Second midterm FYS4480
Quantum mechanics for many-particle systems

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Abstract

The code for this project is available at our GitHub Repository[1]. The project was a joint effort between August Femtehjell and Oskar Idland.

Introduction

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 superfluiditity 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. Thereafter, we present the various exercises.

The Hamiltonian acting in the complete 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

$$\hat{H} = \sum_{\alpha\beta} \langle \alpha | h_0 | \beta \rangle a_\alpha^\dagger a_\beta + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | V | \gamma\delta \rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma,$$

where $a_\alpha^\dagger$ and a_α 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.

[1] https://github.com/augustfe/FYS4480

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 $\mathcal{P}$ is defined by an operator

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

where we assume that $m = \dim(\mathcal{P})$ 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 Fig. 1. The first two single-particle levels define a possible model space, indicated by the label $\mathcal{P}$. The remaining states span the excluded space $\mathcal{Q}$.

We write the Hamiltonian as

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

where

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

and

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

Here, 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, as indicated by the rightmost four-particle state in Fig. 1. There one of the pairs is excited to the state with $p = 9$ and the other to the state $p = 7$. The two middle possibilities are not possible with the present model. We label single-particle states within the model space as hole-states. The single-particle states outside the model space are then particle states.

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.

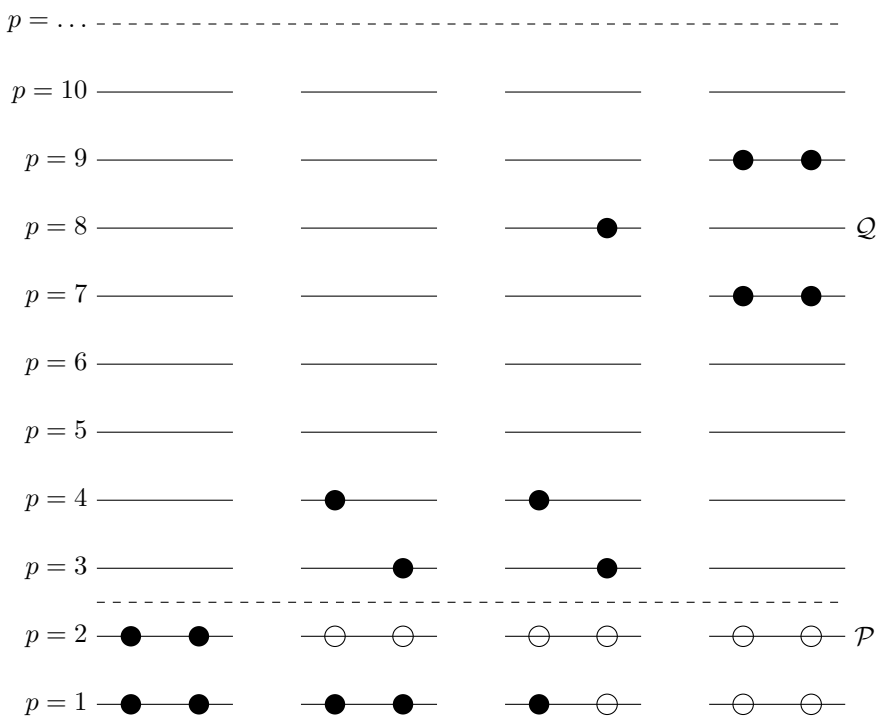


Figure 1: Schematic plot of the possible single-particle levels with double degeneracy. The filled circles indicate occupied particle states while the empty circles represent vacant particle (hole) states. The spacing between each level p is constant in this picture. The first two single-particle levels define our possible model space, indicated by the label $\mathcal{P}$. The remaining states span the excluded space $\mathcal{Q}$. The first state to the left represents a possible ground state representation for a four-fermion system. In the second state to the left, one pair is broken. This possibility is however not included in our interaction.

Exercise 1)

Show that the unperturbed Hamiltonian $\hat{H}_0$ and $\hat{V}$ commute with both the spin projection $\hat{S}_z$ and the total spin $\hat{S}^2$, given by

$$\hat{S}_z := \frac{1}{2}\sum_{p\sigma} \sigma a^\dagger_{p\sigma} a_{p\sigma} \quad \text{and} \quad \hat{S}^2 := \hat{S}_z^2 + \frac{1}{2}(\hat{S}_+\hat{S}_- + \hat{S}_-\hat{S}_+),$$

where

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

This is an important feature of our system that allows us to block-diagonalize the full Hamiltonian. We will focus on total spin $S = 0$. In this case, it is convenient to define the so-called pair creation and pair annihilation operators

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

respectively.

Show that you can rewrite the Hamiltonian (with $\xi = 1$) as

$$\hat{H} = \sum_{p\sigma} (p-1) a^\dagger_{p\sigma} a_{p\sigma} - \frac{1}{2} g \sum_{pq} \hat{P}^+_p \hat{P}^-_q .$$

Show also that pair creation operators commute among themselves.

In this midterm we focus only on a system with no broken pairs. This means that the Hamiltonian can only link two-particle states in so-called spin-reversed states.

Solution

We firstly need to show that the unperturbed Hamiltonian $\hat{H}_0$ and the two-body operator $\hat{V}$ commute with the spin projection $\hat{S}_z$. We have, being careful with the summation indices,

$$\begin{aligned}
\left[\hat{H}_0, \hat{S}_z\right] &= \left[\sum_{p\sigma} (p-1) a^\dagger_{p\sigma} a_{p\sigma}, \frac{1}{2}\sum_{q\tau} \tau a^\dagger_{q\tau} a_{q\tau}\right] \\
&= \frac{1}{2}\sum_{p\sigma} (p-1) \sum_{q\tau} \tau \left[a^\dagger_{p\sigma} a_{p\sigma}, a^\dagger_{q\tau} a_{q\tau}\right] \\
&= \frac{1}{2}\sum_{p\sigma} (p-1) \sum_{q\tau} \tau \left[\hat{n}_{p\sigma}, \hat{n}_{q\tau}\right],
\end{aligned}$$

where we have defined the number operator $\hat{n}_{p\sigma} = a^\dagger_{p\sigma} a_{p\sigma}$. As the number operator commutes with itself, we have that $[\hat{n}_{p\sigma}, \hat{n}_{q\tau}] = 0$, and thus $[\hat{H}_0, \hat{S}_z] = 0$.

Next, we show that the two-body operator $\hat{V}$ commutes with the spin projection $\hat{S}_z$. We have, again being careful with the summation indices,

$$\begin{aligned}\left[\hat{V}, \hat{S}_z\right] &= \left[-\frac{1}{2}g\sum_{pq} a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}, \frac{1}{2}\sum_{r\sigma}\sigma a^\dagger_{r\sigma}a_{r\sigma}\right] \\ &= -\frac{1}{4}g\sum_{pqr\sigma}\sigma\left[a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}, a^\dagger_{r\sigma}a_{r\sigma}\right] \\ &= -\frac{1}{4}g\sum_{pqr\sigma}\sigma\left[a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}, \hat{n}_{r\sigma}\right].\end{aligned}$$

Using the commutation indentity

$$[AB, C] = A\,[B, C] + [A, C]\,B,$$

we have

$$\left[a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}, \hat{n}_{r\sigma}\right] = a^\dagger_{p+}a^\dagger_{p-}\left[a_{q-}a_{q+}, \hat{n}_{r\sigma}\right] + \left[a^\dagger_{p+}a^\dagger_{p-}, \hat{n}_{r\sigma}\right]a_{q-}a_{q+}, \quad (1)$$

and then need to find expressions for

$$\left[a_{q-}a_{q+}, \hat{n}_{r\sigma}\right] \quad \text{and} \quad \left[a^\dagger_{p+}a^\dagger_{p-}, \hat{n}_{r\sigma}\right].$$

Changing the indices for brevity in the intermediate steps, we need to find

$$[a_pa_q, \hat{n}_r] \quad \text{and} \quad \left[a^\dagger_pa^\dagger_q, \hat{n}_r\right],$$

noting that

$$[a_pa_q, \hat{n}_r] = a_p\,[a_q, \hat{n}_r] + [a_p, \hat{n}_r]\,a_q.$$

As

$$\begin{aligned}[a_q, \hat{n}_r] = \left[a_q, a^\dagger_ra_r\right] &= \left[a_q, a^\dagger_r\right]a_r + a^\dagger_r\,[a_q, a_r] \\ &= \delta_{qr}a_r + a^\dagger_r\cdot 0 = \delta_{qr}a_r = a_q,\end{aligned}$$

