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

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

Will only include terms which contribute, and we obtain

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

$$= \{c_{q+}^\dagger c_{q-}^\dagger c_{p-}c_{p+}\} + \{\overline{c_{p-}c_{p+}c_{q+}^\dagger}c_{q-}^\dagger\} + \{c_{p-}\overline{c_{p+}c_{q+}^\dagger}c_{q-}^\dagger\} + \{\overline{c_{p-}\,\overline{c_{p+}c_{q+}^\dagger}c_{q-}^\dagger}\}$$

$$= \{c_{q+}^\dagger c_{q-}^\dagger c_{p-}c_{p+}\} - \delta_{p-q-}c_{p+}c_{q+}^\dagger - \delta_{p+q+}c_{p-}c_{q-}^\dagger + \delta_{p+q+}\delta_{p-q-} \tag{2}$$

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:

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

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:

$$\hat{P}_p\hat{P}_q^\dagger - \hat{P}_q^\dagger\hat{P}_p = -\delta_{pq}c_{q+}^\dagger c_{q+} - \delta_{pq}c_{q-}^\dagger c_{q-} + \delta_{pq}\delta_{qq}$$

$$= \delta_{pq}(1 - c_{q+}^\dagger c_{q+} - c_{q-}^\dagger c_{q-})$$

$$= \delta_{pq}(1 - \hat{n}_q) \tag{4}$$

3.2 e

We have $N = 4$, thus

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

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

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

$$\hat{P} = \sum_{p=1}^{M} \hat{P}_p^\dagger\hat{P}_p \tag{7}$$

$$= \hat{P}_1^\dagger\hat{P}_1 + \hat{P}_2^\dagger\hat{P}_2 + \hat{P}_3^\dagger\hat{P}_3 + \hat{P}_4^\dagger\hat{P}_4 \tag{8}$$

since $M = 4$.

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

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

$$= 2|\Phi\rangle \tag{11}$$

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

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

$$= \frac{1}{2} \Big(c_{1+}^\dagger c_{1+} - c_{1-}^\dagger c_{1-} + c_{2+}^\dagger c_{2+} - c_{2-}^\dagger c_{2-} +$$

$$c_{3+}^\dagger c_{3+} - c_{3-}^\dagger c_{3-} + c_{4+}^\dagger c_{4+} - c_{4-}^\dagger c_{4-} \Big)|-\rangle \tag{13}$$

$$\hat{S}_z|\Phi\rangle = \frac{1}{2} \Big(c_{1+}^\dagger c_{1+} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger - c_{1-}^\dagger c_{1-} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger$$

$$+ c_{2+}^\dagger c_{2+} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger - c_{2-}^\dagger c_{2-} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger \Big)|-\rangle \tag{14}$$

$$= \frac{1}{2} \Big(c_{1+}^\dagger c_{1+} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger - c_{1-}^\dagger c_{1-} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger$$

$$+ c_{2+}^\dagger c_{2+} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger - c_{2-}^\dagger c_{2-} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger \Big)|-\rangle \tag{15}$$

$$= \frac{1}{2} \Big(\delta_{1+1+} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger - \delta_{1-1-} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger$$

$$+ \delta_{2+2+} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger - \delta_{2-2-} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger \Big)|-\rangle \tag{16}$$

