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/evenmn/master/tree/master/FYSKJM4480/Project2`

1 Introduction

Superconductivity might be one of 20th century's most exciting physical discoveries, and for a long time the theory behind was a mystery. In 1957, 46 years after the first observation by Kamerlingh Onnes, John Bardeen, Leon Cooper and John Robert Schrieffer came up with a quantum theory describing superconductivity on microscopic level. This theory was built on Cooper pairs, which is a pair of electrons with lower energy than the Fermi energy, i.e. there is a bounding between them. We can treat the pairs as a particle, which is a boson due to the total spin 1, and this boson-like pair is the reason why the current can flow unhindered in a superconductor.

Furthermore the theory is also used in nuclear physics to describe the paring interaction between nucleons in an atomic nucleus.

This project aims to study such a pairing model, known as BCS-theory after its founders. In the first part we are working with this model independently. Then we will use Configuration-Interaction Doubled (CID) as an approximation to make the equations computer-friendly, and thereafter we repeat this using Coupled-Cluster Doubled (CCD). Finally the results are compared for both the methods, and we will discuss why one method is better than the other.

2 Pairing model

In this project we use a slightly simplified pairing model, which we assume to be carrying a constant strength g. The Hamiltonian is therefore given by

$$\hat{H} = \hat{H}_0 + \hat{V} \tag{1}$$

with

$$\hat{H}_0 = \sum_{p\sigma} \epsilon_p c^\dagger_{p\sigma} c_{p\sigma}, \quad \epsilon_p = \xi \cdot (p-1) \tag{2}$$

and

$$\hat{V} = -\frac{1}{2} g \sum_{pq} c^\dagger_{p+} c^\dagger_{p-} c_{q-} c_{q+}. \tag{3}$$

We will only study systems of a even number of particles, N, and the ground-state wavefunction is then given by the Slater determinant

$$|\Phi\rangle = c^\dagger_{1+} c^\dagger_{1-} \dots c^\dagger_{N/2+} c^\dagger_{N/2-} |\Phi\rangle. \tag{4}$$

Further I will define some operators that will be useful when doing the calculations.

$$\hat{P}^\dagger_p \equiv c^\dagger_{p+} c^\dagger_{p-}, \quad \hat{P}_p \equiv c_{p-} c_{p+} \tag{5}$$

$$\hat{n}_p \equiv \sum_{\sigma} c^\dagger_{p\sigma} c_{p\sigma} \tag{6}$$

$$\hat{P} = \sum_{p} \hat{P}^\dagger_p \hat{P}_p \tag{7}$$

and finally

$$\hat{S}_z = \frac{1}{2} \sum_{p\sigma} \sigma c^\dagger_{p\sigma} c_{p\sigma}. \tag{8}$$

2.1 Exercise 1A

2.2 Exercise 1B

2.3 Exercise 1C

2.4 Exercise 1D

$$[\hat{P}_p, \hat{P}^\dagger_q] = \hat{P}_p \hat{P}^\dagger_q - \hat{P}^\dagger_q \hat{P}_p \tag{9}$$

Will only include terms which contribute, and we obtain

$$
\begin{aligned}
\hat{P}_p\hat{P}_q^\dagger &= \sum_{pq} c_{p-}c_{p+}c_{q+}^\dagger c_{q-}^\dagger \\
&= \{c_{q+}^\dagger c_{q-}^\dagger c_{p-}c_{p+}\} + \{c_{p-}c_{p+}c_{q+}^\dagger c_{q-}^\dagger\} + \{c_{p-}c_{p+}c_{q+}^\dagger c_{q-}^\dagger\} + \{c_{p-}c_{p+}c_{q+}^\dagger c_{q-}^\dagger\} \\
&= \{c_{q+}^\dagger c_{q-}^\dagger c_{p-}c_{p+}\} - \delta_{pq}c_{p+}c_{q+}^\dagger - \delta_{pq}c_{p-}c_{q-}^\dagger + \delta_{pq}\delta_{pq} \qquad (10)
\end{aligned}
$$

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:

$$\hat{P}_q^\dagger\hat{P}_p = \{c_{q+}^\dagger c_{q-}^\dagger c_{p-}c_{p+}\}. \qquad (11)$$