We have

$$\begin{aligned}[a_pa_q, \hat{n}_r] &= a_p\,[a_q, \hat{n}_r] + [a_p, \hat{n}_r]\,a_q \\ &= a_pa_q + a_pa_q = 2a_pa_q.\end{aligned}$$

Similarly, for the creation operators, we have

$$\left[a^\dagger_p, \hat{n}_r\right] = \left[a^\dagger_p, a^\dagger_ra_r\right] = \left[a^\dagger_p, a^\dagger_r\right]a_r + a^\dagger_r\left[a^\dagger_p, a_r\right] = -\delta_{pr}a^\dagger_r = -a^\dagger_p,$$

and thus

$$\begin{aligned}\left[a^\dagger_pa^\dagger_q, \hat{n}_r\right] &= a^\dagger_p\left[a^\dagger_q, \hat{n}_r\right] + \left[a^\dagger_p, \hat{n}_r\right]a^\dagger_q \\ &= -a^\dagger_pa^\dagger_q - a^\dagger_pa^\dagger_q = -2a^\dagger_pa^\dagger_q.\end{aligned}$$

Returning to Eq. (1) with the correct labels, we have

$$\begin{aligned}\left[a_{p+}^\dagger a_{p-}^\dagger a_{q-} a_{q+}, \hat{n}_{r\sigma}\right] &= a_{p+}^\dagger a_{p-}^\dagger \left[a_{q-} a_{q+}, \hat{n}_{r\sigma}\right] + \left[a_{p+}^\dagger a_{p-}^\dagger, \hat{n}_{r\sigma}\right] a_{q-} a_{q+} \\ &= 2a_{p+}^\dagger a_{p-}^\dagger a_{q-} a_{q+} - 2a_{p+}^\dagger a_{p-}^\dagger a_{q-} a_{q+} \\ &= 0,\end{aligned}$$

meaning that

$$\left[\hat{V}, \hat{S}_z\right] = -\frac{1}{4} g \sum_{pqr\sigma} \sigma \left[a_{p+}^\dagger a_{p-}^\dagger a_{q-} a_{q+}, \hat{n}_{r\sigma}\right] = 0.$$

We have thus shown that the unperturbed Hamiltonian $\hat{H}_0$ and the two-body operator $\hat{V}$ commute with the spin projection $\hat{S}_z$.

Next, we want to show the commutations of $\hat{H}_0$ and $\hat{V}$ with the total spin $\hat{S}^2$. Starting with $\hat{H}_0$, we have

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

As we have shown that $\hat{H}_0$ commutes with $\hat{S}_z$, we also have $\left[\hat{H}_0, \hat{S}_z^2\right] = 0$, and thus only need to place our attention on

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

We will only show the commutation of $\hat{H}_0$ with $\hat{S}_\pm \hat{S}_\mp$. Breaking the expression down further, we have

$$\left[\hat{H}_0, \hat{S}_\pm \hat{S}_\mp\right] = \left[\hat{H}_0, \hat{S}_\pm\right] \hat{S}_\mp + \hat{S}_\pm \left[\hat{H}_0, \hat{S}_\mp\right].$$

We then have

$$\begin{aligned}\left[\hat{H}_0, \hat{S}_\pm\right] &= \left[\sum_{p\sigma} (p-1) a_{p\sigma}^\dagger a_{p\sigma}, \sum_q a_{q\pm}^\dagger a_{q\mp}\right] \\ &= \sum_{pq\sigma} (p-1)\left[a_{p\sigma}^\dagger a_{p\sigma}, a_{q\pm}^\dagger a_{q\mp}\right].\end{aligned}$$

Considering the commutation, using the number operator, we have

$$\begin{aligned}\left[\hat{n}_{p\sigma}, a_{q\pm}^\dagger a_{q\mp}\right] &= a_{q\pm}^\dagger \left[\hat{n}_{p\sigma}, a_{q\mp}\right] + \left[\hat{n}_{p\sigma}, a_{q\pm}^\dagger\right] a_{q\mp} \\ &= -a_{q\pm}^\dagger a_{q\mp} + a_{q\pm}^\dagger a_{q\mp} = 0,\end{aligned}$$

and thus

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

We have thus shown that $\left[\hat{H}_0, \hat{S}^2\right] = 0$.

Next, we show that $\hat{V}$ commutes with $\hat{S}^2$. We have

$$\begin{aligned}\left[\hat{V}, \hat{S}^2\right] &= \left[-\frac{1}{2}g\sum_{pq} a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}, \hat{S}_z^2 + \frac{1}{2}(\hat{S}_+\hat{S}_- + \hat{S}_-\hat{S}_+)\right] \\ &= \left[\hat{V}, \hat{S}_z^2\right] + \left[\hat{V}, \frac{1}{2}(\hat{S}_+\hat{S}_- + \hat{S}_-\hat{S}_+)\right].\end{aligned}$$

Again, as we've already shown that $\hat{V}$ commutes with $\hat{S}_z$, we only need to consider the commutation with $\hat{S}_\pm\hat{S}_\mp$. We analogously again have

$$\left[\hat{V}, \hat{S}_\pm\hat{S}_\mp\right] = \left[\hat{V}, \hat{S}_\pm\right]\hat{S}_\mp + \hat{S}_\pm\left[\hat{V}, \hat{S}_\mp\right],$$

where

$$\begin{aligned}\left[\hat{V}, \hat{S}_\pm\right] &= \left[-\frac{1}{2}g\sum_{pq} a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}, \sum_r a^\dagger_{r\pm}a_{r\mp}\right] \\ &= -\frac{1}{2}g\sum_{pqr}\left[a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}, a^\dagger_{r\pm}a_{r\mp}\right].\end{aligned}$$

Breaking the expression down further, we have

$$\begin{aligned}\left[a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}, a^\dagger_{r\pm}a_{r\mp}\right] &= a^\dagger_{p+}a^\dagger_{p-}\left[a_{q-}a_{q+}, a^\dagger_{r\pm}a_{r\mp}\right] \\ &\quad + \left[a^\dagger_{p+}a^\dagger_{p-}, a^\dagger_{r\pm}a_{r\mp}\right]a_{q-}a_{q+}.\end{aligned} \tag{2}$$

Considering the two contractions seperately, starting with the first one:

$$\left[a_{q-}a_{q+}, a^\dagger_{r\pm}a_{r\mp}\right] = a_{q-}\left[a_{q+}, a^\dagger_{r\pm}a_{r\mp}\right] + \left[a_{q-}, a^\dagger_{r\pm}a_{r\mp}\right]a_{q+}.$$

These expressions follow the same pattern, so we only consider $q\pm \mapsto q$.

$$\begin{aligned}\left[a_q, a^\dagger_{r\pm}a_{r\mp}\right] &= \left[a_q, a^\dagger_{r\pm}\right]a_{r\mp} + a^\dagger_{r\pm}\left[a_q, a_{r\mp}\right] \\ &= \delta_{q,r\pm}a_{r\mp} + a^\dagger_{r\pm}\cdot 0 = \delta_{q,r\pm}a_{r\mp}.\end{aligned}$$

We thus only get a contribution when $q = r$ and the spin parities match. We then have

$$\begin{aligned}\left[a_{q-}a_{q+}, a^\dagger_{r\pm}a_{r\mp}\right] &= a_{q-}\left[a_{q+}, a^\dagger_{r\pm}a_{r\mp}\right] + \left[a_{q-}, a^\dagger_{r\pm}a_{r\mp}\right]a_{q+} \\ &= a_{q-}\delta_{q+,r\pm}a_{r\mp} + \delta_{q-,r\pm}a_{r\mp}a_{q+} \\ &= \delta_{q+,r\pm}a_{q-}a_{r\mp} - \delta_{q-,r\pm}a_{q+}a_{r\mp}\end{aligned}$$

Continuing with the second contraction, we have

$$\left[a^\dagger_{p+}a^\dagger_{p-}, a^\dagger_{r\pm}a_{r\mp}\right] = a^\dagger_{p+}\left[a^\dagger_{p-}, a^\dagger_{r\pm}a_{r\mp}\right] + \left[a^\dagger_{p+}, a^\dagger_{r\pm}a_{r\mp}\right]a^\dagger_{p-},$$

which again follow the same pattern. Writing $p\pm \mapsto p$ we have

$$\begin{aligned}\left[a^\dagger_p, a^\dagger_{r\pm}a_{r\mp}\right] &= \left[a^\dagger_p, a^\dagger_{r\pm}\right]a_{r\mp} + a^\dagger_{r\pm}\left[a^\dagger_p, a_{r\mp}\right] \\ &= 0\cdot a_{r\mp} - a^\dagger_{r\pm}\delta_{p,r\mp} = -a^\dagger_{r\pm}\delta_{p,r\mp}.\end{aligned}$$

