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

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

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 h

$$\hat{H} = \hat{H}_0 + \hat{V} \tag{5}$$

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

$$\begin{aligned}
\hat{V} &= -\frac{1}{2}g\sum_{pq} c_{p+}^\dagger c_{p-}^\dagger c_{q-}c_{q+} \\
&= -\frac{1}{2}g\sum_{p}^{M} c_{p+}^\dagger c_{p-}^\dagger \sum_{q}^{M} c_{q-}c_{q+} \\
&= -\frac{1}{2}g\left(\sum_{p=1}^{4}\hat{P}_p^\dagger\right)\left(\sum_{q=1}^{4}\hat{P}_q\right) \qquad (6)
\end{aligned}$$

Similarly we get

$$\begin{aligned}\hat{H}_0 &= \sum_{p\sigma} \varepsilon_p c^\dagger_{p\sigma} c_{p\sigma} \\ &= \sum_p (p-1) \sum_\sigma c^\dagger_{p\sigma} c_{p\sigma} \\ &= \sum_p (p-1)\hat{n}_p. \end{aligned} \tag{7}$$

Thus we end up with

$$\hat{H} = \sum_p (p-1)\hat{n}_p - \frac{1}{2} g \left(\sum_{p=1}^{4} \hat{P}^\dagger_p \right) \left(\sum_{q=1}^{4} \hat{P}_q \right) \tag{8}$$

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