Quantum mechanics for many-particle systems

Department of Physics, University of Oslo, Norway

Joseph P.Vera

Exercises

1. (15/100 points) 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

$$\hat{S}_z := \frac{1}{2}\sum_{p\sigma} \sigma a^\dagger_{p\sigma} a_{p\sigma}$$

and

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

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

$$\hat{P}^+_p = a^\dagger_{p+} a^\dagger_{p-},$$

and

$$\hat{P}^-_p = a_{p-} a_{p+},$$

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
Hamiltonian:

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

where

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

and

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

expand $\sigma = +$ and $-$

$$\hat{S}_z = \frac{1}{2}\sum_{p\sigma} \sigma a^\dagger_{p\sigma} a_{p\sigma} = \frac{1}{2}\sum_p \left(a^\dagger_{p+} a_{p+} - \sigma a^\dagger_{p-} a_{p-} \right)$$

We're going to show

$$[\hat{H}_0, \hat{S}_z] = \left(\xi \sum_{p\sigma} (p-1) a^\dagger_{p\sigma} a_{p\sigma}\right) \left(\frac{1}{2} \sum_{p'\sigma} \sigma a^\dagger_{p'\sigma} a_{p'\sigma}\right) - \left(\frac{1}{2} \sum_{p'\sigma} \sigma a^\dagger_{p'\sigma} a_{p'\sigma}\right) \left(\xi \sum_{p\sigma} (p-1) a^\dagger_{p\sigma} a_{p\sigma}\right)$$

$$[\hat{H}_0, \hat{S}_z] = \frac{1}{2}\xi \sum_{pp'} (p-1) \left[\left(\sum_\sigma a^\dagger_{p\sigma} a_{p\sigma}\right) \left(\sum_\sigma \sigma a^\dagger_{p'\sigma} a_{p'\sigma}\right) - \left(\sum_\sigma \sigma a^\dagger_{p'\sigma} a_{p'\sigma}\right) \left(\sum_\sigma a^\dagger_{p\sigma} a_{p\sigma}\right)\right]$$

$$[\hat{H}_0, \hat{S}_z] = \frac{1}{2}\xi \sum_{pp'} (p-1) \left[\underbrace{\left(a^\dagger_{p+} a_{p+} + a^\dagger_{p-} a_{p-}\right) \left(a^\dagger_{p'+} a_{p'+} - a^\dagger_{p'-} a_{p'-}\right)}_{(i)} - \underbrace{\left(a^\dagger_{p'+} a_{p'+} - a^\dagger_{p'-} a_{p'-}\right) \left(a^\dagger_{p+} a_{p+} + a^\dagger_{p-} a_{p-}\right)}_{(ii)}\right] \tag{1}$$

(i)

$$\left(a^\dagger_{p+} a_{p+} + a^\dagger_{p-} a_{p-}\right) \left(a^\dagger_{p'+} a_{p'+} - a^\dagger_{p'-} a_{p'-}\right) = a^\dagger_{p+} a_{p+} a^\dagger_{p'+} a_{p'+} - a^\dagger_{p+} a_{p+} a^\dagger_{p'-} a_{p'-} + a^\dagger_{p-} a_{p-} a^\dagger_{p'+} a_{p'+} - a^\dagger_{p-} a_{p-} a^\dagger_{p'-} a_{p'-}$$

$$= a^\dagger_{p+}(\delta_{pp'}\delta_{++} - a^\dagger_{p'+} a_{p+}) a_{p'+} - a^\dagger_{p+}(\delta_{pp'}\delta_{+-} - a^\dagger_{p'-} a_{p+}) a_{p'-} + a^\dagger_{p-}(\delta_{pp'}\delta_{-+} - a^\dagger_{p'+} a_{p-}) a_{p'+} - a^\dagger_{p-}(\delta_{pp'}\delta_{--} - a^\dagger_{p'-} a_{p-}) a_{p'-}$$

$$= a^\dagger_{p+} a_{p'+} \delta_{pp'} - a^\dagger_{p+} a^\dagger_{p'+} a_{p+} a_{p'+} + a^\dagger_{p+} a^\dagger_{p'-} a_{p+} a_{p'-} - \underbrace{a^\dagger_{p-} a^\dagger_{p'+}}\,\underbrace{a_{p-} a_{p'+}} - a^\dagger_{p-} a_{p'-} \delta_{pp'} + a^\dagger_{p-} a^\dagger_{p'-} a_{p-} a_{p'-}$$

$$= a^\dagger_{p+} a_{p'+} \delta_{pp'} - a^\dagger_{p+} a^\dagger_{p'+} a_{p+} a_{p'+} + a^\dagger_{p+} a^\dagger_{p'-} a_{p+} a_{p'-} - a^\dagger_{p'+} a^\dagger_{p-} a_{p'+} a_{p-} - a^\dagger_{p-} a_{p'-} \delta_{pp'} + a^\dagger_{p-} a^\dagger_{p'-} a_{p-} a_{p'-}$$

when $p' = p$

$$= a^\dagger_{p+} a_{p+} - a^\dagger_{p+} a^\dagger_{p+} a_{p+} a_{p+} + a^\dagger_{p+} a^\dagger_{p-} a_{p+} a_{p-} - a^\dagger_{p+} a^\dagger_{p-} a_{p+} a_{p-} - a^\dagger_{p-} a_{p-} + a^\dagger_{p-} a^\dagger_{p-} a_{p-} a_{p-}$$

Therefore

$$= a^\dagger_{p+} a_{p+} - a^\dagger_{p+} a^\dagger_{p+} a_{p+} a_{p+} - a^\dagger_{p-} a_{p-} + a^\dagger_{p-} a^\dagger_{p-} a_{p-} a_{p-} \tag{2}$$

(ii)

$$\left(a^\dagger_{p'+} a_{p'+} - a^\dagger_{p'-} a_{p'-}\right) \left(a^\dagger_{p+} a_{p+} + a^\dagger_{p-} a_{p-}\right) = a^\dagger_{p'+} a_{p'+} a^\dagger_{p+} a_{p+} + a^\dagger_{p'+} a_{p'+} a^\dagger_{p-} a_{p-} - a^\dagger_{p'-} a_{p'-} a^\dagger_{p+} a_{p+} - a^\dagger_{p'-} a_{p'-} a^\dagger_{p-} a_{p-}$$

$$= a^\dagger_{p'+}(\delta_{p'p}\delta_{++} - a^\dagger_{p+} a_{p'+}) a_{p+} + a^\dagger_{p'+}(\delta_{p'p}\delta_{+-} - a^\dagger_{p-} a_{p'+}) a_{p-} - a^\dagger_{p'-}(\delta_{p'p}\delta_{-+} - a^\dagger_{p+} a_{p'-}) a_{p+} - a^\dagger_{p'-}(\delta_{p'p}\delta_{--} - a^\dagger_{p-} a_{p'-}) a_{p-}$$

$$= a^\dagger_{p'+} a_{p+} \delta_{p'p} - a^\dagger_{p'+} a^\dagger_{p+} a_{p'+} a_{p+} - a^\dagger_{p'+} a^\dagger_{p-} a_{p'+} a_{p-} + a^\dagger_{p'-} a^\dagger_{p+} a_{p'-} a_{p+} - a^\dagger_{p'-} a_{p-} \delta_{p'p} + a^\dagger_{p'-} a^\dagger_{p-} a_{p'-} a_{p-}$$

$$= a^\dagger_{p'+} a_{p+} \delta_{p'p} - a^\dagger_{p'+} a^\dagger_{p+} a_{p'+} a_{p+} - a^\dagger_{p'+} a^\dagger_{p-} a_{p'+} a_{p-} + \underbrace{a^\dagger_{p'-} a^\dagger_{p+}}\,\underbrace{a_{p'-} a_{p+}} - a^\dagger_{p'-} a_{p-} \delta_{p'p} + a^\dagger_{p'-} a^\dagger_{p-} a_{p'-} a_{p-}$$

$$= a^\dagger_{p'+} a_{p+} \delta_{p'p} - a^\dagger_{p'+} a^\dagger_{p+} a_{p'+} a_{p+} - a^\dagger_{p'+} a^\dagger_{p-} a_{p'+} a_{p-} + a^\dagger_{p+} a^\dagger_{p'-} a_{p+} a_{p'-} - a^\dagger_{p'-} a_{p-} \delta_{p'p} + a^\dagger_{p'-} a^\dagger_{p-} a_{p'-} a_{p-}$$

when $p' = p$

$$= a^\dagger_{p+}a_{p+} - a^\dagger_{p+}a^\dagger_{p+}a_{p+}a_{p+} - a^\dagger_{p+}a^\dagger_{p-}a_{p+}a_{p-} + a^\dagger_{p+}a^\dagger_{p-}a_{p+}a_{p-} - a^\dagger_{p-}a_{p-} + a^\dagger_{p-}a^\dagger_{p-}a_{p-}a_{p-}$$

Therefore

$$= a^\dagger_{p+}a_{p+} - a^\dagger_{p+}a^\dagger_{p+}a_{p+}a_{p+} - a^\dagger_{p-}a_{p-} + a^\dagger_{p-}a^\dagger_{p-}a_{p-}a_{p-} \tag{3}$$

Replacing in the equations (2) and (3) in equation (1)

$$[\hat{H}_0, \hat{S}_z] = \frac{1}{2}\xi\sum_p (p-1)(a^\dagger_{p+}a_{p+} - a^\dagger_{p+}a^\dagger_{p+}a_{p+}a_{p+} - a^\dagger_{p-}a_{p-} + a^\dagger_{p-}a^\dagger_{p-}a_{p-}a_{p-} - a^\dagger_{p+}a_{p+} + a^\dagger_{p+}a^\dagger_{p+}a_{p+}a_{p+}$$
$$+ a^\dagger_{p-}a_{p-} - a^\dagger_{p-}a^\dagger_{p-}a_{p-}a_{p-})$$

Therefore

$$[\hat{H}_0, \hat{S}_z] = 0 \tag{4}$$

$$[\hat{V}, \hat{S}_z] = \left(-\frac{1}{2}g\sum_{pq} a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}\right)\left(\frac{1}{2}\sum_{p'\sigma}\sigma a^\dagger_{p'\sigma}a_{p'\sigma}\right) - \left(\frac{1}{2}\sum_{p'\sigma}\sigma a^\dagger_{p'\sigma}a_{p'\sigma}\right)\left(-\frac{1}{2}g\sum_{pq} a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}\right)$$

$$[\hat{V}, \hat{S}_z] = -\frac{1}{4}g\sum_{pp'q}\left[\left(a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}\right)\left(\sum_\sigma \sigma a^\dagger_{p'\sigma}a_{p'\sigma}\right) - \left(\sum_\sigma \sigma a^\dagger_{p'\sigma}a_{p'\sigma}\right)\left(a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}\right)\right]$$

$$[\hat{V}, \hat{S}_z] = -\frac{1}{4}g\sum_{pp'q}\left[\underbrace{\left(a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}\right)\left(a^\dagger_{p'+}a_{p'+} - a^\dagger_{p'-}a_{p'-}\right)}_{(i)} - \underbrace{\left(a^\dagger_{p'+}a_{p'+} - a^\dagger_{p'-}a_{p'-}\right)\left(a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}\right)}_{(ii)}\right] \tag{5}$$

(i)

$$\left(a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}\right)\left(a^\dagger_{p'+}a_{p'+} - a^\dagger_{p'-}a_{p'-}\right) = a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}a^\dagger_{p'+}a_{p'+} - a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}a^\dagger_{p'-}a_{p'-}$$

$$= a^\dagger_{p+}a^\dagger_{p-}a_{q-}\left(\delta_{qp'}\delta_{++} - a^\dagger_{p'+}a_{q+}\right)a_{p'+} - a^\dagger_{p+}a^\dagger_{p-}a_{q-}\left(\delta_{qp'}\delta_{+-} - a^\dagger_{p'-}a_{q+}\right)a_{p'-}$$

where $q \neq p'$

$$= -a^\dagger_{p+}a^\dagger_{p-}a_{q-}a^\dagger_{p'+}a_{q+}a_{p'+} + a^\dagger_{p+}a^\dagger_{p-}a_{q-}a^\dagger_{p'-}a_{q+}a_{p'-}$$

$$= a^\dagger_{p+}a^\dagger_{p-}a^\dagger_{p'+}a_{q-}a_{q+}a_{p'+} - a^\dagger_{p+}a^\dagger_{p-}a^\dagger_{p'-}a_{q-}a_{q+}a_{p'-}$$

when $p' = p$

$$= a^\dagger_{p+}a^\dagger_{p-}a^\dagger_{p+}a_{q-}a_{q+}a_{p+} - a^\dagger_{p+}a^\dagger_{p-}a^\dagger_{p-}a_{q-}a_{q+}a_{p-} \tag{6}$$

(ii)

$$\left(a^\dagger_{p'+}a_{p'+} - a^\dagger_{p'-}a_{p'-}\right)\left(a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}\right) = a^\dagger_{p'+}a_{p'+}a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+} - a^\dagger_{p'-}a_{p'-}a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}$$

$$= a^\dagger_{p'+}\left(\delta_{p'p}\delta_{++} - a^\dagger_{p+}a_{p'+}\right)a^\dagger_{p-}a_{q-}a_{q+} - a^\dagger_{p'-}\left(\delta_{p'p}\delta_{-+} - a^\dagger_{p+}a_{p'-}\right)a^\dagger_{p-}a_{q-}a_{q+}$$

$$= a^\dagger_{p'+} a^\dagger_{p-} a_{q-} a_{q+} \delta_{p'p} - a^\dagger_{p'+} a^\dagger_{p+} \overbracket{a_{p'+} a^\dagger_{p-}} a_{q-} a_{q+} + a^\dagger_{p'-} a^\dagger_{p+} \overbracket{a_{p'-} a^\dagger_{p-}} a_{q-} a_{q+}$$

$$= a^\dagger_{p'+} a^\dagger_{p-} a_{q-} a_{q+} \delta_{p'p} - a^\dagger_{p'+} a^\dagger_{p+} \left(\delta_{p'p}\delta_{+-} - a^\dagger_{p-} a_{p'+}\right) a_{q-} a_{q+} + a^\dagger_{p'-} a^\dagger_{p+} \left(\delta_{p'p}\delta_{--} - a^\dagger_{p-} a_{p'-}\right) a_{q-} a_{q+}$$

$$= a^\dagger_{p'+} a^\dagger_{p-} a_{q-} a_{q+} \delta_{p'p} + a^\dagger_{p'+} a^\dagger_{p+} a^\dagger_{p-} a_{p'+} a_{q-} a_{q+} + \underbrace{a^\dagger_{p'-} a^\dagger_{p+}} a_{q-} a_{q+} \delta_{p'p} - a^\dagger_{p'-} a^\dagger_{p+} a^\dagger_{p-} a_{p'-} a_{q-} a_{q+}$$

$$= a^\dagger_{p'+} a^\dagger_{p-} a_{q-} a_{q+} \delta_{p'p} + \underbrace{a^\dagger_{p'+} a^\dagger_{p+}} a^\dagger_{p-} \underbrace{a_{p'+} a_{q-}} a_{q+} - a^\dagger_{p+} a^\dagger_{p'-} a_{q-} a_{q+} \delta_{p'p} - \underbrace{a^\dagger_{p'-} a^\dagger_{p+}} a^\dagger_{p-} \underbrace{a_{p'-} a_{q-}} a_{q+}$$

$$= a^\dagger_{p'+} a^\dagger_{p-} a_{q-} a_{q+} \delta_{p'p} + a^\dagger_{p+} \underbrace{a^\dagger_{p'+} a^\dagger_{p-}} a_{q-} \underbrace{a_{p'+} a_{q+}} - a^\dagger_{p+} a^\dagger_{p'-} a_{q-} a_{q+} \delta_{p'p} - a^\dagger_{p+} \underbrace{a^\dagger_{p'-} a^\dagger_{p-}} a_{q-} \underbrace{a_{p'-} a_{q+}}$$

$$= a^\dagger_{p'+} a^\dagger_{p-} a_{q-} a_{q+} \delta_{p'p} + a^\dagger_{p+} a^\dagger_{p-} a^\dagger_{p'+} a_{q-} a_{q+} a_{p'+} - a^\dagger_{p+} a^\dagger_{p'-} a_{q-} a_{q+} \delta_{p'p} - a^\dagger_{p+} a^\dagger_{p-} a^\dagger_{p'-} a_{q-} a_{q+} a_{p'-}$$

when $p' = p$

$$= a^\dagger_{p+} a^\dagger_{p-} a_{q-} a_{q+} + a^\dagger_{p+} a^\dagger_{p-} a^\dagger_{p+} a_{q-} a_{q+} a_{p+} - a^\dagger_{p+} a^\dagger_{p-} a_{q-} a_{q+} - a^\dagger_{p+} a^\dagger_{p-} a^\dagger_{p-} a_{q-} a_{q+} a_{p-}$$

$$= a^\dagger_{p+} a^\dagger_{p-} a^\dagger_{p+} a_{q-} a_{q+} a_{p+} - a^\dagger_{p+} a^\dagger_{p-} a^\dagger_{p-} a_{q-} a_{q+} a_{p-} \tag{7}$$