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:

$$
\begin{aligned}
\hat{P}_p\hat{P}_q^\dagger - \hat{P}_q^\dagger\hat{P}_p &= -\delta_{pq}c_{q+}^\dagger c_{q+} - \delta_{pq}c_{q-}^\dagger c_{q-} + \delta_{pq}\delta_{qq} \\
&= \delta_{pq}(1 - c_{q+}^\dagger c_{q+} - c_{q-}^\dagger c_{q-}) \\
&= \delta_{pq}(1 - \hat{n}_q) \qquad (12)
\end{aligned}
$$

2.5 e

We have $N = 4$, thus

$$
\begin{aligned}
|\Phi\rangle &= c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger|-\rangle \qquad (13)\\
&= \hat{P}_1^\dagger\hat{P}_2^\dagger|-\rangle. \qquad (14)
\end{aligned}
$$

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

$$
\begin{aligned}
\hat{P} &= \sum_{p=1}^{M}\hat{P}_p^\dagger\hat{P}_p \qquad (15)\\
&= \hat{P}_1^\dagger\hat{P}_1 + \hat{P}_2^\dagger\hat{P}_2 + \hat{P}_3^\dagger\hat{P}_3 + \hat{P}_4^\dagger\hat{P}_4 \qquad (16)
\end{aligned}
$$

since $M = 4$.

$$
\begin{aligned}
\hat{P}|\Phi\rangle &= \left(\hat{P}_1^\dagger\hat{P}_1\hat{P}_1^\dagger\hat{P}_2^\dagger + \hat{P}_2^\dagger\hat{P}_2\hat{P}_1^\dagger\hat{P}_2^\dagger + ...\right)|-\rangle \qquad (17)\\
&= \left(\delta_{11}\hat{P}_1^\dagger\hat{P}_2^\dagger + \delta_{22}\hat{P}_1^\dagger\hat{P}_2^\dagger\right)|-\rangle \qquad (18)\\
&= 2|\Phi\rangle \qquad (19)
\end{aligned}
$$

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

$$\hat{S}_z = \frac{1}{2}\sum_{p\sigma} \sigma c^\dagger_{p\sigma} c_{p\sigma} \tag{20}$$

$$\begin{aligned} =&\frac{1}{2}\Big(c^\dagger_{1+}c_{1+} - c^\dagger_{1-}c_{1-} + c^\dagger_{2+}c_{2+} - c^\dagger_{2-}c_{2-} + \\ &c^\dagger_{3+}c_{3+} - c^\dagger_{3-}c_{3-} + c^\dagger_{4+}c_{4+} - c^\dagger_{4-}c_{4-}\Big)|-\rangle \end{aligned} \tag{21}$$

$$\begin{aligned} \hat{S}_z|\Phi\rangle =&\frac{1}{2}\Big(c^\dagger_{1+}c_{1+}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-} - c^\dagger_{1-}c_{1-}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-} \\ &+ c^\dagger_{2+}c_{2+}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-} - c^\dagger_{2-}c_{2-}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-}\Big)|-\rangle \end{aligned} \tag{22}$$

$$\begin{aligned} =&\frac{1}{2}\Big(c^\dagger_{1+}c_{1+}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-} - c^\dagger_{1-}c_{1-}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-} \\ &+ c^\dagger_{2+}c_{2+}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-} - c^\dagger_{2-}c_{2-}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-}\Big)|-\rangle \end{aligned} \tag{23}$$

$$\begin{aligned} =&\frac{1}{2}\Big(\delta_{1+1+}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-} - \delta_{1-1-}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-} \\ &+ \delta_{2+2+}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-} - \delta_{2-2-}c^\dagger_{1+}c^\dagger_{1-}c^\dagger_{2+}c^\dagger_{2-}\Big)|-\rangle \end{aligned} \tag{24}$$

