Second midterm FYS4480
Quantum mechanics for many-particle systems

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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.

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

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

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 $p = 1, 2, \dots$ 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.

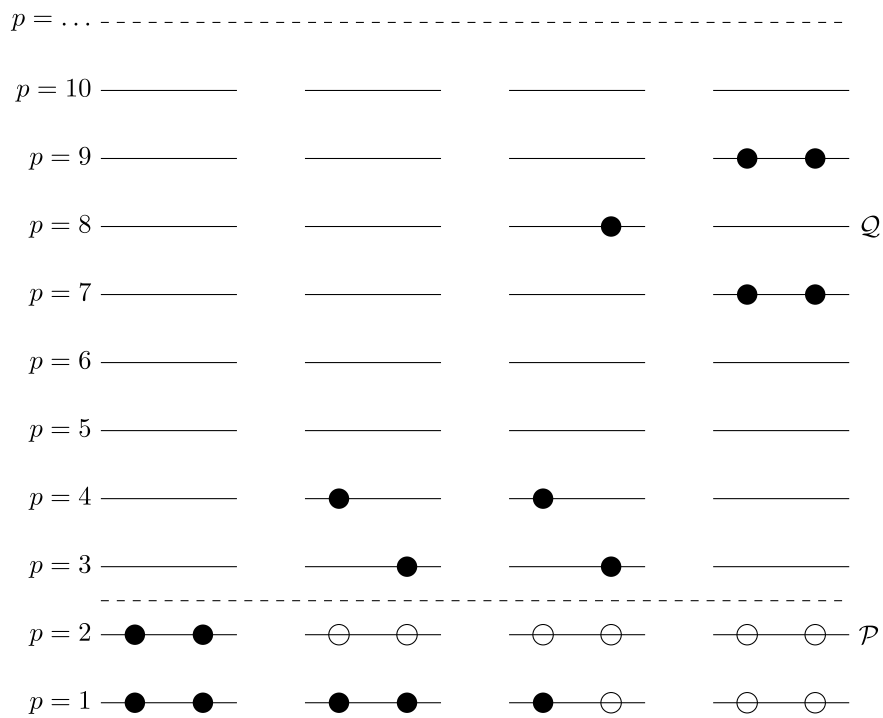

Figure 1: Schematic plot of the possible single-particle levels with double degeneracy. The filled circles indicate occupied particle states while the empty circles represent vacant particle (hole) states. The spacing between each level p is constant in this picture. The first two single-particle levels 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 a)

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 $\hat{S}_+\hat{S}_-$, as the other commutation is analogous. 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

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

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

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

Inserting the expressions back into the commutator, we have

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

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

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

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

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

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

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

For the two-body operator $\hat{V}$, we have, substituting $\hat{P}_p^+ = a_{p+}^\dagger a_{p-}^\dagger$ 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.

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

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

Exercise b)

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.

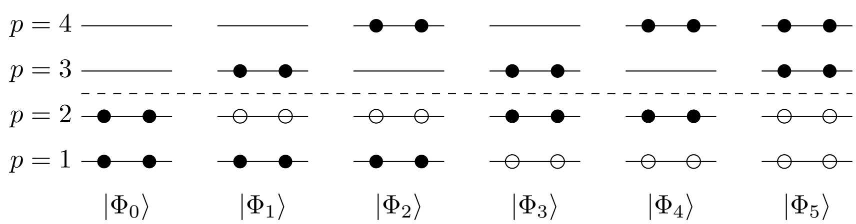

Figure 2: Schematic representation of the six possible Slater determinants for a system with four particles, under the constraint of no broken pairs, total spin $S = 0$, considering only the four lowest levels $p = 1, 2, 3, 4$.

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

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

The other Slater determinants are then

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

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 $|\Phi\rangle_{\alpha,\beta}$, with $\alpha < \beta$, as

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

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

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

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 $|\Phi_0\rangle, |\Phi_1\rangle, \ldots, |\Phi_5\rangle$.

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

Plotted as a function of g, the ground state energy is shown in Fig. 3.

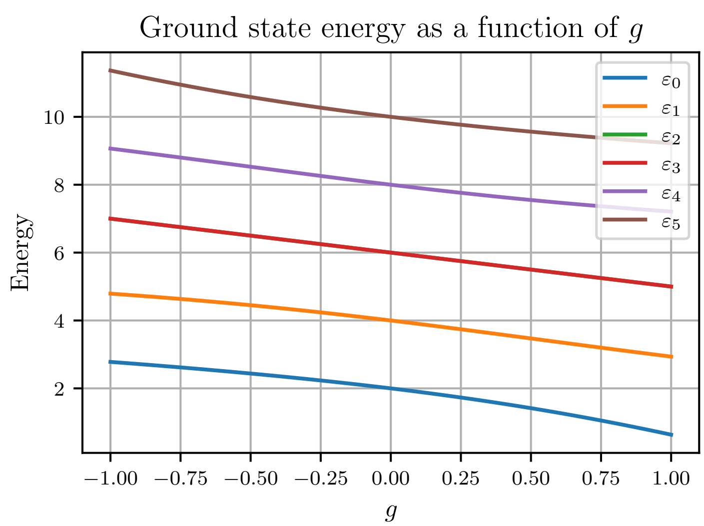

Figure 3: Ground state energy as a function of g for the four-particle system with no broken pairs and total spin $S = 0$. The energy is given in units of the unperturbed ground state energy.

Performing the contractions, we have

groundstate – groundstate:

$$\begin{aligned}
\langle\Phi_0|\hat{H}_0|\Phi_0\rangle &= \langle\Phi_0|\sum_{p\sigma}(p-1)a^\dagger_{p\sigma}a_{p\sigma}|\Phi_0\rangle \\
&= \sum_{p\sigma}(p-1)\langle\Phi_0|a^\dagger_{p\sigma}a_{p\sigma}|\Phi_0\rangle \\
&= \sum_{i=1}^{2}\sum_{\sigma=\pm}(i-1) \\
&= 0+0+1+1 = 2.
\end{aligned}$$

$$\begin{aligned}
\langle\Phi_0|\hat{V}|\Phi_0\rangle &= \langle\Phi_0| - \frac{1}{2}g\sum_{pq}\hat{P}^+_p\hat{P}^-_q|\Phi_0\rangle \\
&= -\frac{1}{2}g\sum_{pq}\langle\Phi_0|\hat{P}^+_p\hat{P}^-_q|\Phi_0\rangle \\
&= -\frac{1}{2}g\sum_{p}\langle\Phi_0|\hat{P}^+_p\hat{P}^-_p|\Phi_0\rangle \\
&= -\frac{1}{2}g\sum_{p=1}^{2}\langle\Phi_0|\Phi_0\rangle \\
&= -\frac{1}{2}g\cdot 2 = -g.
\end{aligned}$$

In order to get a contribution, we then require that