Replacing in the equations (6) and (7) in equation (5)

$$[\hat{V}, \hat{S}_z] = -\frac{1}{4} g \sum_{pq} \left(a^\dagger_{p+} a^\dagger_{p-} a\dagger_{p+} a_{q-} a_{q+} a_{p+} - a^\dagger_{p+} a^\dagger_{p-} a^\dagger_{p-} a_{q-} a_{q+} a_{p-} - a^\dagger_{p+} a^\dagger_{p-} a^\dagger_{p+} a_{q-} a_{q+} a_{p+} + a^\dagger_{p+} a^\dagger_{p-} a^\dagger_{p-} a_{q-} a_{q+} a_{p-} \right)$$

Therefore

$$[\hat{V}, \hat{S}_z] = 0 \tag{8}$$

Now let's demostrate $[\hat{H}_0, \hat{S}_\pm]$ and $[\hat{V}, \hat{S}_\pm]$

$$[\hat{H}_0, \hat{S}_\pm] = \left(\xi \sum_{p\sigma} (p-1) a^\dagger_{p\sigma} a_{p\sigma}\right) \left(\sum_{p'} a^\dagger_{p'\pm} a_{p'\mp}\right) - \left(\sum_{p'} a^\dagger_{p'\pm} a_{p'\mp}\right) \left(\xi \sum_{p\sigma} (p-1) a^\dagger_{p\sigma} a_{p\sigma}\right)$$

$$[\hat{H}_0, \hat{S}_\pm] = \xi \sum_{pp'} (p-1) \left[\left(\sum_\sigma a^\dagger_{p\sigma} a_{p\sigma}\right) \left(a^\dagger_{p'\pm} a_{p'\mp}\right) - \left(a^\dagger_{p'\pm} a_{p'\mp}\right) \left(\sum_\sigma a^\dagger_{p\sigma} a_{p\sigma}\right) \right]$$

$$[\hat{H}_0, \hat{S}_\pm] = \xi \sum_{pp'} (p-1) \left[\underbrace{\left(a^\dagger_{p+} a_{p+} + a^\dagger_{p-} a_{p-}\right) \left(a^\dagger_{p'\pm} a_{p'\mp}\right)}_{(i)} - \underbrace{\left(a^\dagger_{p'\pm} a_{p'\mp}\right) \left(a^\dagger_{p+} a_{p+} + a^\dagger_{p-} a_{p-}\right)}_{(ii)} \right] \tag{9}$$

(i)

$$\left(a^\dagger_{p+} a_{p+} + a^\dagger_{p-} a_{p-}\right) \left(a^\dagger_{p'\pm} a_{p'\mp}\right) = a^\dagger_{p+} \overbracket{a_{p+} a^\dagger_{p'\pm}} a_{p'\mp} + a^\dagger_{p-} \overbracket{a_{p-} a^\dagger_{p'\pm}} a_{p'\mp}$$

$$= a^\dagger_{p+}\left(\delta_{pp'}\delta_{+\pm} - a^\dagger_{p'\pm}a_{p+}\right)a_{p'\mp} + a^\dagger_{p-}\left(\delta_{pp'}\delta_{-\pm} - a^\dagger_{p'\pm}a_{p-}\right)a_{p'\mp}$$

$$= a^\dagger_{p+}a_{p'\mp}\delta_{pp'}\delta_{+\pm} - a^\dagger_{p+}a^\dagger_{p'\pm}a_{p+}a_{p'\mp} + a^\dagger_{p-}a_{p'\mp}\delta_{pp'}\delta_{-\pm} - a^\dagger_{p-}a^\dagger_{p'\pm}a_{p-}a_{p'\mp} \tag{10}$$

(ii)

$$\left(a^\dagger_{p'\pm}a_{p'\mp}\right)\left(a^\dagger_{p+}a_{p+} + a^\dagger_{p-}a_{p-}\right) = a^\dagger_{p'\pm}a_{p'\mp}a^\dagger_{p+}a_{p+} + a^\dagger_{p'\pm}a_{p'\mp}a^\dagger_{p-}a_{p-}$$

$$= a^\dagger_{p'\pm}\left(\delta_{p'p}\delta_{\mp+} - a^\dagger_{p+}a_{p'\mp}\right)a_{p+} + a^\dagger_{p'\pm}\left(\delta_{p'p}\delta_{\mp-} - a^\dagger_{p-}a_{p'\mp}\right)a_{p-}$$

$$= a^\dagger_{p'\pm}a_{p+}\delta_{p'p}\delta_{\mp+} - \underbrace{a^\dagger_{p'\pm}a^\dagger_{p+}}\,\underbrace{a_{p'\mp}a_{p+}} + a^\dagger_{p'\pm}a_{p-}\delta_{p'p}\delta_{\mp-} - \underbrace{a^\dagger_{p'\pm}a^\dagger_{p-}}\,\underbrace{a_{p'\mp}a_{p-}}$$

$$= a^\dagger_{p'\pm}a_{p+}\delta_{p'p}\delta_{\mp+} - a^\dagger_{p+}a^\dagger_{p'\pm}a_{p+}a_{p'\mp} + a^\dagger_{p'\pm}a_{p-}\delta_{p'p}\delta_{\mp-} - a^\dagger_{p-}a^\dagger_{p'\pm}a_{p-}a_{p'\mp} \tag{11}$$

Replacing equations (10) and (11) in equation (9)

$$\begin{aligned}[\hat{H}_0, \hat{S}_\pm] = \xi\sum_{pp'}(p-1)(&a^\dagger_{p+}a_{p'\mp}\delta_{pp'}\delta_{+\pm} - a^\dagger_{p+}a^\dagger_{p'\pm}a_{p+}a_{p'\mp} + a^\dagger_{p-}a_{p'\mp}\delta_{pp'}\delta_{-\pm} - a^\dagger_{p-}a^\dagger_{p'\pm}a_{p-}a_{p'\mp} \\ &- a^\dagger_{p'\pm}a_{p+}\delta_{p'p}\delta_{\mp+} + a^\dagger_{p+}a^\dagger_{p'\pm}a_{p+}a_{p'\mp} - a^\dagger_{p'\pm}a_{p-}\delta_{p'p}\delta_{\mp-} + a^\dagger_{p-}a^\dagger_{p'\pm}a_{p-}a_{p'\mp})\end{aligned}$$

$$[\hat{H}_0, \hat{S}_\pm] = \xi\sum_{pp'}(p-1)\left(a^\dagger_{p+}a_{p'\mp}\delta_{pp'}\delta_{+\pm} + a^\dagger_{p-}a_{p'\mp}\delta_{pp'}\delta_{-\pm} - a^\dagger_{p'\pm}a_{p+}\delta_{p'p}\delta_{\mp+} - a^\dagger_{p'\pm}a_{p-}\delta_{p'p}\delta_{\mp-}\right)$$

For

$$[\hat{H}_0, \hat{S}_+] = \xi\sum_{pp'}(p-1)\left(a^\dagger_{p+}a_{p'-}\delta_{pp'}\delta_{++} + a^\dagger_{p-}a_{p'-}\delta_{pp'}\delta_{-+} - a^\dagger_{p'+}a_{p+}\delta_{p'p}\delta_{-+} - a^\dagger_{p'+}a_{p-}\delta_{p'p}\delta_{--}\right)$$

$$[\hat{H}_0, \hat{S}_+] = \xi\sum_{pp'}(p-1)\left(a^\dagger_{p+}a_{p'-}\delta_{pp'} - a^\dagger_{p'+}a_{p-}\delta_{p'p}\right)$$

when $p' = p$

$$[\hat{H}_0, \hat{S}_+] = \xi\sum_{p}(p-1)\left(a^\dagger_{p+}a_{p-}\delta_{pp} - a^\dagger_{p+}a_{p-}\delta_{pp}\right) = 0$$

For

$$[\hat{H}_0, \hat{S}_-] = \xi\sum_{pp'}(p-1)\left(a^\dagger_{p+}a_{p'+}\delta_{pp'}\delta_{+-} + a^\dagger_{p-}a_{p'+}\delta_{pp'}\delta_{--} - a^\dagger_{p'-}a_{p+}\delta_{p'p}\delta_{++} - a^\dagger_{p'-}a_{p-}\delta_{p'p}\delta_{+-}\right)$$

For

$$[\hat{H}_0, \hat{S}_-] = \xi\sum_{pp'}(p-1)\left(a^\dagger_{p-}a_{p'+}\delta_{pp'} - a^\dagger_{p'-}a_{p+}\delta_{p'p}\right)$$

when $p' = p$

$$[\hat{H}_0, \hat{S}_-] = \xi\sum_{p}(p-1)\left(a^\dagger_{p-}a_{p+}\delta_{pp} - a^\dagger_{p-}a_{p+}\delta_{pp}\right) = 0$$

Therefore

$$[\hat{H}_0, \hat{S}_\pm] = 0 \tag{12}$$

$$[\hat{V}, \hat{S}_\pm] = \left(-\frac{1}{2}g\sum_{pq} a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}\right)\left(\sum_{p'} a^\dagger_{p'\pm}a_{p'\mp}\right) - \left(\sum_{p'} a^\dagger_{p'\pm}a_{p'\mp}\right)\left(-\frac{1}{2}g\sum_{pq} a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}\right)$$

$$[\hat{V}, \hat{S}_\pm] = -\frac{1}{2}g\sum_{pp'q}\left[\underbrace{\left(a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}\right)\left(a^\dagger_{p'\pm}a_{p'\mp}\right)}_{(i)} - \underbrace{\left(a^\dagger_{p'\pm}a_{p'\mp}\right)\left(a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}\right)}_{(ii)}\right] \tag{13}$$

(i)

$$\left(a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}\right)\left(a^\dagger_{p'\pm}a_{p'\mp}\right) = a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}a^\dagger_{p'\pm}a_{p'\mp}$$

$$= a^\dagger_{p+}a^\dagger_{p-}a_{q-}\left(\delta_{qp'}\delta_{+\pm} - a^\dagger_{p'\pm}a_{q+}\right)a_{p'\mp}$$

where $q \neq p'$

$$= -a^\dagger_{p+}a^\dagger_{p-}a_{q-}a^\dagger_{p'\pm}a_{q+}a_{p'\mp} = -a^\dagger_{p+}a^\dagger_{p-}\left(\delta_{qp'}\delta_{-\pm} - a^\dagger_{p'\pm}a_{q-}\right)a_{q+}a_{p'\mp}$$

$$= a^\dagger_{p+}a^\dagger_{p-}a^\dagger_{p'\pm}a_{q-}a_{q+}a_{p'\mp} \tag{14}$$

(ii)

$$\left(a^\dagger_{p'\pm}a_{p'\mp}\right)\left(a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}\right) = a^\dagger_{p'\pm}a_{p'\mp}a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}$$

$$= a^\dagger_{p'\pm}\left(\delta_{p'p}\delta_{\mp+} - a^\dagger_{p+}a_{p'\mp}\right)a^\dagger_{p-}a_{q-}a_{q+} = a^\dagger_{p'\pm}a^\dagger_{p-}a_{q-}a_{q+}\delta_{p'p}\delta_{\mp+} - a^\dagger_{p'\pm}a^\dagger_{p+}a_{p'\mp}a^\dagger_{p-}a_{q-}a_{q+}$$

$$= a^\dagger_{p'\pm}a^\dagger_{p-}a_{q-}a_{q+}\delta_{p'p}\delta_{\mp+} - a^\dagger_{p'\pm}a^\dagger_{p+}\left(\delta_{p'p}\delta_{\mp-} - a^\dagger_{p-}a_{p'\mp}\right)a_{q-}a_{q+}$$

$$= a^\dagger_{p'\pm}a^\dagger_{p-}a_{q-}a_{q+}\delta_{p'p}\delta_{\mp+} - a^\dagger_{p'\pm}a^\dagger_{p+}a_{q-}a_{q+}\delta_{p'p}\delta_{\mp-} + \underbrace{a^\dagger_{p'\pm}a^\dagger_{p+}}\,a^\dagger_{p-}\,\underbrace{a_{p'\mp}a_{q-}}\,a_{q+}$$

$$= a^\dagger_{p'\pm}a^\dagger_{p-}a_{q-}a_{q+}\delta_{p'p}\delta_{\mp+} - a^\dagger_{p'\pm}a^\dagger_{p+}a_{q-}a_{q+}\delta_{p'p}\delta_{\mp-} + a^\dagger_{p+}\,\underbrace{a^\dagger_{p'\pm}a^\dagger_{p-}}\,a_{q-}\,\underbrace{a_{p'\mp}a_{q+}}$$

$$= a^\dagger_{p'\pm}a^\dagger_{p-}a_{q-}a_{q+}\delta_{p'p}\delta_{\mp+} - a^\dagger_{p'\pm}a^\dagger_{p+}a_{q-}a_{q+}\delta_{p'p}\delta_{\mp-} + a^\dagger_{p+}a^\dagger_{p-}a^\dagger_{p'\pm}a_{q-}a_{q+}a_{p'\mp} \tag{15}$$

Replacing equations (14) and (15) in equation (13)

$$[\hat{V}, \hat{S}_\pm] = -\frac{1}{2}g\sum_{pp'q}\left[a^\dagger_{p+}a^\dagger_{p-}a^\dagger_{p'\pm}a_{q-}a_{q+}a_{p'\mp} - a^\dagger_{p'\pm}a^\dagger_{p-}a_{q-}a_{q+}\delta_{p'p}\delta_{\mp+} + a^\dagger_{p'\pm}a^\dagger_{p+}a_{q-}a_{q+}\delta_{p'p}\delta_{\mp-} - a^\dagger_{p+}a^\dagger_{p-}a^\dagger_{p'\pm}a_{q-}a_{q+}a_{p'\mp}\right]$$

$$[\hat{V},\hat{S}_\pm]=-\frac{1}{2}g\sum_{pp'q}\left[-a^\dagger_{p'\pm}a^\dagger_{p-}a_{q-}a_{q+}\delta_{p'p}\delta_{\mp+}+a^\dagger_{p'\pm}a^\dagger_{p+}a_{q-}a_{q+}\delta_{p'p}\delta_{\mp-}\right]$$

