

Midterm 2

Hishem Kløvnnes

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1 Quantum mechanics for many-particle systems

a)

For this exercise, we will use the commutation relations:

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

and

$$[AB, CD] = A[B, C]D + AC[B, D] + [A, C]DB + C[A, D]B$$

We want to show that \hat{H}_0 and \hat{V} commutes with \hat{S}_z and \hat{S}^2 .

The operators are defined as:

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

$$\hat{V} = \sum_{pq} a_{p-}^\dagger a_{p+}^\dagger a_{p-} a_{p+}$$

$$\hat{S}_z = \sum_{p\sigma} \sigma a_{p\sigma}^\dagger a_{p\sigma}$$

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

Where $\hat{S}_\pm = \sum_p a_{p\pm}^\dagger a_{p\mp}$, $\sigma = \pm 1$ for spin and $p = 1, 2, \dots$ is the index for the single-particle states.

We start by showing that \hat{H}_0 commutes with \hat{S}_z :

$$[\hat{H}_0, \hat{S}_z] = \xi \sum_{p\sigma} (p-1) [a_{p\sigma}^\dagger a_{p\sigma}, \sum_{\tau} \tau a_{q\tau}^\dagger a_{q\tau}]$$

Lets take the operators to the side and look at those first:

$$\begin{aligned} & [a_{p\sigma}^\dagger a_{p\sigma}, a_{q\tau}^\dagger a_{q\tau}] \\ &= a_{p\sigma}^\dagger [a_{p\sigma}, a_{q\tau}^\dagger] a_{q\tau} + a_{p\sigma}^\dagger a_{q\tau}^\dagger [a_{p\sigma}, a_{q\tau}] + [a_{p\sigma}^\dagger, a_{q\tau}^\dagger] a_{p\sigma} a_{q\tau} + a_{q\tau}^\dagger [a_{p\sigma}^\dagger, a_{q\tau}] a_{p\sigma} \end{aligned}$$

Two creation operators commute and two annihilation operators commute, so two of them are directly zero, while the other two leaves croenecker deltas

$$\begin{aligned}
&= a_{p\sigma}^\dagger \delta_{pq} \delta_{\sigma\tau} a_{q\tau} - a_{q\tau}^\dagger \delta_{pq} \delta_{\sigma\tau} a_{p\sigma} \\
[\hat{H}_0, \hat{S}_z] &= \xi \sum_{p\sigma} (p-1) [a_{p\sigma}^\dagger a_{p\sigma}, \sum_{\tau} \tau a_{q\tau}^\dagger a_{q\tau}] \\
&= \xi \sum_{p\sigma} (p-1) \sum_{\tau} \tau (a_{p\sigma}^\dagger \delta_{pq} \delta_{\sigma\tau} a_{q\tau} - a_{q\tau}^\dagger \delta_{pq} \delta_{\sigma\tau} a_{p\sigma}) = 0
\end{aligned}$$

Now we want to show that \hat{H}_0 commutes with \hat{S}^2 .

$$[\hat{H}_0, \hat{S}^2] = [H_0, S_z^2] + \frac{1}{2}([H_0, S_+ S_-] + [H_0, S_- S_+])$$

We know that $[H_0, S_z] = 0$ and therefor the first term is zero.

Lets look at the second term:

$$\begin{aligned}
[H_0, S_+ S_-] &= \xi \sum_{pq\sigma} (p-1) [a_{p\sigma}^\dagger a_{p\sigma}, a_{q+}^\dagger a_{q-} a_{q-}^\dagger a_{q+}] \\
&= \xi \sum_{pq\sigma} (p-1) ([a_{p\sigma}^\dagger a_{p\sigma}, a_{q+}^\dagger a_{q-}] a_{q-}^\dagger a_{q+} + a_{q-}^\dagger a_{q+} [a_{p\sigma}^\dagger a_{p\sigma}, a_{q+}^\dagger a_{q-}]) \\
&= \xi \sum_{pq\sigma} (p-1) \left((a_{p\sigma}^\dagger [a_{p\sigma}, a_{q+}^\dagger] a_{q-} + a_{p\sigma}^\dagger a_{q-} [a_{p\sigma}, a_{q+}^\dagger]) a_{q-}^\dagger a_{q+} \right. \\
&\quad \left. + a_{q+}^\dagger a_{q-} (a_{p\sigma}^\dagger [a_{p\sigma}, a_{q-}^\dagger] a_{q+} + a_{p\sigma}^\dagger a_{q+} [a_{p\sigma}, a_{q-}^\dagger]) \right) \\
&= \xi \sum_{p\sigma} (p-1) \left((a_{p+}^\dagger a_{p-} - a_{p-}^\dagger a_{p+}) a_{p-}^\dagger a_{p+} + a_{p+}^\dagger a_{p-} (a_{p-}^\dagger a_{p+} - a_{p-}^\dagger a_{p+}) \right) = 0
\end{aligned}$$

