

FYS-KJM4480 - Quantum mechanics for many-particle systems

Project 2

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- For the Github repository containing programs and results, follow this link: https://github.com/UiO-INF5620/INF5620-evenmn/tree/master/project_2

1 Introduction

Words for motivation

2 Theory

Here I should present all the important equations

3 Exercise 1

3.1 d

$$[\hat{P}_p, \hat{P}_q^\dagger] = \hat{P}_p \hat{P}_q^\dagger - \hat{P}_q^\dagger \hat{P}_p \quad (1)$$

Will only include terms which contribute, and we obtain

$$\begin{aligned} \hat{P}_p \hat{P}_q^\dagger &= c_{p-} c_{p+} c_{q+}^\dagger c_{q-}^\dagger \\ &= \{c_{q+}^\dagger c_{q-}^\dagger c_{p-} c_{p+}\} + \{\overline{c_{p-} c_{p+} c_{q+}^\dagger} c_{q-}^\dagger\} + \{c_{p-} \overline{c_{p+} c_{q+}^\dagger} c_{q-}^\dagger\} + \{\overline{c_{p-} c_{p+} c_{q+}^\dagger} c_{q-}^\dagger\} \\ &= \{c_{q+}^\dagger c_{q-}^\dagger c_{p-} c_{p+}\} - \delta_{p-q-} c_{p+} c_{q+}^\dagger - \delta_{p+q+} c_{p-} c_{q-}^\dagger + \delta_{p+q+} \delta_{p-q-} \end{aligned} \quad (2)$$

due to Wick's theorem. Several terms vanish since a delta function of operators of opposite spin does not contribute, i.e. $\delta_{p+q-} = 0$. Calculating $\hat{P}_q^\dagger \hat{P}_p$ is a simple task:

$$\hat{P}_q^\dagger \hat{P}_p = \{c_{q+}^\dagger c_{q-}^\dagger c_{p-} c_{p+}\}. \quad (3)$$

Furthermore we will omit the spin in delta functions, because it does not affect the delta function as long as the spin is equally directed. We set $p = q$, but not in the Dirac delta functions:

$$\begin{aligned} \hat{P}_p \hat{P}_q^\dagger - \hat{P}_q^\dagger \hat{P}_p &= -\delta_{pq} c_{q+}^\dagger c_{q+} - \delta_{pq} c_{q-}^\dagger c_{q-} + \delta_{pq} \delta_{qq} \\ &= \delta_{pq} (1 - c_{q+}^\dagger c_{q+} - c_{q-}^\dagger c_{q-}) \\ &= \delta_{pq} (1 - \hat{n}_q) \end{aligned} \quad (4)$$

3.2 e

We have $N = 4$, thus

$$|\Phi\rangle = c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger |-\rangle \quad (5)$$

$$= \hat{P}_1^\dagger \hat{P}_2^\dagger |-\rangle. \quad (6)$$

M is the number of states, with p as an index

$$\hat{P} = \sum_{p=1}^M \hat{P}_p^\dagger \hat{P}_p \quad (7)$$

$$= \hat{P}_1^\dagger \hat{P}_1 + \hat{P}_2^\dagger \hat{P}_2 + \hat{P}_3^\dagger \hat{P}_3 + \hat{P}_4^\dagger \hat{P}_4 \quad (8)$$

since $M = 4$.

$$\hat{P}|\Phi\rangle = \left(\hat{P}_1^\dagger \hat{P}_1 \hat{P}_1^\dagger \hat{P}_2^\dagger + \hat{P}_2^\dagger \hat{P}_2 \hat{P}_1^\dagger \hat{P}_2^\dagger + \dots\right)|-\rangle \quad (9)$$

$$= \left(\delta_{11} \hat{P}_1^\dagger \hat{P}_2^\dagger + \delta_{22} \hat{P}_1^\dagger \hat{P}_2^\dagger\right)|-\rangle \quad (10)$$

$$= 2|\Phi\rangle \quad (11)$$

where the two last terms in \hat{P} do not contribute since $|\Phi\rangle$ does not contain creation operators with index 3 or 4. This computation was quite short since we could replace all operators with \hat{P} which is not always the case, something we will see when calculating $\hat{S}_z|\Phi\rangle$.

$$\hat{S}_z = \frac{1}{2} \sum_{p\sigma} \sigma c_{p\sigma}^\dagger c_{p\sigma} \quad (12)$$

$$= \frac{1}{2} \left(c_{1+}^\dagger c_{1+} - c_{1-}^\dagger c_{1-} + c_{2+}^\dagger c_{2+} - c_{2-}^\dagger c_{2-} + \right. \\ \left. c_{3+}^\dagger c_{3+} - c_{3-}^\dagger c_{3-} + c_{4+}^\dagger c_{4+} - c_{4-}^\dagger c_{4-} \right) |-\rangle \quad (13)$$

$$\hat{S}_z|\Phi\rangle = \frac{1}{2} \left(c_{1+}^\dagger c_{1+} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger - c_{1-}^\dagger c_{1-} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger \right. \\ \left. + c_{2+}^\dagger c_{2+} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger - c_{2-}^\dagger c_{2-} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger \right) |-\rangle \quad (14)$$

$$= \frac{1}{2} \left(\delta_{1+1+} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger - \delta_{1-1-} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger \right. \\ \left. + \delta_{2+2+} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger - \delta_{2-2-} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger \right) |-\rangle \quad (15)$$

$$= \frac{1}{2} (1 - 1 + 1 - 1) |\Phi\rangle \quad (16)$$

$$= 0 |\Phi\rangle \quad (17)$$

3.3 h

$$\hat{H} = \hat{H}_0 + \hat{V} \quad (18)$$

We use equation ... and ..., and get

$$\begin{aligned}
\hat{V} &= -\frac{1}{2}g \sum_{pq} c_{p+}^\dagger c_{p-}^\dagger c_{q-} c_{q+} \\
&= -\frac{1}{2}g \sum_p^M c_{p+}^\dagger c_{p-}^\dagger \sum_q^M c_{q-} c_{q+} \\
&= -\frac{1}{2}g \left(\sum_{p=1}^4 \hat{P}_p^\dagger \right) \left(\sum_{q=1}^4 \hat{P}_q \right)
\end{aligned} \tag{19}$$

Similarly we get

$$\begin{aligned}
\hat{H}_0 &= \sum_{p\sigma} \varepsilon_p c_{p\sigma}^\dagger c_{p\sigma} \\
&= \sum_p (p-1) \sum_\sigma c_{p\sigma}^\dagger c_{p\sigma} \\
&= \sum_p (p-1) \hat{n}_p.
\end{aligned} \tag{20}$$

Thus we end up with

$$\hat{H} = \sum_p (p-1) \hat{n}_p - \frac{1}{2}g \left(\sum_{p=1}^4 \hat{P}_p^\dagger \right) \left(\sum_{q=1}^4 \hat{P}_q \right) \tag{21}$$

4 Garbage

Table 1: This table represents the error when solving the system for a constant solution.

Elements	1D	2D	3D
P1	2.77555756e-15	3.55271367e-15	2.60902410e-14
P2	1.26343380e-13	1.39666056e-13	8.69304628e-14