For

$$[\hat{V},\hat{S}_+]=-\frac{1}{2}g\sum_{pp'q}\left[-a^\dagger_{p'+}a^\dagger_{p-}a_{q-}a_{q+}\delta_{p'p}\delta_{-+}+a^\dagger_{p'+}a^\dagger_{p+}a_{q-}a_{q+}\delta_{p'p}\delta_{--}\right]$$

$$[\hat{V},\hat{S}_+]=-\frac{1}{2}g\sum_{pp'q}a^\dagger_{p'+}a^\dagger_{p+}a_{q-}a_{q+}\delta_{p'p}\delta_{--}$$

when $p'=p$

$$[\hat{V},\hat{S}_+]=-\frac{1}{2}g\sum_{pq}a^\dagger_{p'+}a^\dagger_{p+}a_{q-}a_{q+}\delta_{p'p} \tag{16}$$

For

$$[\hat{V},\hat{S}_-]=-\frac{1}{2}g\sum_{pp'q}\left[-a^\dagger_{p'-}a^\dagger_{p-}a_{q-}a_{q+}\delta_{p'p}\delta_{++}+a^\dagger_{p'-}a^\dagger_{p+}a_{q-}a_{q+}\delta_{p'p}\delta_{+-}\right]$$

$$[\hat{V},\hat{S}_-]=-\frac{1}{2}g\sum_{pp'q}-a^\dagger_{p'-}a^\dagger_{p-}a_{q-}a_{q+}\delta_{p'p}\delta_{++}$$

$$[\hat{V},\hat{S}_-]=\frac{1}{2}g\sum_{pq}a^\dagger_{p'-}a^\dagger_{p-}a_{q-}a_{q+}\delta_{p'p} \tag{17}$$

Then, we can show

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

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

Let's use the relation

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

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

Using equations (4) and (12)

$$[\hat{H}_0,\hat{S}^2]=0$$

$$[\hat{V},\hat{S}^2]=\left[\hat{V},\hat{S}_z^2+\frac{1}{2}(\hat{S}_+\hat{S}_-+\hat{S}_-\hat{S}_+)\right]=\left[\hat{V},\hat{S}_z^2\right]+\frac{1}{2}\left[\hat{V},\hat{S}_+\hat{S}_-\right]+\frac{1}{2}\left[\hat{V},\hat{S}_-\hat{S}_+\right]$$

$$[\hat{V},\hat{S}^2]=[\hat{V},\hat{S}_z]\hat{S}_z+\hat{S}_z[\hat{V},\hat{S}_z]+\frac{1}{2}\left([\hat{V},\hat{S}_+]\hat{S}_-+\hat{S}_+[\hat{V},\hat{S}_-]\right)+\frac{1}{2}\left([\hat{V},\hat{S}_-]\hat{S}_++\hat{S}_-[\hat{V},\hat{S}_+]\right)$$

Using equations (8), (16) and (17)

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

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

$$\begin{aligned}[\hat{V},\hat{S}^2] =& -\frac{1}{4}g\sum_{pp'q}\Big[\left(a^\dagger_{p'+}a^\dagger_{p+}a_{q-}a_{q+}\right)\left(a^\dagger_{p'-}a_{p'+}\right) - \left(a^\dagger_{p'+}a_{p'-}\right)\left(a^\dagger_{p'-}a^\dagger_{p-}a_{q-}a_{q+}\right) + \\ &- \left(a^\dagger_{p'-}a^\dagger_{p-}a_{q-}a_{q+}\right)\left(a^\dagger_{p'+}a_{p'-}\right) + \left(a^\dagger_{p'-}a_{p'+}\right)\left(a^\dagger_{p'+}a^\dagger_{p+}a_{q-}a_{q+}\right)\Big]\delta_{p'p}\end{aligned}$$

$$\begin{aligned}[\hat{V},\hat{S}^2] =& -\frac{1}{4}g\sum_{pp'q}\Big[a^\dagger_{p'+}a^\dagger_{p+}a_{q-}a_{q+}a^\dagger_{p'-}a_{p'+} - a^\dagger_{p'+}a_{p'-}a^\dagger_{p'-}a^\dagger_{p-}a_{q-}a_{q+} + \\ &- a^\dagger_{p'-}a^\dagger_{p-}a_{q-}a_{q+}a^\dagger_{p'+}a_{p'-} + a^\dagger_{p'-}a_{p'+}a^\dagger_{p'+}a^\dagger_{p+}a_{q-}a_{q+}\Big]\delta_{p'p}\end{aligned}$$

$$\begin{aligned}[\hat{V},\hat{S}^2] =& -\frac{1}{4}g\sum_{pp'q}\Big[-a^\dagger_{p'+}a^\dagger_{p+}a_{q-}a^\dagger_{p'-}a_{q+}a_{p'+} - a^\dagger_{p'+}a^\dagger_{p-}a_{q-}a_{q+} + a^\dagger_{p'+}a^\dagger_{p'-}a_{p'-}a^\dagger_{p-}a_{q-}a_{q+} + \\ &+ a^\dagger_{p'-}a^\dagger_{p-}a_{q-}a^\dagger_{p'+}a_{q+}a_{p'-} + a^\dagger_{p'-}a^\dagger_{p+}a_{q-}a_{q+} - a^\dagger_{p'-}a^\dagger_{p'+}a_{p'+}a^\dagger_{p+}a_{q-}a_{q+}\Big]\delta_{p'p}\end{aligned}$$

$$\begin{aligned}[\hat{V},\hat{S}^2] =& -\frac{1}{4}g\sum_{pp'q}\Big[a^\dagger_{p'+}a^\dagger_{p+}a^\dagger_{p'-}a_{q-}a_{q+}a_{p'+} - a^\dagger_{p'+}a^\dagger_{p-}a_{q-}a_{q+} + a^\dagger_{p'+}a^\dagger_{p'-}a_{q-}a_{q+}\delta_{p'p} - a^\dagger_{p'+}a^\dagger_{p'-}a^\dagger_{p-}a_{p'-}a_{q-}a_{q+} - \\ &- a^\dagger_{p'-}\underbrace{a^\dagger_{p-}a^\dagger_{p'+}}a_{q-}\underbrace{a_{q+}a_{p'-}} + a^\dagger_{p'-}a^\dagger_{p+}a_{q-}a_{q+} - a^\dagger_{p'-}a^\dagger_{p'+}a_{q-}a_{q+}\delta_{p'p} + \underbrace{a^\dagger_{p'-}a^\dagger_{p'+}}a^\dagger_{p+}\underbrace{a_{p'+}a_{q-}}a_{q+}\Big]\delta_{p'p}\end{aligned}$$

$$\begin{aligned}[\hat{V},\hat{S}^2] =& -\frac{1}{4}g\sum_{pp'q}\Big[a^\dagger_{p'+}a^\dagger_{p+}a^\dagger_{p'-}a_{q-}a_{q+}a_{p'+} - a^\dagger_{p'+}a^\dagger_{p-}a_{q-}a_{q+} + a^\dagger_{p'+}a^\dagger_{p'-}a_{q-}a_{q+}\delta_{p'p} - a^\dagger_{p'+}a^\dagger_{p'-}a^\dagger_{p-}a_{p'-}a_{q-}a_{q+} - \\ &- \underbrace{a^\dagger_{p'-}a^\dagger_{p'+}}a^\dagger_{p-}\underbrace{a_{q-}a_{p'-}}a_{q+} + a^\dagger_{p'-}a^\dagger_{p+}a_{q-}a_{q+} - a^\dagger_{p'-}a^\dagger_{p'+}a_{q-}a_{q+}\delta_{p'p} + a^\dagger_{p'+}\underbrace{a^\dagger_{p'-}a^\dagger_{p+}}a_{q-}\underbrace{a_{p'+}a_{q+}}\Big]\delta_{p'p}\end{aligned}$$

$$\begin{aligned}[\hat{V},\hat{S}^2] =& -\frac{1}{4}g\sum_{pp'q}\Big[a^\dagger_{p'+}a^\dagger_{p+}a^\dagger_{p'-}a_{q-}a_{q+}a_{p'+} - a^\dagger_{p'+}a^\dagger_{p-}a_{q-}a_{q+} + a^\dagger_{p'+}a^\dagger_{p'-}a_{q-}a_{q+}\delta_{p'p} - a^\dagger_{p'+}a^\dagger_{p'-}a^\dagger_{p-}a_{p'-}a_{q-}a_{q+} - \\ &- a^\dagger_{p'+}\underbrace{a^\dagger_{p'-}a^\dagger_{p-}}a_{p'-}a_{q-}a_{q+} + a^\dagger_{p'-}a^\dagger_{p+}a_{q-}a_{q+} - a^\dagger_{p'-}a^\dagger_{p'+}a_{q-}a_{q+}\delta_{p'p} + \underbrace{a^\dagger_{p'+}a^\dagger_{p+}}a^\dagger_{p'-}a_{q-}a_{q+}a_{p'+}\Big]\delta_{p'p}\end{aligned}$$

$$\begin{aligned}[\hat{V},\hat{S}^2] =& -\frac{1}{4}g\sum_{pp'q}\Big[a^\dagger_{p'+}a^\dagger_{p+}a^\dagger_{p'-}a_{q-}a_{q+}a_{p'+} - a^\dagger_{p'+}a^\dagger_{p-}a_{q-}a_{q+} + a^\dagger_{p'+}a^\dagger_{p'-}a_{q-}a_{q+}\delta_{p'p} - a^\dagger_{p'+}a^\dagger_{p'-}a^\dagger_{p-}a_{p'-}a_{q-}a_{q+} + \\ &+ a^\dagger_{p'+}a^\dagger_{p-}a^\dagger_{p'-}a_{p'-}a_{q-}a_{q+} + a^\dagger_{p'-}a^\dagger_{p+}a_{q-}a_{q+} - a^\dagger_{p'-}a^\dagger_{p'+}a_{q-}a_{q+}\delta_{p'p} - a^\dagger_{p+}a^\dagger_{p'+}a^\dagger_{p'-}a_{q-}a_{q+}a_{p'+}\Big]\delta_{p'p}\end{aligned}$$

when $p' = p$

$$[\hat{V}, \hat{S}^2] = -\frac{1}{4}g\sum_{pp'q}\Big[a^\dagger_{p+}a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}a_{p+} - a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+} + a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+} - a^\dagger_{p+}a^\dagger_{p-}a^\dagger_{p-}a_{p-}a_{q-}a_{q+} +$$
$$+a^\dagger_{p+}a^\dagger_{p-}a^\dagger_{p-}a_{p-}a_{q-}a_{q+} + a^\dagger_{p-}a^\dagger_{p+}a_{q-}a_{q+} - a^\dagger_{p-}a^\dagger_{p+}a_{q-}a_{q+} - a^\dagger_{p+}a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}a_{p+}\Big]$$

Therefore

$$[\hat{V}, \hat{S}^2] = 0 \tag{18}$$

Using the relations, Show

$$\hat{P}^+_p = a^\dagger_{p+}a^\dagger_{p-}$$

$$\hat{P}^-_p = a_{p-}a_{p+}$$

with $\xi = 1$, we can express the Hamiltonian

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

like

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

Show $\left[\hat{P}^+_p, \hat{P}^-_q\right]$

$$\left[\hat{P}^+_p, \hat{P}^-_q\right] = a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+} - a_{q-}\underbrace{a_{q+}a^\dagger_{p+}}a^\dagger_{p-}$$

$$= a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+} - a_{q-}\left(\delta_{qp} - a^\dagger_{p+}a_{q+}\right)a^\dagger_{p-} = a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+} - a_{q-}a^\dagger_{p-}\delta_{qp} + \underbrace{a_{q-}a^\dagger_{p+}}a_{q+}a^\dagger_{p-}$$

$$= a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+} - a_{q-}a^\dagger_{p-}\delta_{qp} - a^\dagger_{p+}a_{q-}\underbrace{a_{q+}a^\dagger_{p-}} = a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+} - a_{q-}a^\dagger_{p-}\delta_{qp} + a^\dagger_{p+}\underbrace{a_{q-}a^\dagger_{p-}}a_{q+}$$

$$= a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+} - a_{q-}a^\dagger_{p-}\delta_{qp} + a^\dagger_{p+}\left(\delta_{qp} - a^\dagger_{p-}a_{q-}\right)a_{q+} = a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+} - a_{q-}a^\dagger_{p-}\delta_{qp} + a^\dagger_{p+}a_{q+}\delta_{qp} - a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}$$

$$= -a_{q-}a^\dagger_{p-}\delta_{qp} + a^\dagger_{p+}a_{q+}\delta_{qp}$$

when $p \neq q$

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

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

2. (15/100 points) 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

For this case the systems can draw like

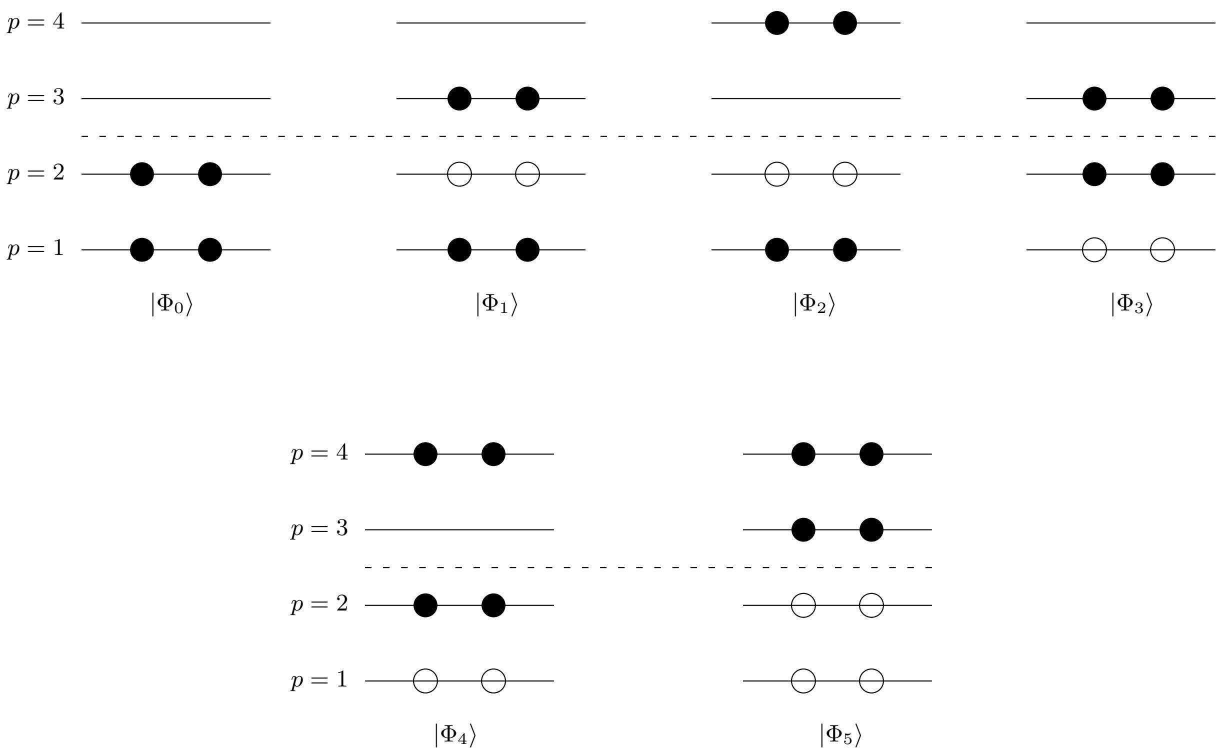


FIG. 1: Systems for no broken pairs

we will have a 6x6 matrix, let's define the general Slater determinant in a general way:

$$\langle\Phi| = \langle 0|a_{p'-}a_{p'+}a_{p-}a_{p+} \qquad\qquad |\Phi\rangle = a^{\dagger}_{p+}a^{\dagger}_{p-}a^{\dagger}_{p'+}a^{\dagger}_{p'-}$$

then for each slater determinant

$$\langle\Phi_0| = \langle 0|a_{2-}a_{2+}a_{1-}a_{1+} \qquad |\Phi_0\rangle = a^{\dagger}_{1+}a^{\dagger}_{1-}a^{\dagger}_{2+}a^{\dagger}_{2-}|0\rangle \tag{19}$$

$$\langle\Phi_1| = \langle 0|a_{3-}a_{3+}a_{1-}a_{1+} \qquad |\Phi_1\rangle = a^{\dagger}_{1+}a^{\dagger}_{1-}a^{\dagger}_{3+}a^{\dagger}_{3-}|0\rangle \tag{20}$$

$$\langle\Phi_2| = \langle 0|a_{4-}a_{4+}a_{1-}a_{1+} \qquad |\Phi_2\rangle = a^{\dagger}_{1+}a^{\dagger}_{1-}a^{\dagger}_{4+}a^{\dagger}_{4-}|0\rangle \tag{21}$$

$$\langle\Phi_3| = \langle 0|a_{3-}a_{3+}a_{2-}a_{2+} \qquad |\Phi_3\rangle = a^{\dagger}_{2+}a^{\dagger}_{2-}a^{\dagger}_{3+}a^{\dagger}_{3-}|0\rangle \tag{22}$$

$$\langle\Phi_4| = \langle 0|a_{4-}a_{4+}a_{2-}a_{2+} \qquad |\Phi_4\rangle = a^{\dagger}_{2+}a^{\dagger}_{2-}a^{\dagger}_{4+}a^{\dagger}_{4-}|0\rangle \tag{23}$$

$$\langle\Phi_5| = \langle 0|a_{4-}a_{4+}a_{3-}a_{3+} \qquad |\Phi_5\rangle = a^{\dagger}_{3+}a^{\dagger}_{3-}a^{\dagger}_{4+}a^{\dagger}_{4-}|0\rangle \tag{24}$$

Matrix is

$$H = \begin{bmatrix}
\langle\Phi_0|\hat{H}|\Phi_0\rangle & \langle\Phi_0|\hat{H}|\Phi_1\rangle & \langle\Phi_0|\hat{H}|\Phi_2\rangle & \langle\Phi_0|\hat{H}|\Phi_3\rangle & \langle\Phi_0|\hat{H}|\Phi_4\rangle & \langle\Phi_0|\hat{H}|\Phi_5\rangle \\
\langle\Phi_1|\hat{H}|\Phi_0\rangle & \langle\Phi_1|\hat{H}|\Phi_1\rangle & \langle\Phi_1|\hat{H}|\Phi_2\rangle & \langle\Phi_1|\hat{H}|\Phi_3\rangle & \langle\Phi_1|\hat{H}|\Phi_4\rangle & \langle\Phi_1|\hat{H}|\Phi_5\rangle \\
\langle\Phi_2|\hat{H}|\Phi_0\rangle & \langle\Phi_2|\hat{H}|\Phi_1\rangle & \langle\Phi_2|\hat{H}|\Phi_2\rangle & \langle\Phi_2|\hat{H}|\Phi_3\rangle & \langle\Phi_2|\hat{H}|\Phi_4\rangle & \langle\Phi_2|\hat{H}|\Phi_5\rangle \\
\langle\Phi_3|\hat{H}|\Phi_0\rangle & \langle\Phi_3|\hat{H}|\Phi_1\rangle & \langle\Phi_3|\hat{H}|\Phi_2\rangle & \langle\Phi_3|\hat{H}|\Phi_3\rangle & \langle\Phi_3|\hat{H}|\Phi_4\rangle & \langle\Phi_3|\hat{H}|\Phi_5\rangle \\
\langle\Phi_4|\hat{H}|\Phi_0\rangle & \langle\Phi_4|\hat{H}|\Phi_1\rangle & \langle\Phi_4|\hat{H}|\Phi_2\rangle & \langle\Phi_4|\hat{H}|\Phi_3\rangle & \langle\Phi_4|\hat{H}|\Phi_4\rangle & \langle\Phi_4|\hat{H}|\Phi_5\rangle \\
\langle\Phi_5|\hat{H}|\Phi_0\rangle & \langle\Phi_5|\hat{H}|\Phi_1\rangle & \langle\Phi_5|\hat{H}|\Phi_2\rangle & \langle\Phi_5|\hat{H}|\Phi_3\rangle & \langle\Phi_5|\hat{H}|\Phi_4\rangle & \langle\Phi_5|\hat{H}|\Phi_5\rangle
\end{bmatrix} \tag{25}$$

Let's calculate

$$\langle\Phi_0|\hat{H}|\Phi_0\rangle = \langle\Phi_0|(\hat{H}_0+\hat{V})|\Phi_0\rangle = \underbrace{\langle\Phi_0|\hat{H}_0|\Phi_0\rangle}_{(i)} + \underbrace{\langle\Phi_0|\hat{V}|\Phi_0\rangle}_{(ii)} \tag{26}$$

For

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

$$\hat{H}_0 = \xi\left[\left(a^\dagger_{2+}a_{2+}+a^\dagger_{2-}a_{2-}\right)+2\left(a^\dagger_{3+}a_{3+}+a^\dagger_{3-}a_{3-}\right)+3\left(a^\dagger_{4+}a_{4+}+a^\dagger_{4-}a_{4-}\right)\right] \tag{27}$$

$$\hat{V} = -\frac{1}{2}g\sum_{pq}a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+} \tag{28}$$

(i) Using equation (33)

$$\begin{aligned}\langle\Phi_0|\hat{H}_0|\Phi_0\rangle = \xi\Big[&\langle 0|a_{2-}a_{2+}a_{1-}a_{1+}a^\dagger_{2+}a_{2+}a^\dagger_{1+}a^\dagger_{1-}a^\dagger_{2+}a^\dagger_{2-}|0\rangle + \langle 0|a_{2-}a_{2+}a_{1-}a_{1+}a^\dagger_{2-}a_{2-}a^\dagger_{1+}a^\dagger_{1-}a^\dagger_{2+}a^\dagger_{2-}|0\rangle\\ &+2\langle 0|a_{2-}a_{2+}a_{1-}a_{1+}a^\dagger_{3+}a_{3+}a^\dagger_{1+}a^\dagger_{1-}a^\dagger_{2+}a^\dagger_{2-}|0\rangle + 2\langle 0|a_{2-}a_{2+}a_{1-}a_{1+}a^\dagger_{3-}a_{3-}a^\dagger_{1+}a^\dagger_{1-}a^\dagger_{2+}a^\dagger_{2-}|0\rangle\\ &+3\langle 0|a_{2-}a_{2+}a_{1-}a_{1+}a^\dagger_{4+}a_{4+}a^\dagger_{1+}a^\dagger_{1-}a^\dagger_{2+}a^\dagger_{2-}|0\rangle + 3\langle 0|a_{2-}a_{2+}a_{1-}a_{1+}a^\dagger_{4-}a_{4-}a^\dagger_{1+}a^\dagger_{1-}a^\dagger_{2+}a^\dagger_{2-}|0\rangle\Big]\end{aligned}$$

It is different to zero only when $p=2$ to other cases it is zero

$$\langle\Phi_0|\hat{H}_0|\Phi_0\rangle = \xi\left[\langle 0|a_{2-}a_{2+}a_{1-}a_{1+}a^\dagger_{2+}a_{2+}a^\dagger_{1+}a^\dagger_{1-}a^\dagger_{2+}a^\dagger_{2-}|0\rangle + \langle 0|a_{2-}a_{2+}a_{1-}a_{1+}a^\dagger_{2-}a_{2-}a^\dagger_{1+}a^\dagger_{1-}a^\dagger_{2+}a^\dagger_{2-}|0\rangle\right]$$

$$\langle\Phi_0|\hat{H}_0|\Phi_0\rangle = 2\xi \tag{29}$$

(ii) Using equation (34)

$$\langle\Phi_0|\hat{V}|\Phi_0\rangle = -\frac{1}{2}g\sum_{pq}\langle 0|a_{2-}a_{2+}a_{1-}a_{1+}a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}a^\dagger_{1+}a^\dagger_{1-}a^\dagger_{2+}a^\dagger_{2-}|0\rangle$$

It is different to zero when $p=1$, $q=1$ and when $p=2$, $q=2$

$$\langle\Phi_0|\hat{V}|\Phi_0\rangle = -\frac{1}{2}g\left[\langle 0|a_{2-}a_{2+}a_{1-}a_{1+}a^\dagger_{1+}a^\dagger_{1-}a_{1-}a_{1+}a^\dagger_{1+}a^\dagger_{1-}a^\dagger_{2+}a^\dagger_{2-}|0\rangle + \langle 0|a_{2-}a_{2+}a_{1-}a_{1+}a^\dagger_{2+}a^\dagger_{2-}a_{2-}a_{2+}a^\dagger_{1+}a^\dagger_{1-}a^\dagger_{2+}a^\dagger_{2-}|0\rangle\right]$$

$$\langle\Phi_0|\hat{V}|\Phi_0\rangle = -\frac{1}{2}g\times 2 = -g \tag{30}$$

Replacing equations (35) and (36) in equation (32)

$$\langle\Phi_0|\hat{H}|\Phi_0\rangle = 2\xi - g \tag{31}$$

$$\langle\Phi_1|\hat{H}|\Phi_1\rangle = \underbrace{\langle\Phi_1|\hat{H}_0|\Phi_1\rangle}_{(i)} + \underbrace{\langle\Phi_1|\hat{V}|\Phi_1\rangle}_{(ii)} \tag{32}$$

(i) Using equation (33), we can see that it is different to zero only when $p=3$

$$\langle\Phi_1|\hat{H}_0|\Phi_1\rangle = 2\xi\left[\langle 0|a_{3-}a_{3+}a_{1-}a_{1+}a^\dagger_{3+}a_{3+}a^\dagger_{1+}a^\dagger_{1-}a^\dagger_{3+}a^\dagger_{3-}|0\rangle + \langle 0|a_{3-}a_{3+}a_{1-}a_{1+}a^\dagger_{3-}a_{3-}a^\dagger_{1+}a^\dagger_{1-}a^\dagger_{3+}a^\dagger_{3-}|0\rangle\right]$$

$$\langle\Phi_1|\hat{H}_0|\Phi_1\rangle = 4\xi \tag{33}$$

(ii) Using equation (34), It is different to zero when $p=1$, $q=1$ and when $p=3$, $q=3$

$$\langle\Phi_1|\hat{V}|\Phi_1\rangle = -\frac{1}{2}g\left[\langle 0|a_{3-}a_{3+}a_{1-}a_{1+}a^\dagger_{1+}a^\dagger_{1-}a_{1-}a_{1+}a^\dagger_{1+}a^\dagger_{1-}a^\dagger_{3+}a^\dagger_{3-}|0\rangle + \langle 0|a_{3-}a_{3+}a_{1-}a_{1+}a^\dagger_{3+}a^\dagger_{3-}a_{3-}a_{3+}a^\dagger_{1+}a^\dagger_{1-}a^\dagger_{3+}a^\dagger_{3-}|0\rangle\right]$$

$$\langle\Phi_1|\hat{V}|\Phi_1\rangle = -\frac{1}{2}g\times 2 = -g \tag{34}$$

Replacing equations (39) and (40) in equation (38)

$$\langle\Phi_1|\hat{H}|\Phi_1\rangle = 4\xi - g \tag{35}$$

$$\langle\Phi_2|\hat{H}|\Phi_2\rangle = \underbrace{\langle\Phi_2|\hat{H}_0|\Phi_2\rangle}_{(i)} + \underbrace{\langle\Phi_2|\hat{V}|\Phi_2\rangle}_{(ii)} \tag{36}$$

(i) Using equation (33), we can see that it is different to zero only when $p=4$

$$\langle\Phi_2|\hat{H}_0|\Phi_2\rangle = 3\xi\left[\langle 0|a_{4-}a_{4+}a_{1-}a_{1+}a^\dagger_{4+}a_{4+}a^\dagger_{1+}a^\dagger_{1-}a^\dagger_{4+}a^\dagger_{4-}|0\rangle + \langle 0|a_{4-}a_{4+}a_{1-}a_{1+}a^\dagger_{4-}a_{4-}a^\dagger_{1+}a^\dagger_{1-}a^\dagger_{4+}a^\dagger_{4-}|0\rangle\right]$$

$$\langle\Phi_1|\hat{H}_0|\Phi_1\rangle = 6\xi \tag{37}$$

(ii) Using equation (34), It is different to zero when $p=1$, $q=1$ and when $p=4$, $q=4$

$$\langle\Phi_2|\hat{V}|\Phi_2\rangle = -\frac{1}{2}g\left[\langle 0|a_{4-}a_{4+}a_{1-}a_{1+}a^\dagger_{1+}a^\dagger_{1-}a_{1-}a_{1+}a^\dagger_{1+}a^\dagger_{1-}a^\dagger_{4+}a^\dagger_{4-}|0\rangle + \langle 0|a_{4-}a_{4+}a_{1-}a_{1+}a^\dagger_{4+}a^\dagger_{4-}a_{4-}a_{4+}a^\dagger_{1+}a^\dagger_{1-}a^\dagger_{4+}a^\dagger_{4-}|0\rangle\right]$$

$$\langle\Phi_1|\hat{V}|\Phi_1\rangle = -\frac{1}{2}g\times 2 = -g \tag{38}$$

Replacing equations (43) and (44) in equation (42)

$$\langle\Phi_2|\hat{H}|\Phi_2\rangle = 6\xi - g \tag{39}$$

$$\langle\Phi_1|\hat{H}|\Phi_0\rangle = \underbrace{\langle\Phi_1|\hat{H}_0|\Phi_0\rangle}_{(i)} + \underbrace{\langle\Phi_1|\hat{V}|\Phi_0\rangle}_{(ii)} \tag{40}$$

(i) In this case i'm going to solve for each case de $\hat{H}_0$, using equation (33)

$$\begin{aligned}\langle\Phi_1|\hat{H}_0|\Phi_0\rangle = \xi\Big[&\langle 0|a_{3-}a_{3+}a_{1-}a_{1+}a^\dagger_{2+}a_{2+}a^\dagger_{1+}a^\dagger_{1-}a^\dagger_{2+}a^\dagger_{2-}|0\rangle + \langle 0|a_{3-}a_{3+}a_{1-}a_{1+}a^\dagger_{2-}a_{2-}a^\dagger_{1+}a^\dagger_{1-}a^\dagger_{2+}a^\dagger_{2-}|0\rangle \\ &+2\langle 0|a_{3-}a_{3+}a_{1-}a_{1+}a^\dagger_{3+}a_{3+}a^\dagger_{1+}a^\dagger_{1-}a^\dagger_{2+}a^\dagger_{2-}|0\rangle + 2\langle 0|a_{3-}a_{3+}a_{1-}a_{1+}a^\dagger_{3-}a_{3-}a^\dagger_{1+}a^\dagger_{1-}a^\dagger_{2+}a^\dagger_{2-}|0\rangle \\ &+3\langle 0|a_{3-}a_{3+}a_{1-}a_{1+}a^\dagger_{4+}a_{4+}a^\dagger_{1+}a^\dagger_{1-}a^\dagger_{2+}a^\dagger_{2-}|0\rangle + 3\langle 0|a_{3-}a_{3+}a_{1-}a_{1+}a^\dagger_{4-}a_{4-}a^\dagger_{1+}a^\dagger_{1-}a^\dagger_{2+}a^\dagger_{2-}|0\rangle\Big]\end{aligned}$$