Inserting the expressions back into the commutator, we have

$$\begin{aligned}\left[a^\dagger_{p+}a^\dagger_{p-}, a^\dagger_{r\pm}a_{r\mp}\right] &= a^\dagger_{p+}\left[a^\dagger_{p-}, a^\dagger_{r\pm}a_{r\mp}\right] + \left[a^\dagger_{p+}, a^\dagger_{r\pm}a_{r\mp}\right]a^\dagger_{p-} \\ &= -a^\dagger_{p+}a^\dagger_{r\pm}\delta_{p-,r\mp} - a^\dagger_{r\pm}\delta_{p+,r\mp}a^\dagger_{p-} \\ &= -\delta_{p-,r\mp}a^\dagger_{p+}a^\dagger_{r\pm} + \delta_{p+,r\mp}a^\dagger_{p-}a^\dagger_{r\pm}.\end{aligned}$$

As the results are getting quite wieldy, we summarize the different cases of spin parities in the commutator.

$$\begin{aligned}\left[a_{q-}a_{q+}, a^\dagger_{r+}a_{r-}\right] &= \delta_{q+,r+}a_{q-}a_{r-} = 0 \\ \left[a_{q-}a_{q+}, a^\dagger_{r-}a_{r+}\right] &= -\delta_{q-,r-}a_{q+}a_{r+} = 0 \\ \left[a^\dagger_{p+}a^\dagger_{p-}, a^\dagger_{r+}a_{r-}\right] &= -\delta_{p-,r-}a^\dagger_{p+}a^\dagger_{r+} = 0 \\ \left[a^\dagger_{p+}a^\dagger_{p-}, a^\dagger_{r-}a_{r+}\right] &= \delta_{p+,r+}a^\dagger_{p-}a^\dagger_{r-} = 0.\end{aligned}$$

We thus have that that Eq. (2) simplifies to

$$\left[a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}, a^\dagger_{r\pm}a_{r\mp}\right] = 0,$$

which means that $\left[\hat{V}, \hat{S}_\pm\right] = 0$, giving us that

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

We have thus shown that both $\hat{H}_0$ and $\hat{V}$ commute with the total spin $\hat{S}^2$.

With $\xi = 1$, the one-body operator $\hat{H}_0$ is defined as

$$\hat{H}_0 = \sum_{p\sigma}(p-1)a^\dagger_{p\sigma}a_{p\sigma}.$$

For the two-body operator $\hat{V}$, we have, substituting $\hat{P}^+_p = a^\dagger_{p+}a^\dagger_{p-}$ and $\hat{P}^-_q = a_{q-}a_{q+}$,

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

This leaves us with the rewritten Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{V} = \sum_{p\sigma}(p-1)a^\dagger_{p\sigma}a_{p\sigma} - \frac{1}{2}g\sum_{pq}\hat{P}^+_p\hat{P}^-_q.$$

Finally, we want to show that the pair creation operators commute among themselves.

$$\begin{aligned}\left[\hat{P}^+_p, \hat{P}^+_q\right] &= \left[a^\dagger_{p+}a^\dagger_{p-}, a^\dagger_{q+}a^\dagger_{q-}\right] \\ &= a^\dagger_{p+}a^\dagger_{p-}a^\dagger_{q+}a^\dagger_{q-} - a^\dagger_{q+}a^\dagger_{q-}a^\dagger_{p+}a^\dagger_{p-} \\ &= a^\dagger_{p+}a^\dagger_{p-}a^\dagger_{q+}a^\dagger_{q-} - (-1)^2a^\dagger_{p+}a^\dagger_{q+}a^\dagger_{q-}a^\dagger_{p-} \\ &= a^\dagger_{p+}a^\dagger_{p-}a^\dagger_{q+}a^\dagger_{q-} - (-1)^4a^\dagger_{p+}a^\dagger_{p-}a^\dagger_{q+}a^\dagger_{q-} \\ &= 0.\end{aligned}$$

Similarly, one can show that the pair annihilation operators also commute among themselves.

Exercise 2)

Construct thereafter the Hamiltonian matrix for a system with no broken pairs and total spin $S = 0$ for the case of the four lowest single-particle levels indicated in the Fig. 1. Our system consists of four particles only. Our single-particle space consists of only the four lowest levels $p = 1, 2, 3, 4$. You need to set up all possible Slater determinants. Find all eigenvalues by diagonalizing the Hamiltonian matrix. Vary your results for values of $g \in [-1, 1]$. We refer to this as the exact calculation. Comment the behavior of the ground state as function of g.

Solution

Due to the requirement of no broken pairs, total spin $S = 0$, and the fact that we have four particles, the number of possible Slater determinants is quite limited. We choose our ansatz $|\Phi_0\rangle$ to be the Slater determinant with all four particles below the Fermi level of $p = 2$. The possible Slater determinants are shown in Fig. 2.

Setting up the Slater determinants in second quantization, we set the ground state to be

$$|\Phi_0\rangle = a^\dagger_{1+}a^\dagger_{1-}a^\dagger_{2+}a^\dagger_{2-}|0\rangle,$$

or equivalently with the pair creation operators

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

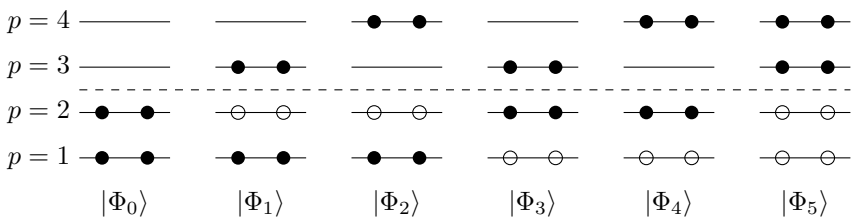


Figure 2: Schematic representation of the six possible Slater determinants for a system with four particles, under the constraint of no broken pairs, total spin $S = 0$, considering only the four lowest levels $p = 1, 2, 3, 4$.

The other Slater determinants are then

$$\begin{aligned} |\Phi_1\rangle &= \hat{P}_1^+ \hat{P}_3^+ |0\rangle, & |\Phi_2\rangle &= \hat{P}_1^+ \hat{P}_4^+ |0\rangle, \\ |\Phi_3\rangle &= \hat{P}_2^+ \hat{P}_3^+ |0\rangle, & |\Phi_4\rangle &= \hat{P}_2^+ \hat{P}_4^+ |0\rangle, \\ |\Phi_5\rangle &= \hat{P}_3^+ \hat{P}_4^+ |0\rangle. \end{aligned}$$

Equivalently, we can write these relative to the ground state as

$$\begin{aligned} |\Phi_1\rangle &= \hat{P}_3^+ \hat{P}_2^- |\Phi_0\rangle, & |\Phi_2\rangle &= \hat{P}_4^+ \hat{P}_2^- |\Phi_0\rangle, \\ |\Phi_3\rangle &= \hat{P}_3^+ \hat{P}_1^- |\Phi_0\rangle, & |\Phi_4\rangle &= \hat{P}_4^+ \hat{P}_1^- |\Phi_0\rangle, \\ |\Phi_5\rangle &= \hat{P}_4^+ \hat{P}_3^+ \hat{P}_1^- \hat{P}_2^- |\Phi_0\rangle. \end{aligned}$$

Note that as the pair creation and annihilation operators commute, the order of the operators in the Slater determinants is not important.

