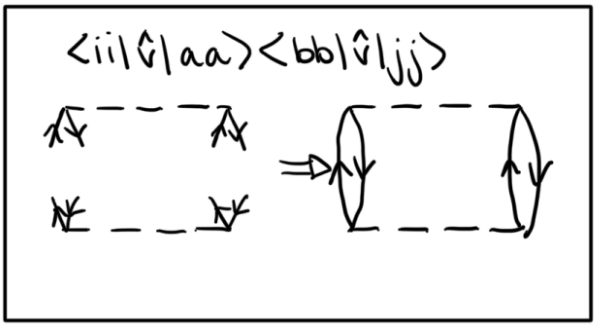


Figure 1.11: *The second order contributions in RSPT on diagrammatic form. This is a Goldstone diagram, meaning that the interaction vertices represent anti-symmetrized matrix elements.*

1.6.3 Third-order contributions

The third order contribution can be written as

$$E^{(3)} = \sum_{pq\neq 0} \frac{\langle\Phi_0|\hat{V}|\Phi_p\rangle\langle\Phi_p|\hat{V}|\Phi_q\rangle\langle\Phi_q|\hat{V}|\Phi_0\rangle}{\langle\Phi_p|\hat{H}_0|\Phi_p\rangle + \langle\Phi_q|\hat{H}_0|\Phi_q\rangle - 2\langle\Phi_0|\hat{H}_0|\Phi_0\rangle} \tag{1.5}$$

$$- E^{(1)} \sum_{pq} \frac{\langle\Phi_0|\hat{H}_0|\Phi_p\rangle\langle\Phi_q|\hat{H}_0|\Phi_0\rangle}{\langle\Phi_p|\hat{H}_0|\Phi_p\rangle + \langle\Phi_q|\hat{H}_0|\Phi_q\rangle - 2\langle\Phi_0|\hat{H}_0|\Phi_0\rangle}. \tag{1.6}$$

We know that q and p only produce non-zero contributions in our basis if they are 2p2h excitations, as the interaction between a 4p4h excitation and the ground state is zero. In this section I will use the pairwise notation for the pair of particles occupying energy level p, $\hat{P}_p^+|0\rangle = |pp\rangle$. The first term in Equation 1.5 contains all the linked diagrams for the third-order contribution to the energy. The terms in the numerator can be written as

$$\begin{aligned}
\langle\Phi_0|\hat{V}|\Phi_i\rangle &= \langle\Phi_0|\hat{P}_p^+\hat{P}_q^-\hat{P}_a^+\hat{P}_i^-|\Phi_0\rangle \\
&= \langle ii|\hat{v}|aa\rangle_{AS} \\
\langle\Phi_i|\hat{V}|\Phi_j\rangle &= \langle\Phi_0|\hat{P}_i^+\hat{P}_a^-\hat{P}_p^+\hat{P}_q^-\hat{P}_b^+\hat{P}_j^-|\Phi_0\rangle \\
&= \langle aa|\hat{v}|bb\rangle_{AS} + \langle jj|\hat{v}|ii\rangle_{AS} \\
\langle\Phi_j|\hat{V}|\Phi_0\rangle &= \langle\Phi_0|\hat{P}_j^+\hat{P}_b^-\hat{P}_p^+\hat{P}_q^-|\Phi_0\rangle \\
&= \langle bb|\hat{v}|jj\rangle_{AS},
\end{aligned}$$

and the product of these is

$$\langle ii|\hat{v}|aa\rangle_{AS}\left(\langle aa|\hat{v}|bb\rangle_{AS} + \langle jj|\hat{v}|ii\rangle_{AS}\right)\langle bb|\hat{v}|jj\rangle_{AS}.$$

This product gives rise to the terms displayed in Figure 1.12.