Since all terms are equal to zero

$$\langle \Phi_1 | \hat{H}_0 | \Phi_0 \rangle = 0 \tag{41}$$

(ii) Using equation (34), It is only differents to zero when $p = 3$ and $q = 2$

$$\langle \Phi_1 | \hat{V} | \Phi_0 \rangle = -\frac{1}{2} g \langle 0 | a_{3-} a_{3+} a_{1-} a_{1+} a^\dagger_{3+} a^\dagger_{3-} a_{2-} a_{2+} a^\dagger_{1+} a^\dagger_{1-} a^\dagger_{2+} a^\dagger_{2-} | 0 \rangle$$

$$\langle \Phi_1 | \hat{V} | \Phi_0 \rangle = -\frac{1}{2} g \tag{42}$$

Replacing equations (47) and (48) in equation (46)

$$\langle \Phi_1 | \hat{H} | \Phi_0 \rangle = -\frac{1}{2} g \tag{43}$$

Since writing the development of the 36 terms of this matrix is very extensive. Now that we know how to solve them, I'm going to write the solution for each matrix element.

$$\begin{aligned}
\langle \Phi_0 | \hat{H} | \Phi_1 \rangle &= -\frac{1}{2} g & \langle \Phi_3 | \hat{H} | \Phi_2 \rangle &= 0 && (44)\\
\langle \Phi_0 | \hat{H} | \Phi_2 \rangle &= -\frac{1}{2} g & \langle \Phi_3 | \hat{H} | \Phi_3 \rangle &= 6\xi - g && (45)\\
\langle \Phi_0 | \hat{H} | \Phi_3 \rangle &= -\frac{1}{2} g & \langle \Phi_3 | \hat{H} | \Phi_4 \rangle &= -\frac{1}{2} g && (46)\\
\langle \Phi_0 | \hat{H} | \Phi_4 \rangle &= -\frac{1}{2} g & \langle \Phi_3 | \hat{H} | \Phi_5 \rangle &= -\frac{1}{2} g && (47)\\
\langle \Phi_0 | \hat{H} | \Phi_5 \rangle &= 0 & \langle \Phi_4 | \hat{H} | \Phi_0 \rangle &= -\frac{1}{2} g && (48)\\
\langle \Phi_1 | \hat{H} | \Phi_2 \rangle &= -\frac{1}{2} g & \langle \Phi_4 | \hat{H} | \Phi_1 \rangle &= 0 && (49)\\
\langle \Phi_1 | \hat{H} | \Phi_3 \rangle &= -\frac{1}{2} g & \langle \Phi_4 | \hat{H} | \Phi_2 \rangle &= -\frac{1}{2} g && (50)\\
\langle \Phi_1 | \hat{H} | \Phi_4 \rangle &= 0 & \langle \Phi_4 | \hat{H} | \Phi_3 \rangle &= -\frac{1}{2} g && (51)\\
\langle \Phi_1 | \hat{H} | \Phi_5 \rangle &= -\frac{1}{2} g & \langle \Phi_4 | \hat{H} | \Phi_4 \rangle &= 8\xi - g && (52)\\
\langle \Phi_2 | \hat{H} | \Phi_0 \rangle &= -\frac{1}{2} g & \langle \Phi_4 | \hat{H} | \Phi_5 \rangle &= -\frac{1}{2} g && (53)\\
\langle \Phi_2 | \hat{H} | \Phi_1 \rangle &= -\frac{1}{2} g & \langle \Phi_5 | \hat{H} | \Phi_0 \rangle &= 0 && (54)\\
\langle \Phi_2 | \hat{H} | \Phi_3 \rangle &= 0 & \langle \Phi_5 | \hat{H} | \Phi_1 \rangle &= -\frac{1}{2} g && (55)\\
\langle \Phi_2 | \hat{H} | \Phi_4 \rangle &= -\frac{1}{2} g & \langle \Phi_5 | \hat{H} | \Phi_2 \rangle &= -\frac{1}{2} g && (56)\\
\langle \Phi_2 | \hat{H} | \Phi_5 \rangle &= -\frac{1}{2} g & \langle \Phi_5 | \hat{H} | \Phi_3 \rangle &= -\frac{1}{2} g && (57)\\
\langle \Phi_3 | \hat{H} | \Phi_0 \rangle &= -\frac{1}{2} g & \langle \Phi_5 | \hat{H} | \Phi_4 \rangle &= -\frac{1}{2} g && (58)\\
\langle \Phi_3 | \hat{H} | \Phi_1 \rangle &= -\frac{1}{2} g & \langle \Phi_5 | \hat{H} | \Phi_5 \rangle &= 10\xi - g && (59)
\end{aligned}$$

Replacing the values of the equations (37), (41), (45), (49) and from (50) to (65), we obtain

$$H = \begin{bmatrix}
2\xi - g & -g/2 & -g/2 & -g/2 & -g/2 & 0 \\
-g/2 & 4\xi - g & -g/2 & -g/2 & 0 & -g/2 \\
-g/2 & -g/2 & 6\xi - g & 0 & -g/2 & -g/2 \\
-g/2 & -g/2 & 0 & 6\xi - g & -g/2 & -g/2 \\
-g/2 & 0 & -g/2 & -g/2 & 8\xi - g & -g/2 \\
0 & -g/2 & -g/2 & -g/2 & -g/2 & 10\xi - g
\end{bmatrix} \tag{60}$$

Now we're going to calculate all eigenvalues for $g \in [-1, 1]$, where we will take $\xi = 1$. For this calculation we will use python.
For $g = -1$

```
In [68]: #Hamiltonian Matrix 6x6
import numpy as np
from sympy import *
from sympy.matrices import Matrix
lamb=symbols('lambda')
xi=symbols('xi')
g,xi=symbols("g,xi")
H= Matrix([[2*xi-g,-g/2,-g/2,-g/2,-g/2,0],[-g/2,4*xi-g,-g/2,-g/2,0,-g/2],[-g/2,-g/2,6*xi-g,0,-g/2,-g/2],[-g/2,-g/2,0,
H
```

Out[68]:

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

```
In [69]: #introduce values
g=-1
xi=1
```

```
In [70]: H= Matrix([[2*xi-g,-g/2,-g/2,-g/2,-g/2,0],[-g/2,4*xi-g,-g/2,-g/2,0,-g/2],[-g/2,-g/2,6*xi-g,0,-g/2,-g/2],[-g/2,-g/2,0,
H
```

Out[70]:

$$\begin{bmatrix} 3 & 0.5 & 0.5 & 0.5 & 0.5 & 0 \\ 0.5 & 5 & 0.5 & 0.5 & 0 & 0.5 \\ 0.5 & 0.5 & 7 & 0 & 0.5 & 0.5 \\ 0.5 & 0.5 & 0 & 7 & 0.5 & 0.5 \\ 0.5 & 0 & 0.5 & 0.5 & 9 & 0.5 \\ 0 & 0.5 & 0.5 & 0.5 & 0.5 & 11 \end{bmatrix}$$

```
In [71]: #Diagonalize-calculate eigenvalues with Characteristic polynomial |A-xI|=0
I=Matrix([[1,0,0,0,0,0],[0,1,0,0,0,0],[0,0,1,0,0,0],[0,0,0,1,0,0],[0,0,0,0,1,0],[0,0,0,0,0,1]])
A= H - lamb*I
A
```

Out[71]:

$$\begin{bmatrix} 3-\lambda & 0.5 & 0.5 & 0.5 & 0.5 & 0 \\ 0.5 & 5-\lambda & 0.5 & 0.5 & 0 & 0.5 \\ 0.5 & 0.5 & 7-\lambda & 0 & 0.5 & 0.5 \\ 0.5 & 0.5 & 0 & 7-\lambda & 0.5 & 0.5 \\ 0.5 & 0 & 0.5 & 0.5 & 9-\lambda & 0.5 \\ 0 & 0.5 & 0.5 & 0.5 & 0.5 & 11-\lambda \end{bmatrix}$$

```
In [72]: #Eigenvalues
C=H.eigenvals()
C
```

```
Out[72]: {2.77987013943789: 1,
 4.79105976082857: 1,
 7.00000000000000: 2,
 9.06461857330913: 1,
 11.3644515264244: 1}
```

Therefore

$$D = \begin{bmatrix} 2.77987 & 0 & 0 & 0 & 0 & 0 \\ 0 & 4.79106 & 0 & 0 & 0 & 0 \\ 0 & 0 & 7.00000 & 0 & 0 & 0 \\ 0 & 0 & 0 & 7.00000 & 0 & 0 \\ 0 & 0 & 0 & 0 & 9.06462 & 0 \\ 0 & 0 & 0 & 0 & 0 & 11.36445 \end{bmatrix} \tag{61}$$

and where $E_0 = 2.77987$

$$P = \begin{bmatrix} 0.972157 & 0.13647 & 0.09371 & -0.11590 & 0.10406 & 0.04059 \\ -0.184926 & 0.92749 & 0.18742 & -0.23179 & 0.01444 & 0.10054 \\ -0.08854 & -0.24234 & -0.18694 & -0.93314 & 0.16970 & 0.15388 \\ -0.08854 & -0.24234 & 0.93661 & 0.00597 & 0.16970 & 0.15388 \\ -0.06601 & 0.04604 & -0.18742 & 0.23179 & 0.90832 & 0.27064 \\ 0.02603 & -0.03937 & -0.09371 & 0.11590 & -0.32608 & 0.93147 \end{bmatrix} \tag{62}$$

Ground state: $|\psi_0\rangle = 0.972157|\Phi_0\rangle - 0.184926|\Phi_1\rangle - 0.08854|\Phi_2\rangle - 0.08854|\Phi_3\rangle - 0.06601|\Phi_4\rangle + 0.02603|\Phi_5\rangle$

For $g = 0$

```
In [2]: #introduce values
        g=0
        xi=1
```

```
In [3]: H= Matrix([[2*xi-g,-g/2,-g/2,-g/2,-g/2,0],[-g/2,4*xi-g,-g/2,-g/2,0,-g/2],[-g/2,-g/2,6*xi-g,0,-g/2,-g/2],[-g/2,-g/2,0,(
        H
```

Out[3]:

$$\begin{bmatrix} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 6 & 0 & 0 & 0 \\ 0 & 0 & 0 & 6 & 0 & 0 \\ 0 & 0 & 0 & 0 & 8 & 0 \\ 0 & 0 & 0 & 0 & 0 & 10 \end{bmatrix}$$

```
In [4]: #Diagonalize-calculate eigenvalues with Characteristic polynomial |A-xI|=0
        I=Matrix([[1,0,0,0,0,0],[0,1,0,0,0,0],[0,0,1,0,0,0],[0,0,0,1,0,0],[0,0,0,0,1,0],[0,0,0,0,0,1]])
        A= H - lamb*I
        A
```

Out[4]:

$$\begin{bmatrix} 2-\lambda & 0 & 0 & 0 & 0 & 0 \\ 0 & 4-\lambda & 0 & 0 & 0 & 0 \\ 0 & 0 & 6-\lambda & 0 & 0 & 0 \\ 0 & 0 & 0 & 6-\lambda & 0 & 0 \\ 0 & 0 & 0 & 0 & 8-\lambda & 0 \\ 0 & 0 & 0 & 0 & 0 & 10-\lambda \end{bmatrix}$$

```
In [5]: #Eigenvalues
        C=H.eigenvals()
        C
```

```
Out[5]: {2: 1, 4: 1, 6: 2, 8: 1, 10: 1}
```

Therefore

$$D = \begin{bmatrix} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 6 & 0 & 0 & 0 \\ 0 & 0 & 0 & 6 & 0 & 0 \\ 0 & 0 & 0 & 0 & 8 & 0 \\ 0 & 0 & 0 & 0 & 0 & 10 \end{bmatrix} \tag{63}$$

and where $E_0 = 2$

$$P = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \tag{64}$$

Ground state: $|\psi_0\rangle = |\Phi_0\rangle$

For $g = 1$

```
In [7]: #introduce values
        g=1
        xi=1
```

```
In [8]: H= Matrix([[2*xi-g,-g/2,-g/2,-g/2,-g/2,0],[-g/2,4*xi-g,-g/2,-g/2,0,-g/2],[-g/2,-g/2,6*xi-g,0,-g/2,-g/2],[-g/2,-g/2,0,(
        H
```

Out[8]:
$$\begin{bmatrix} 1 & -0.5 & -0.5 & -0.5 & -0.5 & 0 \\ -0.5 & 3 & -0.5 & -0.5 & 0 & -0.5 \\ -0.5 & -0.5 & 5 & 0 & -0.5 & -0.5 \\ -0.5 & -0.5 & 0 & 5 & -0.5 & -0.5 \\ -0.5 & 0 & -0.5 & -0.5 & 7 & -0.5 \\ 0 & -0.5 & -0.5 & -0.5 & -0.5 & 9 \end{bmatrix}$$

```
In [9]: #Diagonalize-calculate eigenvalues with Characteristic polynomial |A-xI|=0
        I=Matrix([[1,0,0,0,0,0],[0,1,0,0,0,0],[0,0,1,0,0,0],[0,0,0,1,0,0],[0,0,0,0,1,0],[0,0,0,0,0,1]])
        A= H - lamb*I
        A
```

Out[9]:
$$\begin{bmatrix} 1-\lambda & -0.5 & -0.5 & -0.5 & -0.5 & 0 \\ -0.5 & 3-\lambda & -0.5 & -0.5 & 0 & -0.5 \\ -0.5 & -0.5 & 5-\lambda & 0 & -0.5 & -0.5 \\ -0.5 & -0.5 & 0 & 5-\lambda & -0.5 & -0.5 \\ -0.5 & 0 & -0.5 & -0.5 & 7-\lambda & -0.5 \\ 0 & -0.5 & -0.5 & -0.5 & -0.5 & 9-\lambda \end{bmatrix}$$

```
In [10]: #Eigenvalues
         C=H.eigenvals()
         C
```

```
Out[10]: {0.635548473575598: 1,
          2.93538142669087: 1,
          5.00000000000000: 2,
          7.20894023917143: 1,
          9.22012986056211: 1}
```

Therefore

$$D = \begin{bmatrix} 0.63555 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2.93538 & 0 & 0 & 0 & 0 \\ 0 & 0 & 5.00000 & 0 & 0 & 0 \\ 0 & 0 & 0 & 5.00000 & 0 & 0 \\ 0 & 0 & 0 & 0 & 7.20894 & 0 \\ 0 & 0 & 0 & 0 & 0 & 9.22013 \end{bmatrix} \tag{65}$$

and where $E_0 = 0.63555$

$$P = \begin{bmatrix} 0.93147 & 0.32608 & 0.11986 & -0.04923 & 0.03937 & 0.02603 \\ 0.27064 & -0.90832 & 0.23972 & -0.09847 & -0.04604 & -0.06601 \\ 0.15388 & -0.16970 & -0.03412 & 0.92432 & 0.24234 & -0.08854 \\ 0.15388 & -0.16970 & -0.92476 & -0.53046 & 0.24234 & -0.08854 \\ 0.10054 & -0.01444 & -0.23972 & 0.09847 & -0.92749 & -0.18493 \\ 0.04059 & -0.10406 & -0.11986 & 0.04923 & -0.13647 & 0.97216 \end{bmatrix} \tag{66}$$

Ground state: $|\psi_0\rangle = 0.93147|\Phi_0\rangle + 0.27064|\Phi_1\rangle + 0.15388|\Phi_2\rangle + 0.15388|\Phi_3\rangle + 0.10054|\Phi_4\rangle + 0.04059|\Phi_5\rangle$

Comment: We can see that in this question we have used Full configuration interaction (FCI), which it is an exact method. As g changes from -1 to 1, we can note that ground state will be perturbed or non-perturbed. For example when $g = 0$, system will be non-pertubed. But when $g = -1$ or 1, system will be slightly perturbed. Ground state is written as a linear combination of all Slater determinants.