The same goes for the last term, and therefor $[H_0, S^2] = 0$

Now we can move over to check if \hat{V} commutes with \hat{S}_z and \hat{S}^2 . First we check if \hat{V} commutes with \hat{S}_z :

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

The first term:

$$\begin{aligned}
[a_{q-} a_{q+}, a_{r\sigma}^\dagger a_{r\sigma}] &= a_{q-} [a_{q+}, a_{r\sigma}^\dagger] a_{r\sigma} + a_{q-} a_{r\sigma}^\dagger [a_{q+}, a_{r\sigma}] \\
&\quad + [a_{q-}, a_{r\sigma}^\dagger] a_{r\sigma} a_{q+} + a_{r\sigma}^\dagger [a_{q-}, a_{r\sigma}] a_{q+}
\end{aligned}$$

Where the only surviving term, the ones with one creation and one annihilation operator, are:

$$\begin{aligned}
&= a_{q-} \delta_{qr} \delta_{\sigma+} a_{r\sigma} + a_{q+} \delta_{qr} \delta_{\sigma-} a_{r\sigma} \\
&= a_{q-} a_{q+} + a_{q+} a_{q-}
\end{aligned}$$

Now the second term:

$$\begin{aligned} [a_{p+}^\dagger a_{p-}^\dagger, a_{r\sigma}^\dagger a_{r\sigma}] &= a_{p+}^\dagger [a_{p-}^\dagger, a_{r\sigma}^\dagger] a_{r\sigma} + a_{p+}^\dagger a_{r\sigma}^\dagger [a_{p-}^\dagger, a_{r\sigma}] \\ &\quad + [a_{p+}^\dagger, a_{r\sigma}^\dagger] a_{r\sigma} a_{p-}^\dagger + a_{r\sigma}^\dagger [a_{p+}^\dagger, a_{r\sigma}] a_{p-}^\dagger \end{aligned}$$

Where the only surviving term, the ones with one creation and one annihilation operator, are:

$$\begin{aligned} &= -a_{p+}^\dagger \delta_{pr} \delta_{\sigma-} a_{r\sigma} - a_{p-}^\dagger \delta_{pr} \delta_{\sigma+} a_{r\sigma} \\ &= a_{p+}^\dagger a_{p-} + a_{p-}^\dagger a_{p+} \end{aligned}$$

Now we can put the two results back into the first expression, and we can see that it simply reduces to zero.

$$= \frac{1}{4} g \sum_{pq} \sigma \left(a_{p+}^\dagger a_{p-}^\dagger (a_{q-} a_{q+} + a_{q-} a_{q+}) - a_{q-} a_{q+} (a_{p+}^\dagger a_{p-}^\dagger + a_{p+}^\dagger a_{p-}^\dagger) \right) = 0$$

And now we can check if \hat{V} commutes with \hat{S}^2 :

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

The first term is zero from the fact that \hat{V} commutes with \hat{S}_z . The second term is:

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

I will separate the commutations and look at them one by one. The first term:

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

The second term:

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

The third term:

$$\begin{aligned} [a_{p+}^\dagger a_{p-}^\dagger, a_{r+}^\dagger a_{r-}] &= a_{p+}^\dagger [a_{p-}^\dagger, a_{r+}^\dagger] a_{r-} + a_{p+}^\dagger a_{r+}^\dagger [a_{p-}^\dagger, a_{r-}] + [a_{p+}^\dagger, a_{r+}^\dagger] a_{r-} a_{p-}^\dagger + a_{r+}^\dagger [a_{p+}^\dagger, a_{r-}] a_{p-}^\dagger \\ &= -a_{p+}^\dagger a_{r+}^\dagger \delta_{pr} \delta_{--} - a_{r+}^\dagger \delta_{pr} \delta_{+-} a_{p-}^\dagger = -a_{p+}^\dagger a_{p+}^\dagger \end{aligned}$$

The fourth term:

$$\begin{aligned} [a_{p+}^\dagger a_{p-}^\dagger, a_{r-}^\dagger a_{r+}] &= a_{p+}^\dagger [a_{p-}^\dagger, a_{r-}^\dagger] a_{r+} + a_{p+}^\dagger a_{r-}^\dagger [a_{p-}^\dagger, a_{r+}] + [a_{p+}^\dagger, a_{r-}^\dagger] a_{r+} a_{p-}^\dagger + a_{r-}^\dagger [a_{p+}^\dagger, a_{r+}] a_{p-}^\dagger \\ &= -a_{p+}^\dagger a_{r-}^\dagger \delta_{pr} \delta_{-+} - a_{r-}^\dagger \delta_{pr} \delta_{++} a_{p-}^\dagger = -a_{p-}^\dagger a_{p-}^\dagger \end{aligned}$$