We define an arbitrary four-particle state $|\Phi_{\alpha,\beta}\rangle$, with $\alpha < \beta$, as

$$|\Phi_{\alpha,\beta}\rangle = \hat{P}_\alpha^+ \hat{P}_\beta^+ |0\rangle$$

in order to simplify the computation for the Hamiltonian matrix. For $\langle\Phi_{\alpha,\beta}|\hat{H}_0|\Phi_{\gamma,\delta}\rangle$, we only need to consider the terms where $(\alpha, \beta) = (\gamma, \delta)$, as the other terms vanish due to the orthogonality of the Slater determinants.

$$\begin{aligned} \langle\Phi_{\alpha,\beta}|\hat{H}_0|\Phi_{\alpha,\beta}\rangle &= \langle\Phi_{\alpha,\beta}| \sum_{p\sigma} (p-1) a_{p\sigma}^\dagger a_{p\sigma} |\Phi_{\alpha,\beta}\rangle \\ &= \sum_{p\sigma} (p-1) \langle\Phi_{\alpha,\beta}| a_{p\sigma}^\dagger a_{p\sigma} |\Phi_{\alpha,\beta}\rangle \\ &= \sum_{\substack{p=\alpha,\beta \\ \sigma=\pm}} (p-1) \\ &= 2(\alpha-1) + 2(\beta-1) \\ &= 2(\alpha+\beta-2). \end{aligned}$$

Next, we consider $\langle \Phi_{\alpha,\beta} | \hat{V} | \Phi_{\gamma,\delta} \rangle$.

$$\begin{aligned}
\langle \Phi_{\alpha,\beta} | \hat{V} | \Phi_{\gamma,\delta} \rangle &= -\frac{1}{2} g \sum_{pq} \langle \Phi_{\alpha,\beta} | \hat{P}_p^+ \hat{P}_q^- | \Phi_{\gamma,\delta} \rangle \\
&= -\frac{1}{2} g \sum_{pq} \langle 0 | \hat{P}_\beta^- \hat{P}_\alpha^- \hat{P}_p^+ \hat{P}_q^- \hat{P}_\gamma^+ \hat{P}_\delta^+ | 0 \rangle
\end{aligned}$$

The possible contractions are then

$$(1) \quad \left\langle 0 \middle| \hat{P}_\beta^- \hat{P}_\alpha^- \hat{P}_p^+ \hat{P}_q^- \hat{P}_\gamma^+ \hat{P}_\delta^+ \middle| 0 \right\rangle = \delta_{\beta\delta}\delta_{\alpha p}\delta_{q\gamma}$$

$$(2) \quad \left\langle 0 \middle| \hat{P}_\beta^- \hat{P}_\alpha^- \hat{P}_p^+ \hat{P}_q^- \hat{P}_\gamma^+ \hat{P}_\delta^+ \middle| 0 \right\rangle = \delta_{\beta\gamma}\delta_{\alpha p}\delta_{q\delta}$$

$$(3) \quad \left\langle 0 \middle| \hat{P}_\beta^- \hat{P}_\alpha^- \hat{P}_p^+ \hat{P}_q^- \hat{P}_\gamma^+ \hat{P}_\delta^+ \middle| 0 \right\rangle = \delta_{\beta p}\delta_{\alpha\gamma}\delta_{q\delta}$$

$$(4) \quad \left\langle 0 \middle| \hat{P}_\beta^- \hat{P}_\alpha^- \hat{P}_p^+ \hat{P}_q^- \hat{P}_\gamma^+ \hat{P}_\delta^+ \middle| 0 \right\rangle = \delta_{\beta p}\delta_{\alpha\delta}\delta_{q\gamma}$$

Note the positive sign in the Wick contractions, as all contraction lines are actually between pairs of operators. This means that all labeled lines actually correspond to two lines, such that all crossings labeled actually contain four crossings, and thus a positive sign.

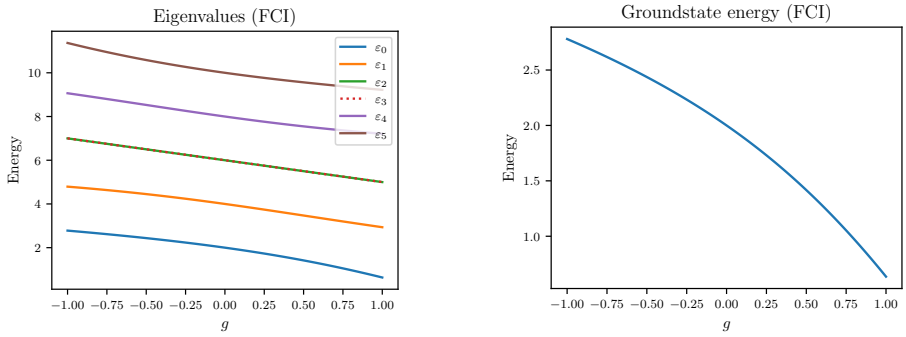
From this, we can then calculate the matrix elements of the Hamiltonian matrix based on the number of matched pairs. When two pairs match, i.e. along the diagonal, we get contributions from (1) and (3). When one pair matches and the other differs, we get contributions from *either* (2) or (4). When no pairs match, the matrix element is zero.

From this, we can set up the Hamiltonian matrix for the system, ordered as $|\Phi_0\rangle, |\Phi_1\rangle, \ldots, |\Phi_5\rangle$.

$$\begin{aligned}
H &= H_0 + V \\
&= \begin{bmatrix} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 6 & 0 & 0 & 0 \\ 0 & 0 & 0 & 6 & 0 & 0 \\ 0 & 0 & 0 & 0 & 8 & 0 \\ 0 & 0 & 0 & 0 & 0 & 10 \end{bmatrix} - \frac{g}{2} \begin{bmatrix} 2 & 1 & 1 & 1 & 1 & 0 \\ 1 & 2 & 1 & 1 & 0 & 1 \\ 1 & 1 & 2 & 0 & 1 & 1 \\ 1 & 1 & 0 & 2 & 1 & 1 \\ 1 & 0 & 1 & 1 & 2 & 1 \\ 0 & 1 & 1 & 1 & 1 & 2 \end{bmatrix} \\
&= \begin{bmatrix} 2-g & -\frac{g}{2} & -\frac{g}{2} & -\frac{g}{2} & -\frac{g}{2} & 0 \\ -\frac{g}{2} & 4-g & -\frac{g}{2} & -\frac{g}{2} & 0 & -\frac{g}{2} \\ -\frac{g}{2} & -\frac{g}{2} & 6-g & 0 & -\frac{g}{2} & -\frac{g}{2} \\ -\frac{g}{2} & -\frac{g}{2} & 0 & 6-g & -\frac{g}{2} & -\frac{g}{2} \\ -\frac{g}{2} & 0 & -\frac{g}{2} & -\frac{g}{2} & 8-g & -\frac{g}{2} \\ 0 & -\frac{g}{2} & -\frac{g}{2} & -\frac{g}{2} & -\frac{g}{2} & 10-g \end{bmatrix}
\end{aligned}$$

We diagonalize this matrix for varying values of $g \in [-1, 1]$ with NumPy, computed in the script `exact_energy.py`. Plotted as a function of g, the

eigenvalues are shown in Fig. 3a, while the ground state energy is shown in Fig. 3b.



(a) Eigenvalues from FCI.

(b) Groundstate energy from FCI.

Figure 3: Eigenvalues and ground state energy of the Hamiltonian matrix for the four-particle system with no broken pairs and total spin $S = 0$, as a function of the pairing strength g.

As the strength of the interaction g increases, the ground state energy decreases. When $g = 0$, we have the non-interaction case, where the ground state energy is simply $\langle \Phi_0 | \hat{H}_0 | \Phi_0 \rangle = 2$. As we are including all states possible states up to a given energy level, we are using FCI theory to solve the system.

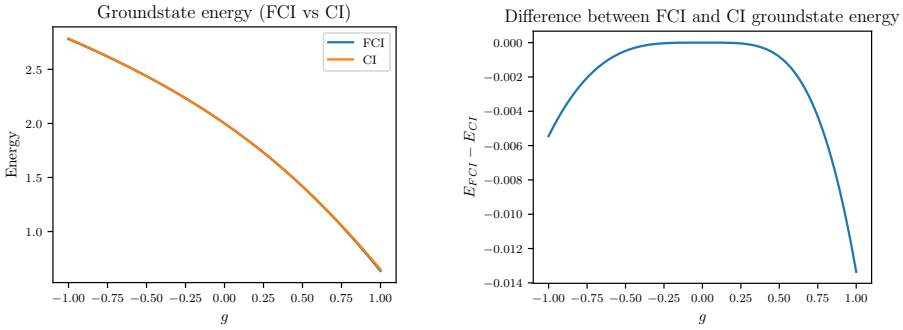
Exercise 3)

Instead of setting up all possible Slater determinants, construct only an approximation to the ground state (where we assume that the four particles are in the two lowest single-particle orbits only) which includes at most two-particle-two-hole excitations. Diagonalize this matrix and compare with the exact calculation and comment your results. Can you set up which diagrams this approximation corresponds to?

Solution

From Fig. 2 we see that all states except $|\Phi_5\rangle$ have states with at most one pair of electrons above the $p = 2$. This corresponds with Configuration Interaction (CI) calculations with at most two-particle-two-hole excitations. Our new approximation of the ground state is then shown in Fig. 4a.

As the figure shows, the approximate energies are very close, regardless of whether we include the four-particle state $|\Phi_5\rangle$. The difference is shown in Fig. 4b, showing that the difference is more substantial for higher values of g. As we are working with variational methods, the energy from the CI calculations will always be higher than the exact energy, as the CI calculations are based on



(a) Groundstate energy from CI.

