

Second midterm FYS4480

Quantum mechanics for many-particle systems

August Femtehjell & Oskar Idland

November 2024

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 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. 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_{α}^{\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

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

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 $p = 1, 2, \dots$ 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

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

and

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

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.

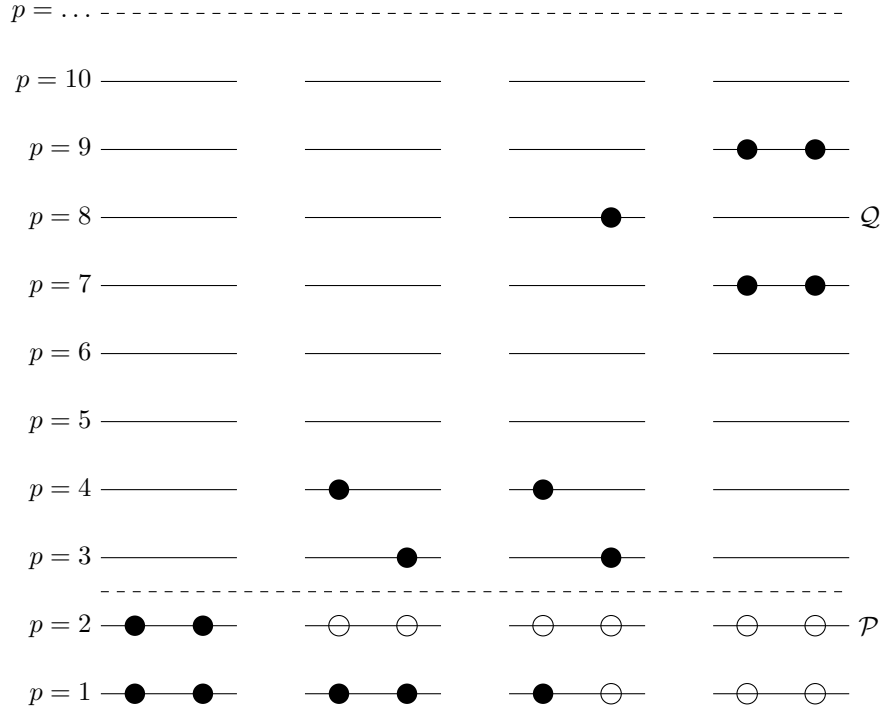


Figure 1: Schematic plot of the possible single-particle levels with double degeneracy. The filled circles indicate occupied particle states while the empty circles represent vacant particle (hole) states. The spacing between each level p is constant in this picture. The first two single-particle levels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

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

where

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

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

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

respectively.

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

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

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,

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

where we have defined the number operator $\hat{n}_{p\sigma} = a_{p\sigma}^\dagger a_{p\sigma}$. 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,

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

Using the commutation identity

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

we have

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

and then need to find expressions for

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

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

$$\left[a_p a_q, \hat{n}_r \right] \quad \text{and} \quad \left[a_p^\dagger a_q^\dagger, \hat{n}_r \right],$$

noting that

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

As

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

We have

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

Similarly, for the creation operators, we have

$$\left[a_p^\dagger, \hat{n}_r \right] = \left[a_p^\dagger, a_r^\dagger a_r \right] = \left[a_p^\dagger, a_r^\dagger \right] a_r + a_r^\dagger \left[a_p^\dagger, a_r \right] = -\delta_{pr} a_r^\dagger = -a_p^\dagger,$$

and thus

$$\begin{aligned} \left[a_p^\dagger a_q^\dagger, \hat{n}_r \right] &= a_p^\dagger \left[a_q^\dagger, \hat{n}_r \right] + \left[a_p^\dagger, \hat{n}_r \right] a_q^\dagger \\ &= -a_p^\dagger a_q^\dagger - a_p^\dagger a_q^\dagger = -2a_p^\dagger a_q^\dagger. \end{aligned}$$

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

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

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

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

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

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

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

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

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

where

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

Breaking the expression down further, we have

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

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

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

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

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

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

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

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 wily, 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 $[\hat{V}, \hat{S}_\pm] = 0$, giving us that

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

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

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

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

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

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