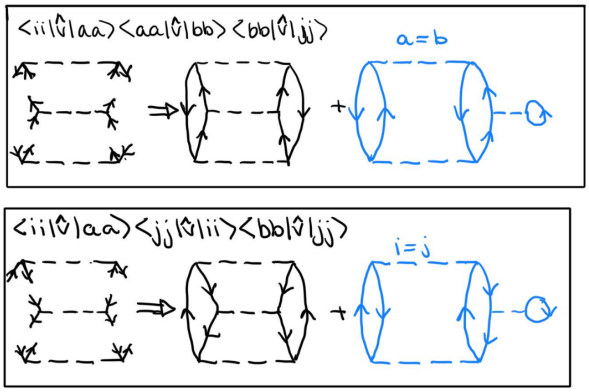
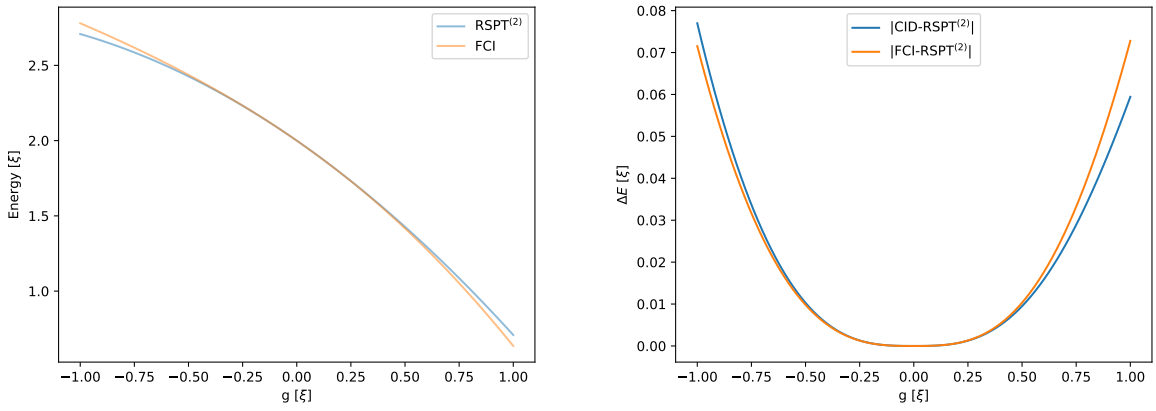


Figure 1.12: *The third order contributions in RSPT on diagrammatic form. These are a Goldstone diagram, meaning that the interaction vertices represent anti-symmetrized matrix elements.*

1.6.4 Energy plots and comparative plots

2nd order RSPT

The second order RSPT approximation to the ground state energy is plotted with the FCI calculation in Figure 1.13(a). It undershoots on the energy for values of $g > 0$, while it is larger than the FCI calculated energy for all values $g < 0$. Figure 1.13(b) displays differences in the RSPT of the second order and the CID and FCI calculations. The error increases fast with increasing $|g|$ value. Because of the undershooting for positive g values, we see an asymmetric curve for the CID-RSPT comparison (CID is always larger than, or equal to, FCI). CID takes into account all 2p2h interactions, while the second-order contribution is only one of many more contributions, lying in the third, fourth, fifth, etc higher orders.