(b) Difference in energy from CI.

Figure 4: Groundstate energy from the CI calculations with at most two-particle-two-hole excitations, compared with the FCI results, as a function of g.

a subset of the full space. The contributing diagrams in this case are shown in Fig. 5.

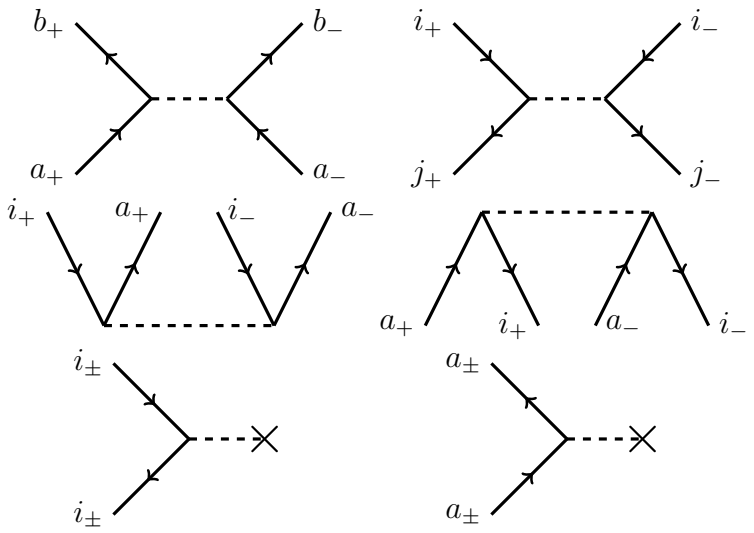


Figure 5: Diagrams corresponding to the approximation of the ground state with at most two-particle-two-hole excitations.

Exercise 4)

We switch now to approximative methods, in our case Hartree-Fock theory and many-body perturbation theory. Hereafter we will define our model space to consist of the single-particle levels $p = 1, 2$. The remaining levels $p = 3, 4$ define our excluded space. This means that our ground state Slater determinant consists of four particles which can be placed in the doubly degenerate orbits $p = 1$ and $p = 2$. Our first step is to perform a Hartree-Fock calculation with the pairing Hamiltonian. Write first the normal-ordered Hamiltonian with respect to the above reference state given by four spin 1/2 fermions in the single-particle levels $p = 1, 2$. Write down the normal-ordered Hamiltonian and set up the standard Hartree-Fock equations for the above system (often called restricted Hartree-Fock due to the fact that we have an equal number of spin-orbitals). These equations are sometimes also called the canonical Hartree-Fock equations. They are the same as those that we discussed earlier. This means that we have a Hartree-Fock Hamiltonian $\hat{h}^{\mathrm{HF}}|p\rangle = \epsilon^{\mathrm{HF}}|p\rangle$, where p are both hole and particle states.

Solution

We begin by writing the normal-ordered form of the single-particle term of the Hamiltonian with respect to the reference state $|\Phi_0\rangle$,

$$\hat{H}_0 = \sum_{p\sigma}(p-1)a^\dagger_{p\sigma}a_{p\sigma}.$$

We have that

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

Next, we have the two-body term of the Hamiltonian,

$$\hat{V} = -\frac{1}{2}g\sum_{pq} a_{p+}^\dagger a_{p-}^\dagger a_{q-}a_{q+}.$$

For the annihilation and creation operators in the two-body term, we have the possible contractions

$$\overbrace{a_{p+}^\dagger a_{p-}^\dagger a_{q-}}a_{q+} = \delta_{pq}n_{p+}a_{p-}^\dagger a_{q-},$$
$$a_{p+}^\dagger \overbrace{a_{p-}^\dagger a_{q-}}a_{q+} = \delta_{pq}n_{p-}a_{p+}^\dagger a_{q+},$$
$$\overbrace{a_{p+}^\dagger \overbrace{a_{p-}^\dagger a_{q-}}a_{q+}} = \delta_{pq}n_{p+}n_{p-}a_{p+}^\dagger a_{q+}a_{p-}^\dagger a_{q-},$$

where $n_{p\sigma} = 1$ if $p = 1, 2$ and $n_{p\sigma} = 0$ otherwise. Note that as we have terms $n_{p\pm}a_{p\mp}^\dagger a_{p\mp}$, we only get contributions when both spins at a given level is occupied, i.e., from unbroken pairs.

We switch now to particle-hole formalism, where we denote states below the Fermi level as $i, j, \ldots \in \{1, 2\}$, states above the Fermi level as $a, b, \ldots \in \{3, 4\}$, and unrestricted indices as $p, q, \ldots$. The normal-ordered form of the two-body term is then

$$\begin{aligned}\hat{V} =& -\frac{1}{2}g\sum_{pq}\{a_{p+}^\dagger a_{p-}^\dagger a_{q-}a_{q+}\} - \frac{1}{2}g\sum_i\left[a_{p-}^\dagger a_{p-} + a_{p+}^\dagger a_{p+}\right] \\ & -\frac{1}{2}g\sum_i 1 \\ =& -\frac{1}{2}g\sum_{pq}\{a_{p+}^\dagger a_{p-}^\dagger a_{q-}a_{q+}\} - \frac{1}{2}g\sum_{i\sigma} a_{i\sigma}^\dagger a_{i\sigma} - g.\end{aligned}$$

Grouping the terms of parts involving no particles, one particle, and two particles respectively, we have the normal-ordered Hamiltonian as

$$\hat{H} = E_0^{\text{Ref}} + \hat{H}_0^N + \hat{V}^N,$$

where

$$\begin{aligned}E_0^{\text{Ref}} &= 2 - g \\ \hat{H}_0^N &= \sum_{p\sigma}(p-1)\{a_{p\sigma}^\dagger a_{p\sigma}\} - \frac{1}{2}g\sum_{i\sigma}\{a_{i\sigma}^\dagger a_{i\sigma}\} \\ \hat{V}^N &= -\frac{1}{2}g\sum_{pq}\{a_{p+}^\dagger a_{p-}^\dagger a_{q-}a_{q+}\}.\end{aligned}$$

We begin by defining the single-particle operator $\hat{f}$, which in the general case is given by

$$\langle p|\hat{f}|q\rangle = \langle p|\hat{H}_0|q\rangle + \sum_j \langle pj|\hat{V}|qj\rangle_{AS}.$$

Due to the nature of our Hamiltonian, we have that $\langle p|\hat{f}|q\rangle = 0$ for $p \neq q$. In second quantization, we then have that the operator becomes

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

In writing the operator in normal order, we have

$$\overbrace{a_p^\dagger a_p} = \{a_p^\dagger a_p\} + \delta_{pq} n_p,$$

and thus

$$\hat{F} = \sum_p \langle p|\hat{f}|p\rangle \{a_p^\dagger a_p\} + \sum_i \langle i|\hat{f}|i\rangle.$$

The canonical Hartree-Fock equations are then given by

$$\hat{f}|p\rangle = \sum_q \epsilon_{qp}|q\rangle.$$

Exercise 5)

We will now set up the Hartree-Fock equations by varying the coefficients of the single-particle functions. The single-particle basis functions are defined as

$$\psi_p = \sum_\lambda C_{p\lambda}\psi_\lambda.$$

where in our case $p = 1, 2, 3, 4$ and $\lambda = 1, 2, 3, 4$, that is the first four lowest single-particle orbits of Fig. 1. Set up the Hartree-Fock equations for this system by varying the coefficients $C_{p\lambda}$ and solve them for values of $g \in [-1, 1]$. Comment your results and compare with the exact solution. Discuss also which diagrams in Fig. 6 that can be affected by a Hartree-Fock basis. Compute the total ground state energy using a Hartree-Fock basis and comment your results.

We will now study the system using non-degenerate Rayleigh-Schrödinger perturbation theory to third order in the interaction. If we exclude the first order contribution, all possible diagrams (so-called anti-symmetric Goldstone diagrams) are shown in Fig. 6.

Based on the form of the interaction, which diagrams contribute to the energy of the ground state? Write down the expressions for the diagrams that contribute and find the contribution to the ground state energy as function $g \in [-1, 1]$. Comment your results. Compare these results with those you obtained in 2) and 3).