$$=\frac{1}{2}(1-1+1-1)|\Phi\rangle \tag{25}$$

$$=0|\Phi\rangle \tag{26}$$

2.6 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 the arithmetic series

$$n_M = \sum_{m=1}^{M-1}(M-m). \tag{27}$$

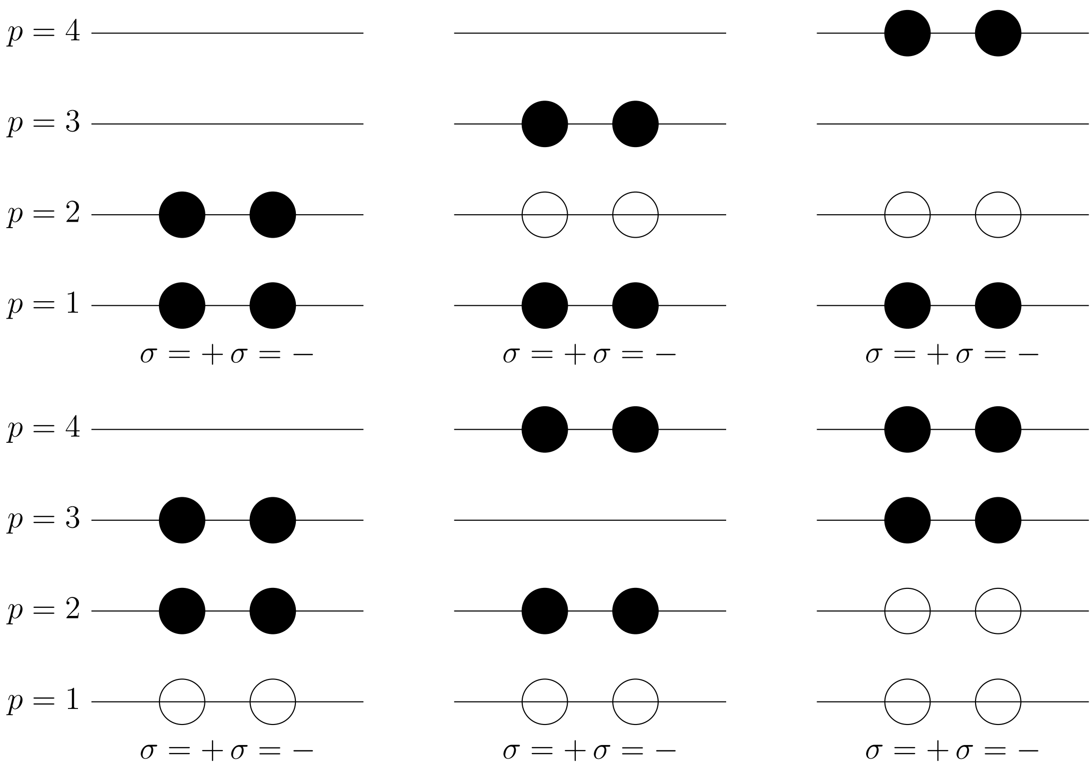

Figure 1: Need good caption here.

2.7 g

2.8 h

$$\hat{H} = \hat{H}_0 + \hat{V} \tag{28}$$

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

$$\begin{aligned}\hat{V} &= -\frac{1}{2}g\sum_{pq} c^\dagger_{p+}c^\dagger_{p-}c_{q-}c_{q+} \\ &= -\frac{1}{2}g\sum_{p}^{M} c^\dagger_{p+}c^\dagger_{p-}\sum_{q}^{M} c_{q-}c_{q+} \\ &= -\frac{1}{2}g\left(\sum_{p=1}^{4}\hat{P}^\dagger_p\right)\left(\sum_{q=1}^{4}\hat{P}_q\right)\end{aligned} \tag{29}$$

Similarly we get

$$\begin{aligned}\hat{H}_0 &= \sum_{p\sigma}\varepsilon_p c^\dagger_{p\sigma}c_{p\sigma} \\ &= \sum_{p}(p-1)\sum_{\sigma}c^\dagger_{p\sigma}c_{p\sigma} \\ &= \sum_{p}(p-1)\hat{n}_p.\end{aligned} \tag{30}$$

Thus we end up with

$$\hat{H} = \sum_{p}(p-1)\hat{n}_p - \frac{1}{2}g\left(\sum_{p=1}^{4}\hat{P}^\dagger_p\right)\left(\sum_{q=1}^{4}\hat{P}_q\right) \tag{31}$$

3 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