3. (10/100 points)

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

If we are going to include at most two-particle-two-hole excitations, following the Fig.1 we will take $|\Phi_0\rangle$, $|\Phi_1\rangle$, $|\Phi_2\rangle$, $|\Phi_3\rangle$ and $|\Phi_4\rangle$. Constructing the matrix is the same case as question 2:

$$H = \begin{bmatrix} \langle \Phi_0|\hat{H}|\Phi_0\rangle & \langle \Phi_0|\hat{H}|\Phi_1\rangle & \langle \Phi_0|\hat{H}|\Phi_2\rangle & \langle \Phi_0|\hat{H}|\Phi_3\rangle & \langle \Phi_0|\hat{H}|\Phi_4\rangle \\ \langle \Phi_1|\hat{H}|\Phi_0\rangle & \langle \Phi_1|\hat{H}|\Phi_1\rangle & \langle \Phi_1|\hat{H}|\Phi_2\rangle & \langle \Phi_1|\hat{H}|\Phi_3\rangle & \langle \Phi_1|\hat{H}|\Phi_4\rangle \\ \langle \Phi_2|\hat{H}|\Phi_0\rangle & \langle \Phi_2|\hat{H}|\Phi_1\rangle & \langle \Phi_2|\hat{H}|\Phi_2\rangle & \langle \Phi_2|\hat{H}|\Phi_3\rangle & \langle \Phi_2|\hat{H}|\Phi_4\rangle \\ \langle \Phi_3|\hat{H}|\Phi_0\rangle & \langle \Phi_3|\hat{H}|\Phi_1\rangle & \langle \Phi_3|\hat{H}|\Phi_2\rangle & \langle \Phi_3|\hat{H}|\Phi_3\rangle & \langle \Phi_3|\hat{H}|\Phi_4\rangle \\ \langle \Phi_4|\hat{H}|\Phi_0\rangle & \langle \Phi_4|\hat{H}|\Phi_1\rangle & \langle \Phi_4|\hat{H}|\Phi_2\rangle & \langle \Phi_4|\hat{H}|\Phi_3\rangle & \langle \Phi_4|\hat{H}|\Phi_4\rangle \\ \langle \Phi_5|\hat{H}|\Phi_0\rangle & \langle \Phi_5|\hat{H}|\Phi_1\rangle & \langle \Phi_5|\hat{H}|\Phi_2\rangle & \langle \Phi_5|\hat{H}|\Phi_3\rangle & \langle \Phi_5|\hat{H}|\Phi_4\rangle \end{bmatrix} \tag{67}$$

solutions are iquals, therefore

$$H = \begin{bmatrix} 2\xi - g & -g/2 & -g/2 & -g/2 & -g/2 \\ -g/2 & 4\xi - g & -g/2 & -g/2 & 0 \\ -g/2 & -g/2 & 6\xi - g & 0 & -g/2 \\ -g/2 & -g/2 & 0 & 6\xi - g & -g/2 \\ -g/2 & 0 & -g/2 & -g/2 & 8\xi - g \end{bmatrix} \tag{68}$$

We will use the same conditions as question 2: $g \in [-1, 1]$, where we will take $\xi = 1$
For $g = -1$

In [1]:
```
#Hamiltonian Matrix 6x6
import numpy as np
from sympy import *
from sympy.matrices import Matrix
lamb=symbols('lambda')
xi=symbols('xi')
g,xi=symbols("g,xi")
H= Matrix([[2*xi-g,-g/2,-g/2,-g/2,-g/2],[-g/2,4*xi-g,-g/2,-g/2,0],[-g/2,-g/2,6*xi-g,0,-g/2],[-g/2,-g/2,0,6*xi-g,-g/2]
H
```

Out[1]:

$$\begin{bmatrix} -g + 2\xi & -\frac{g}{2} & -\frac{g}{2} & -\frac{g}{2} & -\frac{g}{2} \\ -\frac{g}{2} & -g + 4\xi & -\frac{g}{2} & -\frac{g}{2} & 0 \\ -\frac{g}{2} & -\frac{g}{2} & -g + 6\xi & 0 & -\frac{g}{2} \\ -\frac{g}{2} & -\frac{g}{2} & 0 & -g + 6\xi & -\frac{g}{2} \\ -\frac{g}{2} & 0 & -\frac{g}{2} & -\frac{g}{2} & -g + 8\xi \end{bmatrix}$$

In [2]:
```
#introduce values
g=-1
xi=1
```

In [5]:
```
H= Matrix([[2*xi-g,-g/2,-g/2,-g/2,-g/2],[-g/2,4*xi-g,-g/2,-g/2,0],[-g/2,-g/2,6*xi-g,0,-g/2],[-g/2,-g/2,0,6*xi-g,-g/2]
H
```

Out[5]:

$$\begin{bmatrix} 3 & 0.5 & 0.5 & 0.5 & 0.5 \\ 0.5 & 5 & 0.5 & 0.5 & 0 \\ 0.5 & 0.5 & 7 & 0 & 0.5 \\ 0.5 & 0.5 & 0 & 7 & 0.5 \\ 0.5 & 0 & 0.5 & 0.5 & 9 \end{bmatrix}$$

In [7]:
```
#Diagonalize-calculate eigenvalues with Characteristic polynomial |A-xI|=0
I=Matrix([[1,0,0,0,0],[0,1,0,0,0],[0,0,1,0,0],[0,0,0,1,0],[0,0,0,0,1]])
A= H - lamb*I
A
```

Out[7]:

$$\begin{bmatrix} 3 - \lambda & 0.5 & 0.5 & 0.5 & 0.5 \\ 0.5 & 5 - \lambda & 0.5 & 0.5 & 0 \\ 0.5 & 0.5 & 7 - \lambda & 0 & 0.5 \\ 0.5 & 0.5 & 0 & 7 - \lambda & 0.5 \\ 0.5 & 0 & 0.5 & 0.5 & 9 - \lambda \end{bmatrix}$$

In [8]:
```
#Eigenvalues
C=H.eigenvals()
C
```

Out[8]:
```
{7.00000000000000: 1,
 2.78531449939237: 1,
 4.80030641112605: 1,
 7.09292722101003: 1,
 9.32145186847155: 1}
```

Therefore

$$D = \begin{bmatrix} 7.00000 & 0 & 0 & 0 & 0 \\ 0 & 2.78531 & 0 & 0 & 0 \\ 0 & 0 & 4.80031 & 0 & 0 \\ 0 & 0 & 0 & 7.09293 & 0 \\ 0 & 0 & 0 & 0 & 9.32145 \end{bmatrix} \tag{69}$$

and where $E_0 = 7.00000$

$$P = \begin{bmatrix} 1.59979 \times 10^{-63} & -0.97376 & -0.13036 & -0.14517 & 0.11712 \\ 2.88665 \times 10^{-63} & 0.18082 & -0.92527 & -0.32618 & 0.06921 \\ 0.70711 & 0.08642 & 0.24995 & -0.61008 & 0.24054 \\ -0.70711 & 0.08642 & 0.24995 & -0.61008 & 0.24054 \\ -2.69047 \times 10^{-63} & 0.06444 & -0.04400 & 0.35797 & 0.93047 \end{bmatrix} \tag{70}$$

Ground state: $|\psi_0\rangle = 1.59979 \times 10^{-63}|\Phi_0\rangle + 2.88665 \times 10^{-63}|\Phi_1\rangle + 0.70711|\Phi_2\rangle - 0.70711|\Phi_3\rangle - 2.69047 \times 10^{-63}|\Phi_4\rangle$

For $g = 0$

In [25]:
```
#introduce values
g=0
xi=1
```

In [26]:
```
H= Matrix([[2*xi-g,-g/2,-g/2,-g/2,-g/2],[-g/2,4*xi-g,-g/2,-g/2,0],[-g/2,-g/2,6*xi-g,0,-g/2],[-g/2,-g/2,0,6*xi-g,-g/2]
H
```

Out[26]:

$$\begin{bmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 \\ 0 & 0 & 6 & 0 & 0 \\ 0 & 0 & 0 & 6 & 0 \\ 0 & 0 & 0 & 0 & 8 \end{bmatrix}$$

In [27]:
```
#Diagonalize-calculate eigenvalues with Characteristic polynomial |A-xI|=0
I=Matrix([[1,0,0,0,0],[0,1,0,0,0],[0,0,1,0,0],[0,0,0,1,0],[0,0,0,0,1]])
A= H - lamb*I
A
```

Out[27]:

$$\begin{bmatrix} 2-\lambda & 0 & 0 & 0 & 0 \\ 0 & 4-\lambda & 0 & 0 & 0 \\ 0 & 0 & 6-\lambda & 0 & 0 \\ 0 & 0 & 0 & 6-\lambda & 0 \\ 0 & 0 & 0 & 0 & 8-\lambda \end{bmatrix}$$

In [28]:
```
#Eigenvalues
C=H.eigenvals()
C
```

Out[28]:
```
{2: 1, 4: 1, 6: 2, 8: 1}
```

Therefore

$$D = \begin{bmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 \\ 0 & 0 & 6 & 0 & 0 \\ 0 & 0 & 0 & 6 & 0 \\ 0 & 0 & 0 & 0 & 8 \end{bmatrix} \tag{71}$$

and where $E_0 = 2$

$$P = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \tag{72}$$

Ground state: $|\psi_0\rangle = |\Phi_0\rangle$

For $g = 1$

```
In [20]: #introduce values
         g=1
         xi=1
```

```
In [21]: H= Matrix([[2*xi-g,-g/2,-g/2,-g/2,-g/2],[-g/2,4*xi-g,-g/2,-g/2,0],[-g/2,-g/2,6*xi-g,0,-g/2],[-g/2,-g/2,0,6*xi-g,-g/2]
         H
```

Out[21]:
$$\begin{bmatrix} 1 & -0.5 & -0.5 & -0.5 & -0.5 \\ -0.5 & 3 & -0.5 & -0.5 & 0 \\ -0.5 & -0.5 & 5 & 0 & -0.5 \\ -0.5 & -0.5 & 0 & 5 & -0.5 \\ -0.5 & 0 & -0.5 & -0.5 & 7 \end{bmatrix}$$

```
In [22]: #Diagonalize-calculate eigenvalues with Characteristic polynomial |A-xI|=0
         I=Matrix([[1,0,0,0,0],[0,1,0,0,0],[0,0,1,0,0],[0,0,0,1,0],[0,0,0,0,1]])
         A= H - lamb*I
         A
```

Out[22]:
$$\begin{bmatrix} 1-\lambda & -0.5 & -0.5 & -0.5 & -0.5 \\ -0.5 & 3-\lambda & -0.5 & -0.5 & 0 \\ -0.5 & -0.5 & 5-\lambda & 0 & -0.5 \\ -0.5 & -0.5 & 0 & 5-\lambda & -0.5 \\ -0.5 & 0 & -0.5 & -0.5 & 7-\lambda \end{bmatrix}$$

```
In [23]: #Eigenvalues
         C=H.eigenvals()
         C
```

```
Out[23]: {3.00000000000000: 1,
          5.00000000000000: 1,
          0.648906553603944: 1,
          5.10219551695516: 1,
          7.24889792944090: 1}
```

Therefore

$$D = \begin{bmatrix} 3.00000 & 0 & 0 & 0 & 0 \\ 0 & 5.00000 & 0 & 0 & 0 \\ 0 & 0 & 0.64891 & 0 & 0 \\ 0 & 0 & 0 & 5.10220 & 0 \\ 0 & 0 & 0 & 0 & 7.24890 \end{bmatrix} \tag{73}$$

and where $E_0 = 3.00000$

$$P = \begin{bmatrix} -0.30861 & -7.21757\times 10^{-64} & -0.93661 & -0.15929 & 0.04636 \\ 0.92582 & -5.37937\times 10^{-63} & -0.26255 & -0.26613 & -0.05569 \\ 0.15430 & -0.70711 & -0.14897 & 0.63910 & 0.21342 \\ 0.15430 & 0.70711 & -0.14897 & 0.63910 & 0.21342 \\ -2.10526\times 10^{-65} & 2.65998\times 10^{-63} & -0.09719 & 0.29479 & -0.95061 \end{bmatrix} \tag{74}$$

Ground state: $|\psi_0\rangle = -0.30861|\Phi_0\rangle + 0.92582\times 10^{-63}|\Phi_1\rangle + 0.15430|\Phi_2\rangle + 0.15430|\Phi_3\rangle - 2.10526\times 10^{-65}|\Phi_4\rangle$

Comment: In this case we have calculated an approximation for FCI, which it is possible to calculate in practice. This method is useful because it is variational, which ensures that the result will be equal or bigger to the real result. Instead, results for FCI (question 2) are ideals, that means, it is not possible in practice since we should have a complete and finite Slater determinant basis for the system.