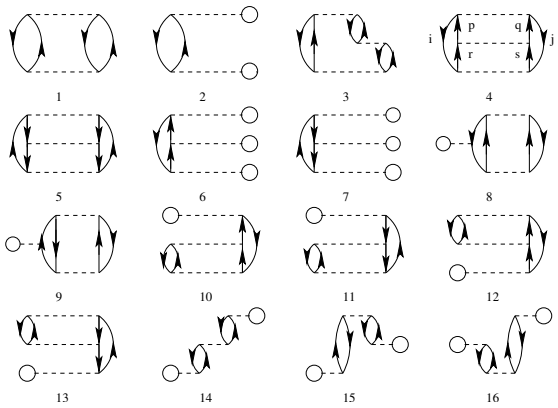


Figure 6: Diagrams to third order in the interaction. The first order term is excluded. All interaction vertices represent anti-symmetrized matrix elements.

Solution

Hartree-Fock

In the previous midterm, we found that the Hartree-Fock equations by way of varying coefficients are

$$\sum_{\gamma} h^{\mathrm{HF}}_{\alpha\gamma} C_{p\gamma} = \varepsilon_p C_{p\alpha},$$

where the Hartree-Fock matrix elements are

$$h^{\mathrm{HF}}_{\alpha\gamma} = \langle\alpha|\hat{h}_0|\gamma\rangle + \sum_{\beta\delta} \rho_{\beta\delta}\langle\alpha\beta|V|\gamma\delta\rangle.$$

In order to simplify the calculations, we begin by computing the matrix elements of the one-body operator $\hat{h}_0$. As computed previously, we have that

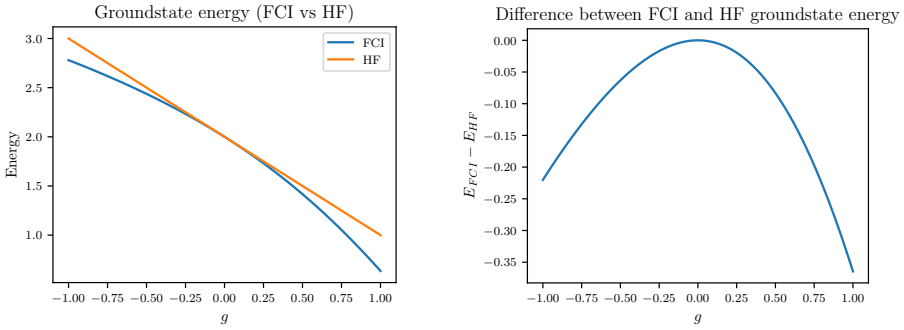
$$\langle\alpha|\hat{h}_0|\gamma\rangle = \delta_{\alpha\gamma}(\alpha - 1).$$

Next, we need to compute the matrix elements of the two-body operator V. We require that the energy levels of bra and ket states match within, and that the spins differ.

Writing $\bar{\alpha}$ as the quantum number with the same energy level as α but with opposite spin, we have that

$$\begin{aligned} h^{\mathrm{HF}}_{\alpha\gamma} &= \delta_{\alpha\gamma}(\alpha - 1) + \rho_{\bar{\alpha}\bar{\gamma}}\langle\alpha\bar{\alpha}|V|\gamma\bar{\gamma}\rangle \\ &= \delta_{\alpha\gamma}(\alpha - 1) - \rho_{\bar{\alpha}\bar{\gamma}}\frac{1}{2}g. \end{aligned}$$

We choose our initial guess for the coefficients to be the identity matrix, $C_{p\lambda} = \delta_{p\lambda}$, or equivalently $C = I \in \mathbb{C}^{8\times 8}$. We then solve the Hartree-Fock equations for $g \in [-1, 1]$.



(a) Groundstate energy from HF.

(b) Difference in energy from HF.

Figure 7: Groundstate energy from the Hartree-Fock calculations, compared with the FCI results, as a function of g.

Because of our initial guess for the coefficients, we have that the density matrix is

$$\rho = C^* C^T = I^* I^T = I.$$

This means that the Hartree-Fock matrix is initially entirely diagonal, with diagonal elements $\alpha - 1 - \frac{1}{2}g$. As the matrix is diagonal, the eigenvalue problem is already solved, with

$$\varepsilon_p = p - 1 - \frac{1}{2}g,$$

where p denotes the energy level, regardless of spin. We realized this after having implemented a solver, in the file `hartree_fock.py`.

As the coefficients are the identity matrix, we have that

$$E[\Phi^{\text{HF}}] = E[\Phi_0] = 2 - g.$$

As we see in Figs. 7a and 7b, the Hartree-Fock approximation serves as a poor approximation to the exact solution, with the difference in energy increasing as $|g|$ increases. However, as it is also a variational method, the energy from the Hartree-Fock calculations will always be higher than the exact energy. The diagrams in Fig. 6 that can be affected in the canonical Hartree-Fock case are diagrams 1, 3, 4, and 5.

Rayleigh-Schrödinger Perturbation Theory

We consider now Rayleigh-Schrödinger perturbation theory. For a diagram to be considered possible, we require that no pairs are broken. We can thus eliminate all diagrams but 1, 4, 5, and 8.

As equations, the first diagram contains $n_h = 2$ hole lines, $n_l = 2$ loops, and $n_{ep} = 2$ equivalent pairs. We thus get a factor of

$$\frac{(-1)^{n_h + n_l}}{2^{n_{ep}}} = \frac{(-1)^{2+2}}{2^2} = \frac{1}{4}.$$

The expression for diagram 1 is then

$$\frac{1}{4}\sum_{abij}\frac{\langle ij|V|ab\rangle\langle ab|V|ij\rangle}{\varepsilon_i+\varepsilon_j-\varepsilon_a-\varepsilon_b}=\frac{1}{4}\sum_{ai}\frac{\langle i\bar{i}|V|a\bar{a}\rangle\langle a\bar{a}|V|i\bar{i}\rangle}{2(\varepsilon_i-\varepsilon_a)}$$

We have that

$$\varepsilon_i-\varepsilon_a=\left(i-1-\frac{1}{2}g\right)-\left(a-1-\frac{1}{2}g\right)=i-a,$$

so the expression simplifies to

$$\frac{1}{4}\sum_{ai}\frac{(-\frac{1}{2}g)(-\frac{1}{2}g)}{2(i-a)}=\frac{1}{32}\sum_{ai}\frac{g^2}{i-a}.$$

For diagram 4 we have $n_h=2$, $n_l=2$ and $n_{ep}=3$. The expression is then

$$\begin{aligned}\frac{1}{8}\sum_{\substack{abcd\\ij}}\frac{\langle ij|V|cd\rangle\langle cd|V|ab\rangle\langle ab|V|ij\rangle}{(\varepsilon_i+\varepsilon_j-\varepsilon_a-\varepsilon_b)(\varepsilon_i+\varepsilon_j-\varepsilon_c-\varepsilon_d)}&=\frac{1}{8}\sum_{aci}\frac{\langle i\bar{i}|V|c\bar{c}\rangle\langle c\bar{c}|V|a\bar{a}\rangle\langle a\bar{a}|V|i\bar{i}\rangle}{4(\varepsilon_i-\varepsilon_a)(\varepsilon_i-\varepsilon_c)}\\&=\frac{1}{32}\left(-\frac{1}{2}\right)^3\sum_{aci}\frac{g^3}{(i-a)(i-c)}\\&=-\frac{1}{256}\sum_{aci}\frac{g^3}{(i-a)(i-c)}\end{aligned}$$

Similarly, we have for diagram 5 that $n_h=4$, $n_l=2$ and $n_{ep}=3$, which gives the expression

$$\frac{1}{8}\sum_{\substack{ab\\ijkl}}\frac{\langle ij|V|kl\rangle\langle kl|V|ab\rangle\langle ab|V|ij\rangle}{(\varepsilon_i+\varepsilon_j-\varepsilon_a-\varepsilon_b)(\varepsilon_k+\varepsilon_l-\varepsilon_a-\varepsilon_b)}=-\frac{1}{256}\sum_{aik}\frac{g^3}{(i-a)(k-a)}.$$

Diagram 8 has $n_h=4$, $n_l=3$ and $n_{ep}=1$, which gives

$$-\frac{1}{2}\sum_{\substack{ab\\ijkl}}\frac{\langle li|V|lk\rangle\langle kj|V|ab\rangle\langle ab|V|ij\rangle}{(\varepsilon_i+\varepsilon_j-\varepsilon_a-\varepsilon_b)(\varepsilon_k+\varepsilon_j-\varepsilon_a-\varepsilon_b)}$$

