FYS-KJM4480 - Quantum mechanics for many-particle systems

Project 2

Even Marius Nordhagen

November 13, 2017

- 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

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

Will only include terms which contribute, and we obtain

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

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:

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

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:

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

3.2 e

We have $N = 4$, thus

$$\begin{aligned}
|\Phi\rangle &= c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger|-\rangle \qquad (5) \\
&= \hat{P}_1^\dagger\hat{P}_2^\dagger|-\rangle. \qquad (6)
\end{aligned}$$

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

$$\begin{aligned}
\hat{P} &= \sum_{p=1}^{M}\hat{P}_p^\dagger\hat{P}_p \qquad (7) \\
&= \hat{P}_1^\dagger\hat{P}_1 + \hat{P}_2^\dagger\hat{P}_2 + \hat{P}_3^\dagger\hat{P}_3 + \hat{P}_4^\dagger\hat{P}_4 \qquad (8)
\end{aligned}$$

since $M = 4$.

$$\hat{P}|\Phi\rangle = \Big(\hat{P}_1^\dagger \hat{P}_1 \hat{P}_1^\dagger \hat{P}_2^\dagger + \hat{P}_2^\dagger \hat{P}_2 \hat{P}_1^\dagger \hat{P}_2^\dagger + ...\Big)|-\rangle \tag{9}$$
$$= \Big(\delta_{11}\hat{P}_1^\dagger \hat{P}_2^\dagger + \delta_{22}\hat{P}_1^\dagger \hat{P}_2^\dagger\Big)|-\rangle \tag{10}$$
$$= 2|\Phi\rangle \tag{11}$$

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 $\hat{S}_z|\Phi\rangle$.

$$\hat{S}_z = \frac{1}{2}\sum_{p\sigma} \sigma c_{p\sigma}^\dagger c_{p\sigma} \tag{12}$$
$$= \frac{1}{2}\Big(c_{1+}^\dagger c_{1+} - c_{1-}^\dagger c_{1-} + c_{2+}^\dagger c_{2+} - c_{2-}^\dagger c_{2-} + c_{3+}^\dagger c_{3+} - c_{3-}^\dagger c_{3-} + c_{4+}^\dagger c_{4+} - c_{4-}^\dagger c_{4-}\Big)|-\rangle \tag{13}$$

$$\hat{S}_z|\Phi\rangle = \frac{1}{2}\Big(c_{1+}^\dagger c_{1+} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger - c_{1-}^\dagger c_{1-} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger + c_{2+}^\dagger c_{2+} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger - c_{2-}^\dagger c_{2-} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger\Big)|-\rangle \tag{14}$$
$$= \frac{1}{2}\Big(\delta_{1+1+} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger - \delta_{1-1-} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger + \delta_{2+2+} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger - \delta_{2-2-} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger\Big)|-\rangle \tag{15}$$
$$= \frac{1}{2}(1 - 1 + 1 - 1)|\Phi\rangle \tag{16}$$
$$= 0|\Phi\rangle \tag{17}$$

3.3 f

Observe that $|1\bar{1}2\bar{2}\rangle = |\Phi\rangle$.

From figure (1) one can observe that the dimension of the subspace for $M = 4$ is $3 + 2 + 1 = 6$, which is the number of possible states. We can easily imagine that for $M = 2$ we would get 1 state, with $M = 5$ we would get $4 + 3 + 2 + 1 = 10$ states and so on. Thus the dimension of the subspace for an arbitrary M is given by