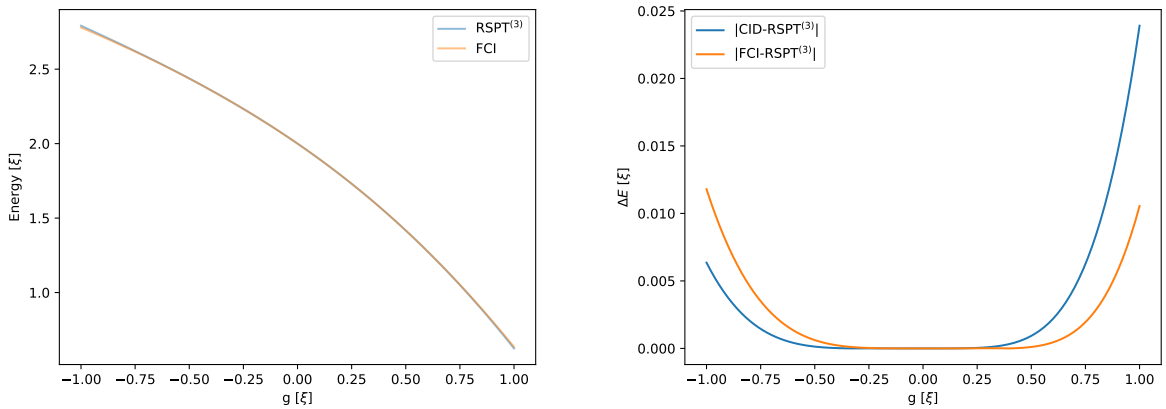
(a) **(b)**

Figure 1.13: *(a) FCI and 2nd order RSPT against $g \in [-1, 1]$. (b) The absolute difference between CID and 2nd order RSPT, and the absolute difference between FCI and 2nd order RSPT against $g \in [-1, 1]$.*

3rd order RSPT

The third order RSPT approximation to the ground state energy is plotted with the FCI calculation in Figure 1.14(a). It undershoots on the energy for values of $g < 0$, while it is

larger than the FCI calculated energy for all values $g > 0$. The (b) figure in Figure 1.14 displays the differences between the RSPT approximation to the third order and the CID and FCI calculations.



(a) (b)

Figure 1.14: *(a) FCI and 3rd order RSPT against $g \in [-1, 1]$. (b) The absolute difference between CID and 3rd order RSPT, and the absolute difference between FCI and 3rd order RSPT against $g \in [-1, 1]$*

1.7 Rayleigh-Schrödinger Perturbation Theory to the Fourth Order

1.7.1 Linked and Unlinked Diagrams

A linked diagram can be thought of as a graph where there exists a path from every node to every other node in the graph. In contrast, we have the unlinked diagrams, which can be seen as a product of two (or more) diagrams, which are not connected. Figure 1.15 displays an example of a linked diagram (left) and an unlinked diagram (right).

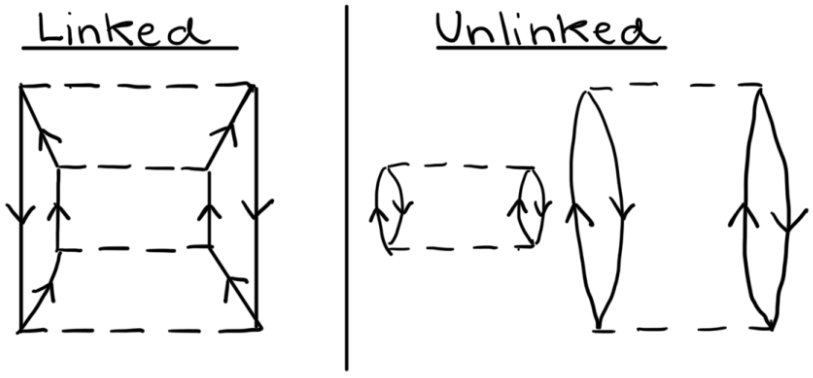


Figure 1.15: *An example of a linked diagram (left) and an unlinked diagram (right).*

1.7.2 Goldstone's Linked Diagram Theorem

The idea behind the Linked Diagram Theorem is that the unlinked diagrams cancel terms among the linked diagrams, which needs to be cancelled. It can be shown through insertion of the the unlinked parts of the unlinked diagrams that they exactly cancel terms of the linked chains of the MBPT order term, and are often called renormalization terms. The denominators are shown through the factorization-theorem to exactly match up between the linked and unlinked terms. The idea is that we can "insert" the unlinked parts at a specific place, which will create one of the linked diagrams, and that all possible insertions will each correspond to a linked diagram, and therefore cancel.