Looking closer at the expression, we see that we require $j=\bar{i}$ in order to get a contribution, and then $k=\bar{j}=i$, and also $l=\bar{i}$. This gives the expression

$$\begin{aligned}-\frac{1}{2}\sum_{ai}\frac{\langle\bar{i}i|V|\bar{i}i\rangle\langle i\bar{i}|V|a\bar{a}\rangle\langle a\bar{a}|V|i\bar{i}\rangle}{4(\varepsilon_i-\varepsilon_a)(\varepsilon_i-\varepsilon_a)}&=-\frac{1}{8}\left(-\frac{1}{2}\right)^3\sum_{ai}\frac{g^3}{(i-a)^2}\\&=\frac{1}{64}\sum_{ai}\frac{g^3}{(i-a)^2}\end{aligned}$$

Note that in these sums we sum over all possible quantum numbers a and i, not simply the energy levels, but also the spins. In finding the final expressions for the energy, we now resolve the sums of the spins. With n_q as the number of quantum numbers, we get a factor of 2^{n_q}, when changing the sums to sums over the energy levels only. The final expressions for the energy, per diagram, are then

$$\text{(1)} \qquad \frac{2^2}{32}\sum_{ai}\frac{g^2}{i-a} = \frac{1}{8}\sum_{ai}\frac{g^2}{i-a}$$

$$\text{(4)} \qquad -\frac{2^3}{256}\sum_{aci}\frac{g^3}{(i-a)(i-c)} = -\frac{1}{32}\sum_{aci}\frac{g^3}{(i-a)(i-c)}$$

$$\text{(5)} \qquad -\frac{2^3}{256}\sum_{aik}\frac{g^3}{(i-a)(k-a)} = -\frac{1}{32}\sum_{aik}\frac{g^3}{(i-a)(k-a)}$$

$$\text{(8)} \qquad \frac{2^2}{64}\sum_{ai}\frac{g^3}{(i-a)^2} = \frac{1}{16}\sum_{ai}\frac{g^3}{(i-a)^2}$$

Our total estimate for the Energy with Rayleigh-Schrödinger perturbation theory to third order of interactions, with

$$E^{(0)} = 2 \quad \text{and} \quad E^{(1)} = -g,$$

is then

$$E^{(3)}_{RS} = 2 - g + (1) + (4) + (5) + (8)$$

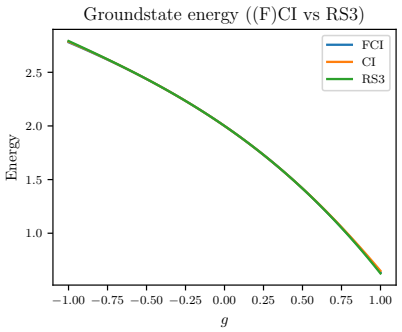
Evaluating the sums for $a, c \in \{3, 4\}$ and $i, k \in \{1, 2\}$, we find

$$E^{(3)}_{RS} = 2 - g - \frac{7}{24}g^2 - \frac{1}{12}g^3.$$

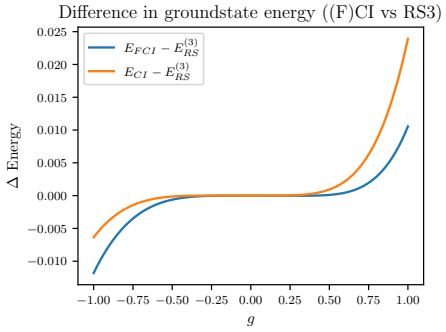
Comparing the results from the Rayleigh-Schrödinger perturbation theory to third order with the exact solution, we see in Figs. 8a and 8b that the perturbation theory serves as a good approximation to the exact solution. Note however that the perturbation theory is not variational, and the energy will not necessarily be bounded from below by the exact energy.

Exercise 6)

Diagram 1 in Fig. 6 represents a second-order contribution to the energy and a so-called $2p-2h$ contribution to the intermediate states. Write down the expression for the wave operator in this case and compare the possible contributions with the configuration interaction calculations of exercise 3). Comment your results for various values of $g \in [-1, 1]$.



(a) Groundstate energy from RSPT.



(b) Difference in energy from RSPT.

Figure 8: Groundstate energy from the Rayleigh-Schrödinger perturbation theory to third-order, compared with the FCI & CI results, as a function of g.

Solution

For a second-order contribution to the energy, we get a contribution from the first-order wave operator, which is given by

$$\begin{aligned}|\Psi^{(1)}\rangle = \frac{\hat{Q}}{\mathcal{E}_0 - \hat{H}_0}\hat{V}|\Phi_0\rangle &= \frac{1}{4}\sum_{\substack{ab\\ij}} \frac{\langle ab|V|ij\rangle}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}|\Phi_{ij}^{ab}\rangle \\ &= \frac{1}{8}\sum_{ai} \frac{\langle i\bar{i}|V|a\bar{a}\rangle}{i-a}|\Phi_{i\bar{i}}^{a\bar{a}}\rangle \\ &= -\frac{1}{4}\sum_{ai} \frac{g}{i-a}|\Phi_{i\bar{i}}^{a\bar{a}}\rangle,\end{aligned}$$

where we've again reduced the sum to just sum over the energy levels, and introduced a factor of 2 per spin state. Here we are interested in each coefficient

$$\frac{g}{4(i-a)}|\Phi_{i\bar{i}}^{a\bar{a}}\rangle,$$

which we can compare with those found from the CI calculations. The coefficients of the wave operator $\Psi^{(1)}$ are shown in Fig. 9.

The second-order energy contribution is given by

$$\begin{aligned}\langle\Phi_0|\hat{V}|\Psi^{(1)}\rangle &= \frac{1}{4}\sum_{\substack{ab\\ij}} \frac{\langle ab|V|ij\rangle}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}\langle\Phi_0|\hat{V}|\Phi_{ij}^{ab}\rangle \\ &= \frac{1}{4}\sum_{\substack{ab\\ij}} \frac{\langle ij|V|ab\rangle\langle ab|V|ij\rangle}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b} \\ &= \frac{1}{4}\sum_{ai} \frac{\langle i\bar{i}|V|a\bar{a}\rangle\langle a\bar{a}|V|i\bar{i}\rangle}{2(\varepsilon_i - \varepsilon_a)}\end{aligned}$$

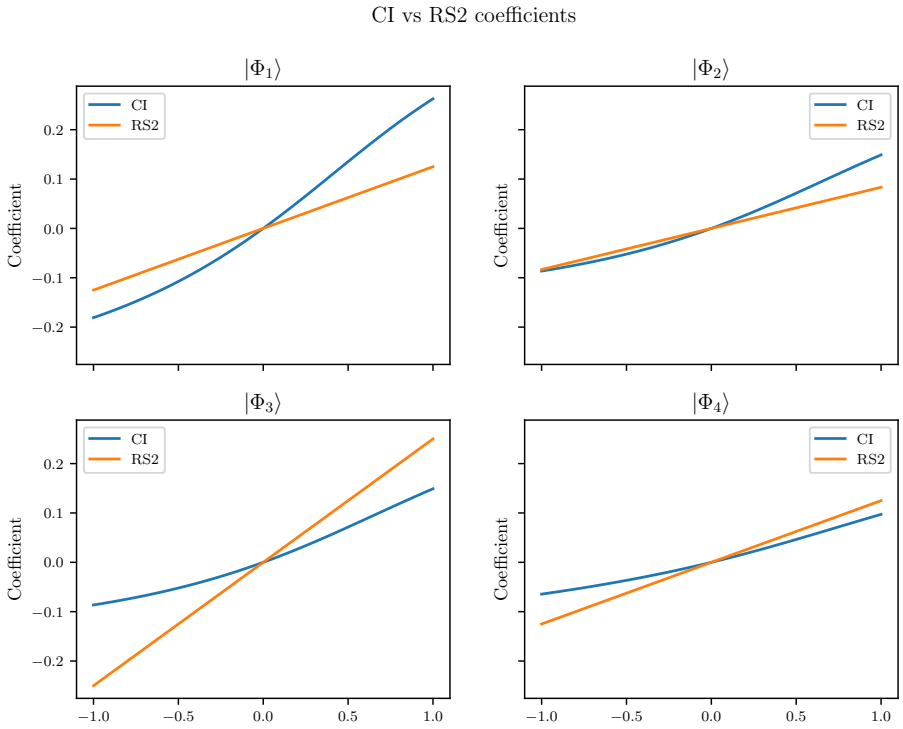
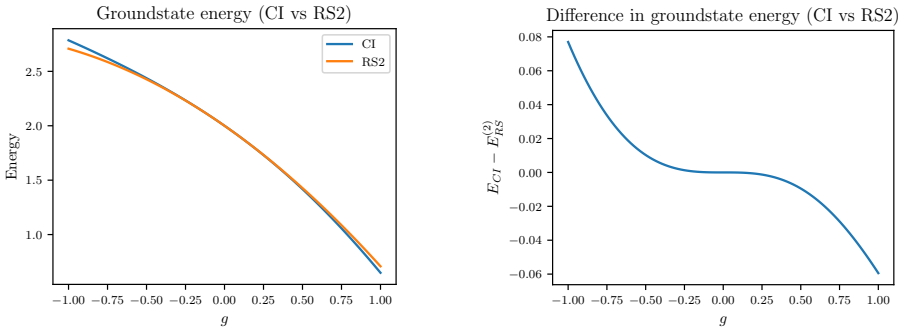


Figure 9: Coefficients of the wave operator $\Psi^{(1)}$ as a function of g, compared with those from the CI calculations.