Now we can put the results back into the expression, and since r is equal to either p or q , we can adjust according to this:

$$\begin{aligned} &= -\frac{1}{2}g \sum_{pq} \left(a_{p+}^\dagger a_{p-}^\dagger a_{q-} a_{q-} a_{q-}^\dagger a_{q+} \right. \\ &\quad + a_{p+}^\dagger a_{p-}^\dagger a_{q+} a_{q-} a_{q+} a_{q+} \\ &\quad - a_{p+}^\dagger a_{p+}^\dagger a_{p-}^\dagger a_{p+} a_{q-} a_{q+} \\ &\quad \left. - a_{p+}^\dagger a_{p-}^\dagger a_{p-}^\dagger a_{p-} a_{q-} a_{q+} \right) \end{aligned}$$

All of these terms are zero, because if we look closely, we can either see that each term is trying to annihilate the same state twice. For the second and third term this happens directly, while for the first and last term, this happens when trying to normal order the operators.

The last term is the same as the second term, because of the commutation relations between \hat{S}_+ and \hat{S}_- , and therefore the result is zero.

This means that \hat{V} commutes with \hat{S}^2 .

We can now introduce the pair-creation and pair-annihilation operators:

$$\begin{aligned} \hat{P}_p^+ &= a_{p+}^\dagger a_{p-}^\dagger \\ \hat{P}_p^- &= a_{p-} a_{p+} \end{aligned}$$

Lets re-introduce the \hat{V} operator:

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

From this we can easily see that we can write \hat{V} as:

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

And therefore we can write the \hat{H} , with $\xi = 1$ as:

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

And lastly we want to show that the pair creation operators commutes among themselves:

$$[\hat{P}_p^+, \hat{P}_q^+] = [a_{p+}^\dagger a_{p-}^\dagger, a_{q+}^\dagger a_{q-}^\dagger]$$

$$a_{p+}^\dagger [a_{p-}^\dagger, a_{q+}^\dagger] a_{q-}^\dagger + a_{p+}^\dagger a_{q+}^\dagger [a_{p-}^\dagger, a_{q-}^\dagger] + [a_{p+}^\dagger, a_{q+}^\dagger] a_{q-}^\dagger a_{p-}^\dagger + a_{q+}^\dagger [a_{p+}^\dagger, a_{q-}^\dagger] a_{p-}^\dagger$$

All these terms are zero, because commuting two creation or annihilation operators will give zero.

b)

For this part we want to construct the Hamiltonian matrix for a system with no broken pairs and total spin of $S = 0$, for the case of the four lowest single-particle states.

We can start by defining a state with total spin $S = 0$:

$$|\Phi_{\alpha\beta}\rangle = P_{\alpha}^{+} P_{\beta}^{+} |0\rangle$$

We will start by finding the expectation value of the one body term:

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

Here $\sigma = \pm 1$ and p can have the values $p = \alpha, \beta$, and therefor we can write the expression as:

$$\langle \Phi_{\alpha\beta} | \hat{H}_0 | \Phi_{\alpha\beta} \rangle = 2(\alpha-1) + 2(\beta-1) = 2(\alpha + \beta - 2)$$

For the interaction term \hat{V} , we will use the indexes $\alpha, \beta, \gamma, \delta$ to represent the four lowest single-particle states. We can write the expectation value as:

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

For this we will need to use contractions.

$$\begin{aligned} \overbrace{P_{\beta}^{-} P_{\alpha}^{-} P_p^{+} P_q^{-} P_{\gamma}^{+} P_{\delta}^{+}} &= \delta_{\beta\delta} \delta_{\alpha p} \delta_{q\gamma} \\ \overbrace{P_{\beta}^{-} P_{\alpha}^{-} P_p^{+} P_q^{-} P_{\gamma}^{+} P_{\delta}^{+}} &= \delta_{\beta\gamma} \delta_{\alpha p} \delta_{q\delta} \\ \overbrace{P_{\beta}^{-} P_{\alpha}^{-} P_p^{+} P_q^{-} P_{\gamma}^{+} P_{\delta}^{+}} &= \delta_{\beta p} \delta_{\alpha\gamma} \delta_{q\delta} \\ \overbrace{P_{\beta}^{-} P_{\alpha}^{-} P_p^{+} P_q^{-} P_{\gamma}^{+} P_{\delta}^{+}} &= \delta_{\beta p} \delta_{\alpha\delta} \delta_{q\gamma} \end{aligned}$$

Usually, when we work with contraction, we will notice how many of the lines cross to determine if the term is negative or positive. One cross, and the term is negative, while two crosses and the term is positive.