1.7.3 Remaining Diagrams for the Fourth Order Correction term

The interactions of the kind $\left\langle \Phi_{i+i-}^{a+a-} \middle| \hat{V} \middle| \Phi_{i+i-j+j-}^{a+a-b+b-} \right\rangle$ will look like

$$\begin{aligned}\left\langle \Phi_{i+i-}^{a+a-} \middle| \hat{V} \middle| \Phi_{i+i-j+j-}^{a+a-b+b-} \right\rangle &= \langle jj| \hat{v} |bb\rangle_{AS} \\ \left\langle \Phi_{i+i-j+j-}^{a+a-b+b-} \middle| \hat{V} \middle| \Phi_{i+i-}^{a+a-} \right\rangle &= \langle bb| \hat{v} |jj\rangle_{AS} ,\end{aligned}$$

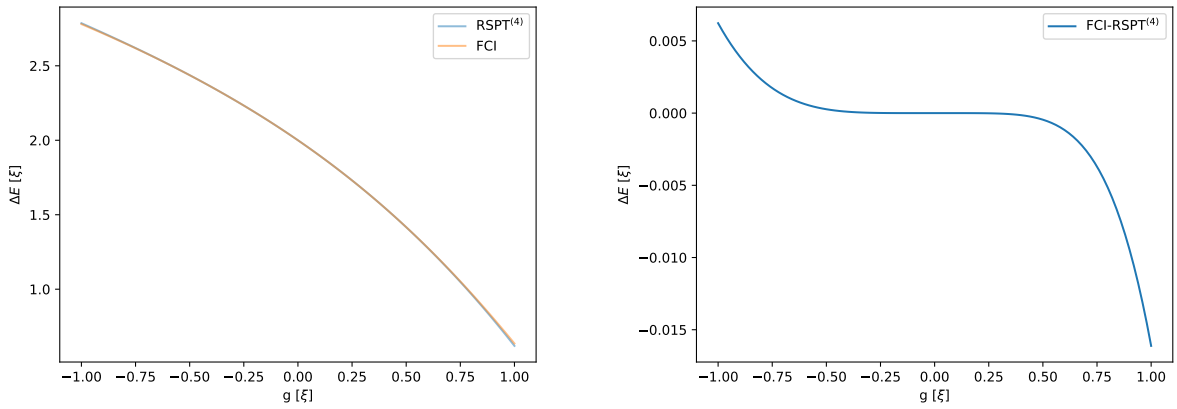
and there will be terms of the kind

$$\frac{\langle ii| \hat{v} |aa\rangle \langle jj| \hat{v} |bb\rangle \langle bb| \hat{v} |jj\rangle \langle aa| \hat{v} |ii\rangle}{(2\epsilon_a - 2\epsilon_i)(2\epsilon_a + 2\epsilon_b - 2\epsilon_j - 2\epsilon_i)^2(2\epsilon_a - 2\epsilon_i)},$$

which will be cancelled by the renormalization terms. More specifically, the unlinked diagrams 33 and 41 will cancel all contributions from 4p4h (all diagrams in Figure 6 in (Hjorth-Jensen, 2022)), and we will have our 2p2h terms in Figure 4 from (Hjorth-Jensen, 2022).

1.7.4 Results from RSPT of the Fourth Order

Figure 1.16(a) displays the calculated energy with contributions up to the fourth order using the RSPT method, and it is plotted alongside the FCI implementation. In Figure 1.16(b) you can see the difference between the FCI and the fourth order approximation. Notice that the fourth order approximation undershoots for $g < 0$, while it gives an approximation with higher energy for $g > 0$. As the 4p4h excitations has not yet contributed anything to the energy, for all $g \in [-0.5, 0.5]$ gives decent approximations to the ground state energy, while it has troubles when the interaction strength approaches ξ.



(a) **(b)**

Figure 1.16: *(a) FCI and 4th order RSPT against $g \in [-1, 1]$. (b) The absolute difference between FCI and 4th order RSPT against $g \in [-1, 1]$*

References

Hjorth-Jensen, Morten (Nov. 2022). “Second Midterm problem set”. In: (cit. on pp. 2, 25).