4. (10/100 points) 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

$$\hat{H} = \sum_{p\sigma}(p-1)a^\dagger_{p\sigma}a_{p\sigma} - \frac{1}{2}g\sum_{pq}a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+} \tag{75}$$

We can write equation (75) separating states below and above the Fermi energy

$$\hat{H} = \sum_{p=1,\sigma}^{2} (p-1)a^{\dagger}_{p\sigma}a_{p\sigma} + \sum_{q=3,\sigma}^{4} (q-1)a^{\dagger}_{q\sigma}a_{q\sigma} - \frac{1}{2}g\sum_{p=1}^{2} a^{\dagger}_{p+}a^{\dagger}_{p-}a_{p-}a_{p+} - \frac{1}{2}g\sum_{q=3}^{4} a^{\dagger}_{q+}a^{\dagger}_{q-}a_{q-}a_{q+} \\ - \frac{1}{2}g\sum_{pq} a^{\dagger}_{p+}a^{\dagger}_{p-}a_{q-}a_{q+} - \frac{1}{2}g\sum_{qp} a^{\dagger}_{q+}a^{\dagger}_{q-}a_{p-}a_{p+} \tag{76}$$

Following the system with $p = 1, 2$, which is below the Fermi energy. Let's use from equation (76) the terms for this case and we will write in the normal-ordered

$$\hat{H} = \sum_{p=1,\sigma}^{2} (p-1)a^{\dagger}_{p\sigma}a_{p\sigma} - \frac{1}{2}g\sum_{p=1}^{2} a^{\dagger}_{p+}a^{\dagger}_{p-}a_{p-}a_{p+} \tag{77}$$

reference energy

$$E_{ref} = \langle\Phi_0|\hat{H}|\Phi_0\rangle$$

Then

$$\hat{H} = E_{ref} + \sum_{p=1,\sigma}^{2} (p-1)a^{\dagger}_{p\sigma}a_{p\sigma} - \frac{1}{2}g\sum_{p=1}^{2} a^{\dagger}_{p+}a^{\dagger}_{p-}a_{p-}a_{p+}$$

$$E[\Phi] = \langle\Phi|\hat{H}|\Phi\rangle = E_{ref}\langle\Phi|\Phi\rangle + \langle\Phi|\hat{H}'|\Phi\rangle = E_{ref} + \langle\Phi|\hat{H}'|\Phi\rangle$$

$$E[\Phi] = E_{ref}\langle p|p'\rangle + \sum_{p}\langle p|h|p'\rangle + \frac{1}{2}\sum_{p}\langle pp'|v|pp'\rangle$$

Using new basis

$$|p\rangle = \sum_{\lambda} C_{p\lambda}|\lambda\rangle$$

then

$$E[\Phi^{HF}] = C^{*}_{p\lambda}C_{p\lambda'}E_{ref}\langle\lambda|\lambda'\rangle + \sum_{p}\sum_{\lambda\lambda'} C^{*}_{p\lambda}C_{p\lambda'}\langle\lambda|h|\lambda'\rangle + \frac{1}{2}\sum_{p}\sum_{\lambda\lambda'} C^{*}_{p\lambda}C^{*}_{p\lambda'}C_{p\lambda'}C_{p\lambda}\langle\lambda\lambda'|v|\lambda\lambda'\rangle_{AS}$$

We can see that this equation is similar to the general form

$$E[\Phi^{HF}] = \sum_{i=1}^{N}\sum_{\alpha\beta} C^{*}_{i\alpha}C_{i\beta}\langle\alpha|h|\beta\rangle + \frac{1}{2}\sum_{i,j=1}^{N}\sum_{\alpha\beta\gamma\delta} C^{*}_{i\alpha}C^{*}_{j\beta}C_{i\gamma}C_{j\delta}\langle\alpha\beta|v|\gamma\delta\rangle_{AS}$$

If we minimizing with respect to $C^{*}_{i\alpha}$, we obtain

$$\sum_{\beta} C_{i\beta}\langle\alpha|h|\beta\rangle + \sum_{j=1}^{N}\sum_{\beta\gamma\delta} C^{*}_{j\beta}C_{i\gamma}C_{j\delta}\langle\alpha\beta|v|\gamma\delta\rangle_{AS} = \epsilon^{HF}_{i}C_{i\alpha}$$

$$\sum_{\beta}\left\{\langle\alpha|h|\beta\rangle + \sum_{j=1}^{N}\sum_{\beta\gamma\delta} C^{*}_{j\gamma}C_{j\delta}\langle\alpha\gamma|v|\beta\delta\rangle_{AS}\right\}C_{i\beta} = \epsilon^{HF}_{i}C_{i\alpha}$$

then

$$h^{HF}_{\alpha\beta} = \langle\alpha|h|\beta\rangle + \sum_{j=1}^{N}\sum_{\gamma\delta} C^{*}_{j\gamma}C_{j\delta}\langle\alpha\gamma|v|\beta\delta\rangle_{AS} \tag{78}$$

$$\sum_{\beta} h^{HF}_{\alpha\beta} C_{i\beta} = \epsilon^{HF}_{i} C_{i\alpha} \tag{79}$$

so we can use the equation (78), replacing

$$h^{HF}_{\alpha\beta} = \langle\alpha| \left(E_{ref} + \sum_{p=1,\sigma}^{2} (p-1) a^{\dagger}_{p\sigma} a_{p\sigma} \right) |\beta\rangle - \sum_{j=1}^{N} \sum_{\gamma\delta} C^{*}_{j\gamma} C_{j\delta} \langle\alpha\gamma| \frac{1}{2} g \sum_{p=1}^{2} a^{\dagger}_{p+} a^{\dagger}_{p-} a_{p-} a_{p+} |\beta\delta\rangle_{AS}$$

$$h^{HF}_{\alpha\beta} = E_{ref} \langle\alpha|\beta\rangle + \sum_{p=1}^{2} (p-1) \underbrace{\langle\alpha| \sum_{\sigma} a^{\dagger}_{p\sigma} a_{p\sigma} |\beta\rangle}_{(i)} - \frac{1}{2} g \sum_{j=1}^{N} \sum_{\gamma\delta} \sum_{p=1}^{2} C^{*}_{j\gamma} C_{j\delta} \underbrace{\langle\alpha\gamma| a^{\dagger}_{p+} a^{\dagger}_{p-} a_{p-} a_{p+} |\beta\delta\rangle_{AS}}_{(ii)} \tag{80}$$

Applying Wick's theorem
(i)

$$\langle\alpha| \sum_{\sigma} a^{\dagger}_{p\sigma} a_{p\sigma} |\beta\rangle = \langle\alpha| a^{\dagger}_{p+} a_{p+} |\beta\rangle + \langle\alpha| a^{\dagger}_{p-} a_{p-} |\beta\rangle$$

When $\alpha = \beta = p$

$$= \langle 0| a^{\dagger}_{\alpha-} a^{\dagger}_{\alpha+} a^{\dagger}_{p+} a_{p+} a_{\beta+} a_{\beta-} |0\rangle + \langle 0| a^{\dagger}_{\alpha-} a^{\dagger}_{\alpha+} a^{\dagger}_{p-} a_{p-} a_{\beta+} a_{\beta-} |0\rangle = 1 \tag{81}$$

(ii)

$$\sum_{\gamma\delta} C^{*}_{j\gamma} C_{j\delta} \sum_{p=1}^{2} \langle\alpha\gamma| a^{\dagger}_{p+} a^{\dagger}_{p-} a_{p-} a_{p+} |\beta\delta\rangle_{AS} = \sum_{\gamma\delta} C^{*}_{j\gamma} C_{j\delta} \langle\alpha\gamma| a^{\dagger}_{1+} a^{\dagger}_{1-} a_{1-} a_{1+} |\beta\delta\rangle_{AS} + \sum_{\gamma\delta} C^{*}_{j\gamma} C_{j\delta} \langle\alpha\gamma| a^{\dagger}_{2+} a^{\dagger}_{2-} a_{2-} a_{2+} |\beta\delta\rangle_{AS}$$

When $\alpha = \beta = \gamma = \delta = 1$ and $\alpha = \beta = \gamma = \delta = 2$

$$= C^{*}_{j1} C_{j1} \langle 11| a^{\dagger}_{1+} a^{\dagger}_{1-} a_{1-} a_{1+} |11\rangle + C^{*}_{j2} C_{j2} \langle 22| a^{\dagger}_{2+} a^{\dagger}_{2-} a_{2-} a_{2+} |22\rangle$$

$$\begin{aligned} =& C^{*}_{j1} C_{j1} \langle 0| a^{\dagger}_{1-} a^{\dagger}_{1+} a^{\dagger}_{1-} a^{\dagger}_{1+} a^{\dagger}_{1+} a^{\dagger}_{1-} a_{1-} a_{1+} a_{1+} a_{1-} a_{1+} a_{1-} |0\rangle + C^{*}_{j2} C_{j2} \langle 0| a^{\dagger}_{2-} a^{\dagger}_{2+} a^{\dagger}_{2-} a^{\dagger}_{2+} a^{\dagger}_{2+} a^{\dagger}_{2-} a_{2-} a_{2+} a_{2+} a_{2-} a_{2+} a_{2-} |0\rangle \\ &= C^{*}_{j1} C_{j1} + C^{*}_{j2} C_{j2} \end{aligned} \tag{82}$$

Replacing equations (81) and (82) in equation (80)

$$h^{HF}_{\alpha\beta} = E_{ref} + 2 \sum_{p=1}^{2} (p-1) - \frac{1}{2} g \sum_{j=1}^{N} \left(C^{*}_{j1} C_{j1} + C^{*}_{j2} C_{j2} \right)$$

$$h^{HF}_{\alpha\beta} = E_{ref} + 2 \sum_{p=1}^{2} (p-1) - \frac{1}{2} g \sum_{j=1}^{N} (\delta_{j1} + \delta_{j2}) = E_{ref} + 2 - g \tag{83}$$

Using equation (79), for this case

$$h^{HF}_{\alpha\beta} C_{i\alpha} = \epsilon^{HF}_{i} C_{i\alpha}$$

$$\epsilon^{HF}_{i} - E_{ref} = 2 - g \tag{84}$$

5. (15/100 points) 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.2 that can be affected by a Hartree-Fock basis. Compute the total binding 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.2.

Based on the form of the interaction, which diagrams contribute to the binding 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).

Solution

For this case we're going to use the Hamiltonian of the equation (76), now we consider the states above the Fermi energy and also both cases (below and above the Fermi level). For the first part (below the Fermi level), we can take the answer in equation (83).

$$\begin{aligned}\hat{H} = & \underbrace{\sum_{p=1,\sigma}^{2}(p-1)a^\dagger_{p\sigma}a_{p\sigma} + \sum_{q=3,\sigma}^{4}(q-1)a^\dagger_{q\sigma}a_{q\sigma}}_{\text{Question 3}} \underbrace{- \frac{1}{2}g\sum_{p=1}^{2}a^\dagger_{p+}a^\dagger_{p-}a_{p-}a_{p+} - \frac{1}{2}g\sum_{q=3}^{4}a^\dagger_{q+}a^\dagger_{q-}a_{q-}a_{q+}}_{\text{Similar to question 3}} \\ & \underbrace{- \frac{1}{2}g\sum_{pq}a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+} - \frac{1}{2}g\sum_{qp}a^\dagger_{q+}a^\dagger_{q-}a_{p-}a_{p+}}_{\text{No calculated}}\end{aligned} \tag{85}$$

If we calculate the term "Similar to question 3", obtain

$$h^{HF}_{\alpha\beta} = 2\sum_{q=3}^{4}(q-1) - \frac{1}{2}g\sum_{j=1}^{N}(\delta_{j3}+\delta_{j4}) = 10 - g \tag{86}$$

we're going to work with the term "No calculated". As it is only two-bodies operator, replace in second part of the equation (78)

$$h^{HF\prime}_{\alpha\beta} = \sum_{j=1}^{N}\sum_{\gamma\delta}C^*_{j\gamma}C_{j\delta}\langle\alpha\gamma|v|\beta\delta\rangle_{AS}$$

$$h^{HF\prime}_{\alpha\beta} = -\sum_{j=1}^{N}\sum_{\gamma\delta}C^*_{j\gamma}C_{j\delta}\langle\alpha\gamma|\frac{1}{2}g\sum_{pq}a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}|\beta\delta\rangle_{AS} - \sum_{j=1}^{N}\sum_{\gamma\delta}C^*_{j\gamma}C_{j\delta}\langle\alpha\gamma|\frac{1}{2}g\sum_{qp}a^\dagger_{q+}a^\dagger_{q-}a_{p-}a_{p+}|\beta\delta\rangle_{AS}$$

$$h^{HF\prime}_{\alpha\beta} = -\frac{1}{2}g\sum_{j=1}^{N}\sum_{\gamma\delta}\sum_{pq}C^*_{j\gamma}C_{j\delta}\underbrace{\langle\alpha\gamma|a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}|\beta\delta\rangle_{AS}}_{(i)} - \frac{1}{2}g\sum_{j=1}^{N}\sum_{\gamma\delta}\sum_{qp}C^*_{j\gamma}C_{j\delta}\underbrace{\langle\alpha\gamma|a^\dagger_{q+}a^\dagger_{q-}a_{p-}a_{p+}|\beta\delta\rangle_{AS}}_{(ii)}$$

(i)

$$\langle\alpha\gamma|a^\dagger_{p+}a^\dagger_{p-}a_{q-}a_{q+}|\beta\delta\rangle_{AS} \tag{87}$$

we set values for α and β, and vary γ, δ

		+		+	+
α	γ	p	q	β	δ
1	1	1	3	3	1
1	2	2	3	3	1
1	2	1	3	3	2
1	3	1	2	3	2
1	3	1	3	3	3
1	3	1	4	3	4
1	4	1	3	3	4

Table 1

Table 1 is all possible combinations for equation (85), therefore

$$\langle\alpha\gamma|a_{p+}^\dagger a_{p-}^\dagger a_{q-}a_{q+}|\beta\delta\rangle_{AS} = \sum_j^N \left(C_{j1}^*C_{j1} + C_{j2}^*C_{j1} + C_{j2}^*C_{j2} + C_{j3}^*C_{j2} + C_{j3}^*C_{j3} + C_{j3}^*C_{j4} + C_{j4}^*C_{j4}\right)$$

$$\langle\alpha\gamma|a_{p+}^\dagger a_{p-}^\dagger a_{q-}a_{q+}|\beta\delta\rangle_{AS} = C_{11}^*C_{11} + C_{22}^*C_{22} + C_{33}^*C_{33} + C_{44}^*C_{44} = \delta_{11} + \delta_{22} + \delta_{33} + \delta_{44} = 4 \tag{88}$$

(ii) Similar to the previous calculation

$$\langle\alpha\gamma|a_{q+}^\dagger a_{q-}^\dagger a_{p-}a_{p+}|\beta\delta\rangle_{AS}$$

		+		+	+
α	γ	q	p	β	δ
3	1	3	1	1	1
3	1	3	2	1	2
3	2	3	1	1	2
3	2	2	1	1	3
3	3	3	1	1	3
3	4	4	1	1	3
3	4	3	1	1	4

Table 2

$$\langle\alpha\gamma|a_{q+}^\dagger a_{q-}^\dagger a_{p-}a_{p+}|\beta\delta\rangle_{AS} = \sum_j^N \left(C_{j1}^*C_{j1} + C_{j1}^*C_{j2} + C_{j2}^*C_{j2} + C_{j2}^*C_{j3} + C_{j3}^*C_{j3} + C_{j4}^*C_{j3} + C_{j4}^*C_{j4}\right)$$

$$\langle\alpha\gamma|a_{p+}^\dagger a_{p-}^\dagger a_{q-}a_{q+}|\beta\delta\rangle_{AS} = C_{11}^*C_{11} + C_{22}^*C_{22} + C_{33}^*C_{33} + C_{44}^*C_{44} = \delta_{11} + \delta_{22} + \delta_{33} + \delta_{44} = 4 \tag{89}$$

Therefore

$$h_{\alpha\beta}^{HF\prime} = -\frac{1}{2}g \times 4 - \frac{1}{2}g \times 4 = -4g \tag{90}$$

Taking solutions of equations (83), (86) and (90), we can write

$$h_{\alpha\beta}^{HF} = E_{ref} + 2 - g + 10 - g - 4g = E_{ref} + 12 - 6g$$

and

$$\epsilon_i^{HF} - E_{ref} = 12 - 6g = 6(2 - g) \tag{91}$$

For $g = -1$

$$\epsilon_i^{HF} - E_{ref} = 18$$

For $g = 0$

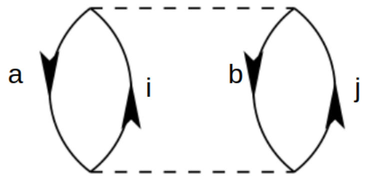
$$\epsilon_i^{HF} - E_{ref} = 12$$

For $g = 1$

$$\epsilon_i^{HF} - E_{ref} = 6$$

6. (10/100 points) Diagram 1 in Fig.2 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 $g \in [-1,1]$.