For these operators, each of them contain either two creation or two annihilation operators, and therefor the result will always be positive.

Now we can set up the matrices:

$$\hat{H}_0 = \begin{bmatrix} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 6 & 0 & 0 & 0 \\ 0 & 0 & 0 & 6 & 0 & 0 \\ 0 & 0 & 0 & 0 & 8 & 0 \\ 0 & 0 & 0 & 0 & 0 & 10 \end{bmatrix}$$

$$\hat{V} = -\frac{1}{2}g \begin{bmatrix} 2 & 1 & 1 & 1 & 1 & 0 \\ 1 & 2 & 1 & 1 & 0 & 1 \\ 1 & 1 & 2 & 0 & 1 & 1 \\ 1 & 1 & 0 & 2 & 1 & 1 \\ 1 & 0 & 1 & 1 & 2 & 1 \\ 0 & 1 & 1 & 1 & 1 & 2 \end{bmatrix}$$

The total Hamiltonian matrix will be:

$$\hat{H} = \hat{H}_0 + \hat{V} = \begin{bmatrix} 2-g & -\frac{1}{2}g & -\frac{1}{2}g & -\frac{1}{2}g & -\frac{1}{2}g & 0 \\ -\frac{1}{2}g & 4-g & -\frac{1}{2}g & -\frac{1}{2}g & 0 & -\frac{1}{2}g \\ -\frac{1}{2}g & -\frac{1}{2}g & 6-g & 0 & -\frac{1}{2}g & -\frac{1}{2}g \\ -\frac{1}{2}g & -\frac{1}{2}g & 0 & 6-g & -\frac{1}{2}g & -\frac{1}{2}g \\ -\frac{1}{2}g & 0 & -\frac{1}{2}g & -\frac{1}{2}g & 8-g & -\frac{1}{2}g \\ 0 & -\frac{1}{2}g & -\frac{1}{2}g & -\frac{1}{2}g & -\frac{1}{2}g & 10-g \end{bmatrix}$$

The following plot and the matrix elements are calculated with the code in `energies.py`

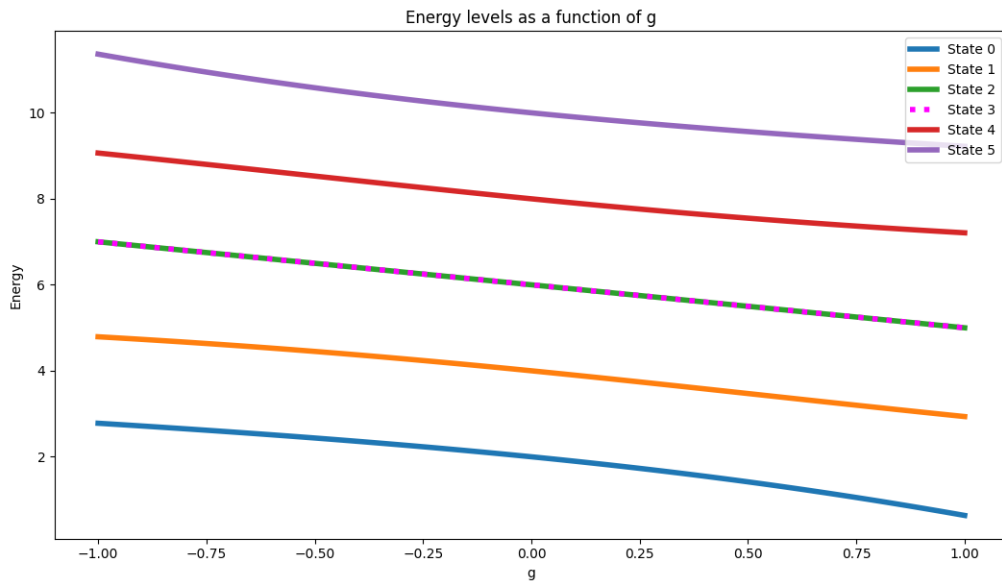


Figure 1: The Hamiltonian matrix for a system with no broken pairs and total spin of $S = 0$, for the case of the four lowest single-particle states. Energies as a function of the strength of the interaction g . The dashed lines are to show the degeneracy of the states.

- c)
- d)
- e)
- f)
- g)