(a) Groundstate energy from RSPT.

(b) Difference in energy from RSPT.

Figure 10: Groundstate energy from the Rayleigh-Schrödinger perturbation theory to second-order, compared with the CI results, as a function of g.

Changing the summation to just sum over the energy levels, we again need to introduce a factor of 2 per spin state, giving

$$\frac{1}{2}\sum_{ai}\frac{\langle i\bar{i}|V|a\bar{a}\rangle\langle a\bar{a}|V|i\bar{i}\rangle}{i-a}=\frac{1}{8}\sum_{ai}\frac{g^2}{i-a}=-\frac{7}{24}g^2$$

We thus get a total contribution with RSPT to second order of

$$2-g-\frac{7}{24}g^2.$$

As we see in Fig. 10, the RSPT calculations serve as a good approximation for g close to 0, but differs both from above and below for larger values of $|g|$.

Exercise 7)

We limit now the discussion to the Hartree-Fock basis we discussed above. To fourth order in perturbation theory we can produce diagrams with $1p-1h$ intermediate excitations as shown in Fig. ??, $2p-2h$ excitations, see Fig. ??, $3p-3h$ excitations as shown in Fig. ?? and finally so-called diagrams with intermediate four-particle-four-hole excitations, see Fig. ??[2].

Based on the linked diagram theorem and the form of the pairing Hamiltonian, which diagrams will contribute to fourth order? Here we recommend reading Shavitt and Bartlett's chapter 4–6, and chapter 6 in particular about the linked diagram theorem.

Calculate the energy to fourth order with the Hartree-Fock basis defined earlier for $g\in[-1,1]$ and compare with the full diagonalization case in exercise 2). Discuss the results.

Solution

Based on the pairing nature of the Hamiltonian, we can immediately exclude the $1p-1h$ and $3p-3h$ diagrams. We can furthermore reduce the possible $2p-2h$ diagrams to diagrams 5, 6, 14, 15. The $4p-4h$ diagrams which are possible based on the pairing, are diagrams 33, 36, 37 and 41.

With diagrams 33 and 41, we now have to be careful as they are unlinked diagrams. By the linked diagram theorem, we can exlude these diagrams, and only consider the contributions from the linked diagrams, rather than considering the principal and renormalization terms.

Beginning with diagrams 5 and 6, both have $n_h=4$, $n_l=2$ and $n_{ep}=4$. As the notation is quite wieldy, we adopt the convention of writing

$$\varepsilon_i^a=\varepsilon_i-\varepsilon_a,\quad \varepsilon_{ij}^{ab}=\varepsilon_i+\varepsilon_j-\varepsilon_a-\varepsilon_b,\quad \text{etc.}$$

[2]We were unable to render the `.ps` files.

The contributions from these diagrams are then

$$(5)\quad (-1)^6\frac{1}{2^4}\sum_{\substack{abcd\\ijkl}}\frac{\langle ij|V|kl\rangle\langle kl|V|cd\rangle\langle cd|V|ab\rangle\langle ab|V|ij\rangle}{\varepsilon_{ij}^{ab}\cdot\varepsilon_{kl}^{ab}\cdot\varepsilon_{kl}^{cd}}$$

$$(6)\quad (-1)^6\frac{1}{2^4}\sum_{\substack{abcd\\ijkl}}\frac{\langle ij|V|kl\rangle\langle kl|V|cd\rangle\langle cd|V|ab\rangle\langle ab|V|ij\rangle}{\varepsilon_{ij}^{ab}\cdot\varepsilon_{ij}^{cd}\cdot\varepsilon_{kl}^{cd}}$$

which by the previous method simplify to

$$(5)\quad \frac{1}{128}\sum_{\substack{ac\\ik}}\frac{g^4}{(i-a)(k-a)(k-c)}$$

$$(6)\quad \frac{1}{128}\sum_{\substack{ac\\ik}}\frac{g^4}{(i-a)(i-c)(k-c)}$$

summing now just over energy levels.

For diagrams 14 and 15 we have $n_h = 2$ and $n_h = 6$ respectively, with $n_l = 2$ and $n_{ep} = 4$. The contributions from these diagrams are then

$$(14)\quad (-1)^4\frac{1}{2^4}\sum_{\substack{abcdef\\ij}}\frac{\langle ij|V|ef\rangle\langle ef|V|cd\rangle\langle cd|V|ab\rangle\langle ab|V|ij\rangle}{\varepsilon_{ij}^{ab}\cdot\varepsilon_{ij}^{cd}\cdot\varepsilon_{ij}^{ef}}$$

$$(15)\quad (-1)^8\frac{1}{2^4}\sum_{\substack{ab\\ijklmn}}\frac{\langle ij|V|kl\rangle\langle kl|V|mn\rangle\langle mn|V|ab\rangle\langle ab|V|ij\rangle}{\varepsilon_{ij}^{ab}\cdot\varepsilon_{kl}^{ab}\cdot\varepsilon_{mn}^{ab}}$$

which simplify to

$$(14)\quad \frac{1}{128}\sum_{\substack{ace\\i}}\frac{g^4}{(i-a)(i-c)(i-e)}$$

$$(15)\quad \frac{1}{128}\sum_{\substack{a\\ikm}}\frac{g^4}{(i-a)(k-a)(m-a)}$$

For diagram 36 we have $n_h = 4$, $n_l = 0$ and $n_{ep} = 4$, and then the expression

$$(36)\quad (-1)^6\frac{1}{2^4}\sum_{\substack{abcd\\ijkl}}\frac{\langle ij|V|cd\rangle\langle cd|V|kl\rangle\langle kl|V|ab\rangle\langle ab|V|ij\rangle}{\varepsilon_{ij}^{ab}\cdot\varepsilon_{ijkl}^{abcd}\cdot\varepsilon_{ij}^{cd}}$$

which simplifies to

$$(36)\quad \frac{1}{128}\sum_{\substack{ac\\ik}}\frac{g^4}{(i-a)(i+k-a-c)(i-c)}.$$

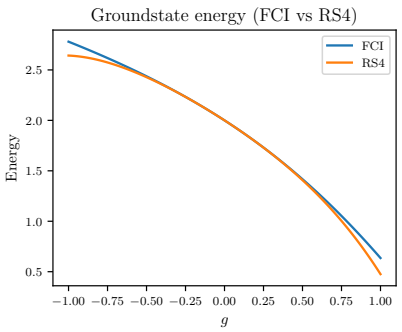
By symmetry, we have

$$\frac{1}{128}\sum_{\substack{ac\\ik}}\frac{g^4}{(i-a)(i+k-a-c)(k-a)}. \tag{37}$$

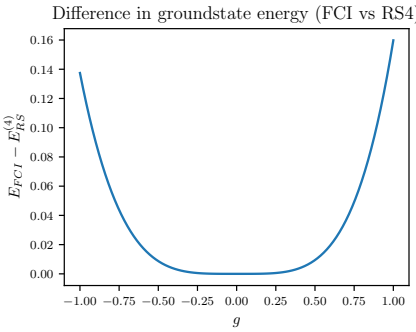
Performing the summations, we get an additional contribution to the energy of

$$-\frac{2063}{13824}g^4 \approx -0.149g^4.$$

For higher and higher powers, the additional contributions become smaller for values of g further from ± 1. As we see in Figs. 11a and 11b, the fourth-order RSPT seem to be a worse approximation, as compared with the third-order RSPT. This is not an entirely unexpected result, as pertubation theories give no guarantees of better convergence for each higher term included. Again, the approximate energy falls below the exact energy computed with FCI, as RSPT is not variational.



(a) Groundstate energy from RSPT.



(b) Difference in energy from RSPT.

Figure 11: Groundstate energy from the Rayleigh-Schrödinger perturbation theory to fourth-order, compared with the FCI results, as a function of g.