Solution



This diagram represents a case of $2p2h$, expression is

$$\Delta E^{(2)} = \frac{1}{4}\sum_{ijab}\frac{\langle ab|v|ij\rangle\langle ij|v|ab\rangle}{\epsilon_{ab}^{ij}}$$

Where $\epsilon_{ab}^{ij} = \epsilon_a + \epsilon_b - \epsilon_i - \epsilon_j$

$$\Delta E^{(2)} = \sum_{i<j,a<b}\frac{\langle ab|v|ij\rangle\langle ij|v|ab\rangle}{\epsilon_{ab}^{ij}}$$

Then following the Fig. 1 only for $2p2h$, we can write

$$\Delta E^{(2)} = \frac{\langle 2_-2_+|v|3_+3_-\rangle\langle 3_+3_-|v|2_-2_+\rangle}{\epsilon_{2_+}+\epsilon_{2_-}-\epsilon_{3_+}-\epsilon_{3_-}} + \frac{\langle 2_-2_+|v|4_+4_-\rangle\langle 4_+4_-|v|2_-2_+\rangle}{\epsilon_{2_+}+\epsilon_{2_-}-\epsilon_{4_+}-\epsilon_{4_-}} + \frac{\langle 1_-1_+|v|3_+3_-\rangle\langle 3_+3_-|v|1_-1_+\rangle}{\epsilon_{1_+}+\epsilon_{1_-}-\epsilon_{3_+}-\epsilon_{3_-}} + \frac{\langle 1_-1_+|v|4_+4_-\rangle\langle 4_+4_-|v|1_-1_+\rangle}{\epsilon_{1_+}+\epsilon_{1_-}-\epsilon_{4_+}-\epsilon_{4_-}}$$

or

$$\Delta E^{(2)} = \frac{\langle\Phi_0|v|\Phi_{2_-2_+}^{3_+3_-}\rangle\langle\Phi_{2_-2_+}^{3_+3_-}|v|\Phi_0\rangle}{\epsilon_{2_+}+\epsilon_{2_-}-\epsilon_{3_+}-\epsilon_{3_-}} + \frac{\langle\Phi_0|v|\Phi_{2_-2_+}^{4_+4_-}\rangle\langle\Phi_{2_-2_+}^{4_+4_-}|v|\Phi_0\rangle}{\epsilon_{2_+}+\epsilon_{2_-}-\epsilon_{4_+}-\epsilon_{4_-}} + \frac{\langle\Phi_0|v|\Phi_{1_-1_+}^{3_+3_-}\rangle\langle\Phi_{1_-1_+}^{3_+3_-}|v|\Phi_0\rangle}{\epsilon_{1_+}+\epsilon_{1_-}-\epsilon_{3_+}-\epsilon_{3_-}} + \frac{\langle\Phi_0|v|\Phi_{1_-1_+}^{4_+4_-}\rangle\langle\Phi_{1_-1_+}^{4_+4_-}|v|\Phi_0\rangle}{\epsilon_{1_+}+\epsilon_{1_-}-\epsilon_{4_+}-\epsilon_{4_-}}$$

$$\Delta E^{(2)} = \frac{\langle\Phi_0|v|\Phi_{2_-2_+}^{3_+3_-}\rangle^2}{\epsilon_{2_+}+\epsilon_{2_-}-\epsilon_{3_+}-\epsilon_{3_-}} + \frac{\langle\Phi_0|v|\Phi_{2_-2_+}^{4_+4_-}\rangle^2}{\epsilon_{2_+}+\epsilon_{2_-}-\epsilon_{4_+}-\epsilon_{4_-}} + \frac{\langle\Phi_0|v|\Phi_{1_-1_+}^{3_+3_-}\rangle^2}{\epsilon_{1_+}+\epsilon_{1_-}-\epsilon_{3_+}-\epsilon_{3_-}} + \frac{\langle\Phi_0|v|\Phi_{1_-1_+}^{4_+4_-}\rangle^2}{\epsilon_{1_+}+\epsilon_{1_-}-\epsilon_{4_+}-\epsilon_{4_-}} \tag{92}$$

Where follow the Fig. 1

$$|\Phi_1\rangle = |\Phi_{2_-2_+}^{3_+3_-}\rangle = a_{3+}^\dagger a_{3-}^\dagger a_{2+}a_{2-}|\Phi_0\rangle \qquad |\Phi_2\rangle = |\Phi_{2_-2_+}^{4_+4_-}\rangle = a_{4+}^\dagger a_{4-}^\dagger a_{2+}a_{2-}|\Phi_0\rangle \tag{93}$$

$$|\Phi_3\rangle = |\Phi_{1_-1_+}^{3_+3_-}\rangle = a_{3+}^\dagger a_{3-}^\dagger a_{1+}a_{1-}|\Phi_0\rangle \qquad |\Phi_4\rangle = |\Phi_{1_-1_+}^{4_+4_-}\rangle = a_{4+}^\dagger a_{4-}^\dagger a_{1+}a_{1-}|\Phi_0\rangle \tag{94}$$

Using

$$\epsilon_i = \langle i|h|i\rangle + \sum_j \langle ij|v|ij\rangle$$

We can calculate the energy for each single-particle:

$$\epsilon_{1_+} = -\frac{g}{2} \qquad \epsilon_{1_-} = -\frac{g}{2} \tag{95}$$

$$\epsilon_{2_+} = 1-\frac{g}{2} \qquad \epsilon_{2_-} = 1-\frac{g}{2} \tag{96}$$

$$\epsilon_{3_+} = 2 \qquad \epsilon_{3_-} = 2 \tag{97}$$

$$\epsilon_{4_+} = 3 \qquad \epsilon_{4_-} = 3 \tag{98}$$

Now using equations (19), (93) and (94), we're going to calculate the numerators of the equation (92) with

$$\hat{v} = -\frac{g}{2}\sum_{pq} a^{\dagger}_{p+}a^{\dagger}_{p-}a_{q-}a_{q+}$$

$$\langle\Phi_0|v|\Phi^{3+3-}_{2-2+}\rangle = -\frac{g}{2}\langle 0|a_{2-}a_{2+}a_{1-}a_{1+}a^{\dagger}_{p+}a^{\dagger}_{p-}a_{q-}a_{q+}a^{\dagger}_{3+}a^{\dagger}_{3-}a_{2+}a_{2-}a^{\dagger}_{1+}a^{\dagger}_{1-}a^{\dagger}_{2+}a^{\dagger}_{2-}|0\rangle$$

when $p = 2$ and $q = 3$, other cases are zero

$$\langle\Phi_0|v|\Phi^{3+3-}_{2-2+}\rangle = -\frac{g}{2}\langle 0|a_{2-}a_{2+}a_{1-}a_{1+}a^{\dagger}_{2+}a^{\dagger}_{2-}a_{3-}a_{3+}a^{\dagger}_{3+}a^{\dagger}_{3-}a_{2+}a_{2-}a^{\dagger}_{1+}a^{\dagger}_{1-}a^{\dagger}_{2+}a^{\dagger}_{2-}|0\rangle = -\frac{g}{2} \tag{99}$$

$$\langle\Phi_0|v|\Phi^{4+4-}_{2-2+}\rangle = -\frac{g}{2}\langle 0|a_{2-}a_{2+}a_{1-}a_{1+}a^{\dagger}_{p+}a^{\dagger}_{p-}a_{q-}a_{q+}a^{\dagger}_{4+}a^{\dagger}_{4-}a_{2+}a_{2-}a^{\dagger}_{1+}a^{\dagger}_{1-}a^{\dagger}_{2+}a^{\dagger}_{2-}|0\rangle$$

when $p = 2$ and $q = 4$, other cases are zero

$$\langle\Phi_0|v|\Phi^{4+4-}_{2-2+}\rangle = -\frac{g}{2}\langle 0|a_{2-}a_{2+}a_{1-}a_{1+}a^{\dagger}_{2+}a^{\dagger}_{2-}a_{4-}a_{4+}a^{\dagger}_{4+}a^{\dagger}_{4-}a_{2+}a_{2-}a^{\dagger}_{1+}a^{\dagger}_{1-}a^{\dagger}_{2+}a^{\dagger}_{2-}|0\rangle = -\frac{g}{2} \tag{100}$$

$$\langle\Phi_0|v|\Phi^{3+3-}_{1-1+}\rangle = -\frac{g}{2}\langle 0|a_{2-}a_{2+}a_{1-}a_{1+}a^{\dagger}_{p+}a^{\dagger}_{p-}a_{q-}a_{q+}a^{\dagger}_{3+}a^{\dagger}_{3-}a_{1+}a_{1-}a^{\dagger}_{1+}a^{\dagger}_{1-}a^{\dagger}_{2+}a^{\dagger}_{2-}|0\rangle$$

when $p = 1$ and $q = 3$, other cases are zero

$$\langle\Phi_0|v|\Phi^{3+3-}_{1-1+}\rangle = -\frac{g}{2}\langle 0|a_{2-}a_{2+}a_{1-}a_{1+}a^{\dagger}_{1+}a^{\dagger}_{1-}a_{3-}a_{3+}a^{\dagger}_{3+}a^{\dagger}_{3-}a_{1+}a_{1-}a^{\dagger}_{1+}a^{\dagger}_{1-}a^{\dagger}_{2+}a^{\dagger}_{2-}|0\rangle = -\frac{g}{2} \tag{101}$$

$$\langle\Phi_0|v|\Phi^{4+4-}_{1-1+}\rangle = -\frac{g}{2}\langle 0|a_{2-}a_{2+}a_{1-}a_{1+}a^{\dagger}_{p+}a^{\dagger}_{p-}a_{q-}a_{q+}a^{\dagger}_{4+}a^{\dagger}_{4-}a_{1+}a_{1-}a^{\dagger}_{1+}a^{\dagger}_{1-}a^{\dagger}_{2+}a^{\dagger}_{2-}|0\rangle$$

when $p = 1$ and $q = 4$, other cases are zero

$$\langle\Phi_0|v|\Phi^{4+4-}_{1-1+}\rangle = -\frac{g}{2}\langle 0|a_{2-}a_{2+}a_{1-}a_{1+}a^{\dagger}_{1+}a^{\dagger}_{1-}a_{4-}a_{4+}a^{\dagger}_{4+}a^{\dagger}_{4-}a_{1+}a_{1-}a^{\dagger}_{1+}a^{\dagger}_{1-}a^{\dagger}_{2+}a^{\dagger}_{2-}|0\rangle = -\frac{g}{2} \tag{102}$$

Replacing equations from (95) to (102) in equation (92)

$$\Delta E^{(2)} = \frac{\left(-\frac{g}{2}\right)^2}{1-\frac{g}{2}+1-\frac{g}{2}-2-2} + \frac{\left(-\frac{g}{2}\right)^2}{1-\frac{g}{2}+1-\frac{g}{2}-3-3} + \frac{\left(-\frac{g}{2}\right)^2}{-\frac{g}{2}+-\frac{g}{2}-2-2} + \frac{\left(-\frac{g}{2}\right)^2}{-\frac{g}{2}+-\frac{g}{2}-3-3}$$

$$\Delta E^{(2)} = \frac{\left(-\frac{g}{2}\right)^2}{-2-g} + \frac{\left(-\frac{g}{2}\right)^2}{-4-g} + \frac{\left(-\frac{g}{2}\right)^2}{-4-g} + \frac{\left(-\frac{g}{2}\right)^2}{-6-g}$$

$$\Delta E^{(2)} = -\frac{g^2}{4}\left(\frac{1}{2+g} + \frac{1}{4+g} + \frac{1}{4+g} + \frac{1}{6+g}\right) \tag{103}$$

For $g = -1$

$$\Delta E^{(2)} = -0.46667$$

For $g = 0$

$$\Delta E^{(2)} = 0$$

For $g = 1$

$$\Delta E^{(2)} = -0.21905$$

7. (25/100 points) 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.3, $2p-2h$ excitations, see Fig.4, $3p-3h$ excitations as shown in Fig.5 and finally so-called diagrams with intermediate four-particle-four-hole excitations, see Fig.6.
Define first linked and unlinked diagrams and explain briefly Goldstone's linked diagram theorem. Based on the linked diagram theorem and the form of the pairing Hamiltonian, which diagrams will contribute to fourth order?

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
We can define an unliked diagrams as a diagram that contain unlinked parts or insertions, or some combinations of these. That's means that have disconnected closed parts, while linked diagrams are the opposite.
Goldstone's linked diagram theorem mentions that in an exact theory all unlinked diagrams cancel each other. It means that only linked diagrams contribute to the final energy.

If we take into account our hamiltonian, where it is a system with no broken pairs and Goldstone's linked diagram theorem. Looking the diagrams:

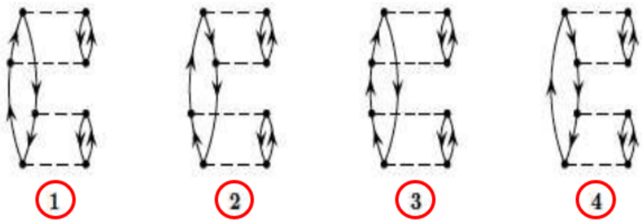


FIG. 3: One-particle-one-hole excitations to fourth order.

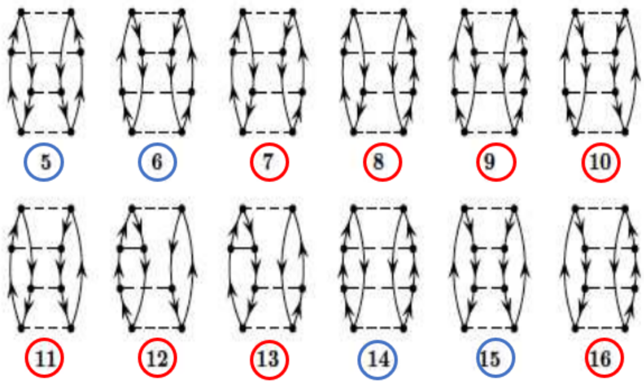


FIG. 4: Two-particle-two-hole excitations to fourth order.

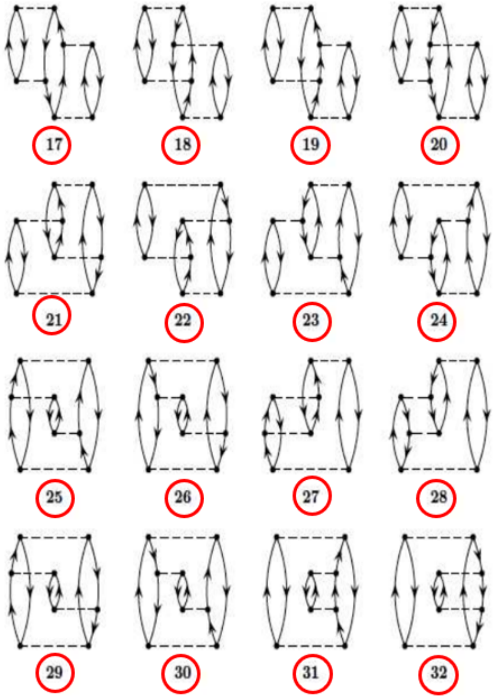


FIG. 5: Three-particle-three-hole excitations to fourth order.

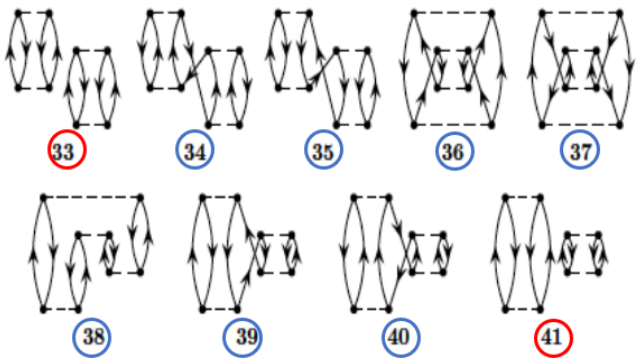


FIG. 6: Four-particle-four-hole excitations to fourth order.

Only the diagrams with blue circle contribute to fourth order, while diagrams with red circle vanishes.