$$= \frac{1}{2}(1 - 1 + 1 - 1)|\Phi\rangle \tag{17}$$

$$= 0|\Phi\rangle \tag{18}$$

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
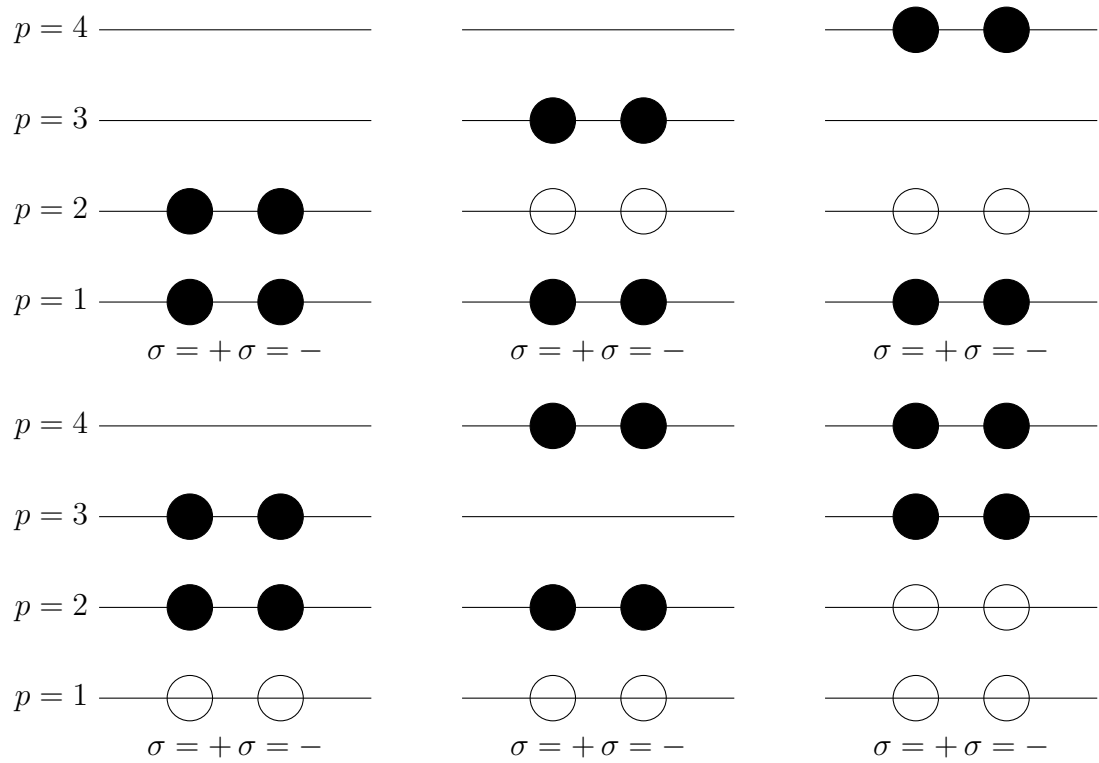
Figure 1: Need good caption here.

get $4 + 3 + 2 + 1 = 10$ states and so on. Thus the dimension of the subspace for an arbitrary M is given by the arithmetic series

$$n_M = \sum_{m=1}^{M-1} (M - m).\tag{19}$$

3.4   g

3.5   h

$$\hat{H} = \hat{H}_0 + \hat{V}\tag{20}$$

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

$$\begin{aligned}\hat{V} &= -\frac{1}{2}g \sum_{pq} c_{p+}^\dagger c_{p-}^\dagger c_{q-} c_{q+} \\ &= -\frac{1}{2}g \sum_p^M c_{p+}^\dagger c_{p-}^\dagger \sum_q^M c_{q-} c_{q+} \\ &= -\frac{1}{2}g \left(\sum_{p=1}^4 \hat{P}_p^\dagger \right) \left(\sum_{q=1}^4 \hat{P}_q \right)\end{aligned}\tag{21}$$

Similarly we get

$$\begin{aligned}\hat{H}_0 &= \sum_{p\sigma} \varepsilon_p c_{p\sigma}^\dagger c_{p\sigma} \\ &= \sum_p (p - 1) \sum_\sigma c_{p\sigma}^\dagger c_{p\sigma} \\ &= \sum_p (p - 1) \hat{n}_p.\end{aligned}\tag{22}$$

Thus we end up with

$$\hat{H} = \sum_p (p - 1) \hat{n}_p - \frac{1}{2}g \left(\sum_{p=1}^4 \hat{P}_p^\dagger \right) \left(\sum_{q=1}^4 \hat{P}_q \right)\tag{23}$$

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