$$n_M = \sum_{m=1}^{M}(M - m) = \sum_{m=1}^{M-1}(M - m) = ... \tag{18}$$

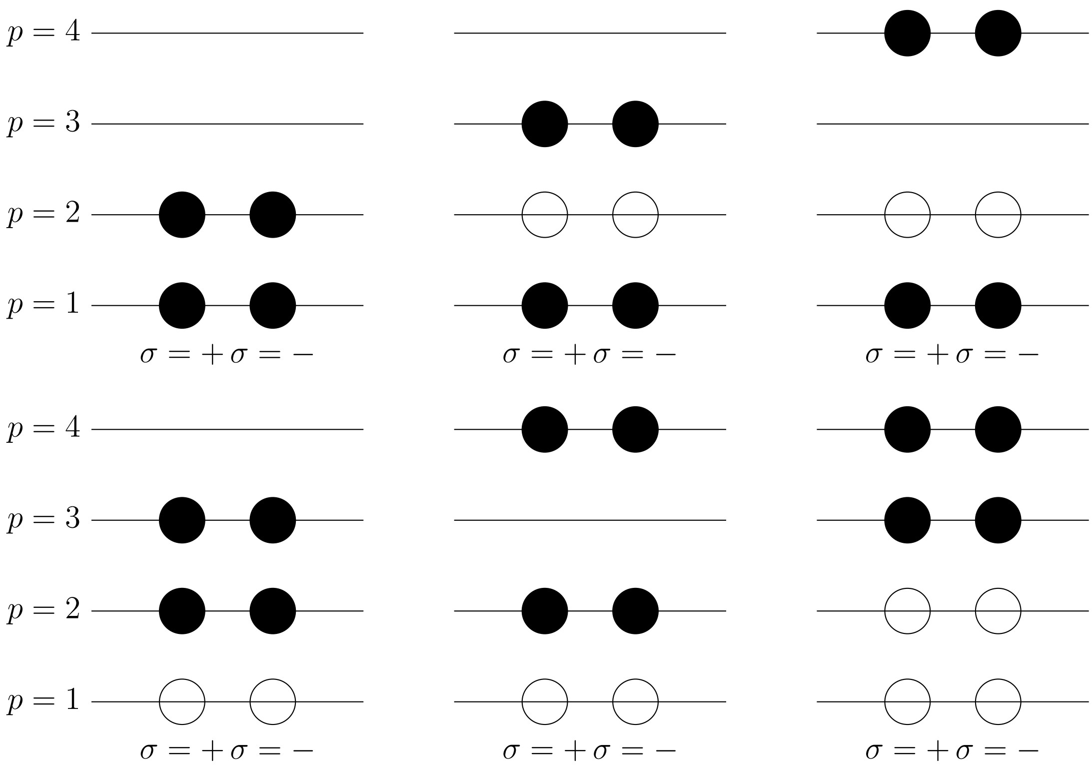

Figure 1: Need good caption here.

3.4 h

$$\hat{H} = \hat{H}_0 + \hat{V} \tag{19}$$

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

$$\begin{aligned}
\hat{V} &= -\frac{1}{2} g \sum_{pq} c^\dagger_{p+} c^\dagger_{p-} c_{q-} c_{q+} \\
&= -\frac{1}{2} g \sum_{p}^{M} c^\dagger_{p+} c^\dagger_{p-} \sum_{q}^{M} c_{q-} c_{q+} \\
&= -\frac{1}{2} g \left(\sum_{p=1}^{4} \hat{P}^\dagger_p \right) \left(\sum_{q=1}^{4} \hat{P}_q \right)
\end{aligned} \tag{20}$$

Similarly we get

$$\begin{aligned}
\hat{H}_0 &= \sum_{p\sigma} \varepsilon_p c^\dagger_{p\sigma} c_{p\sigma} \\
&= \sum_{p} (p-1) \sum_{\sigma} c^\dagger_{p\sigma} c_{p\sigma} \\
&= \sum_{p} (p-1) \hat{n}_p.
\end{aligned} \tag{21}$$

Thus we end up with

$$\hat{H} = \sum_{p} (p-1)\hat{n}_p - \frac{1}{2} g \left(\sum_{p=1}^{4} \hat{P}^\dagger_p \right) \left(\sum_{q=1}^{4} \hat{P}_q \right) \tag{22}$$

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