

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 pairing 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

$$\hat{H} = \hat{H}_0 + \hat{V} \quad (1)$$

with

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

and

$$\hat{V} = -\frac{1}{2}g \sum_{pq} c_{p+}^\dagger c_{p-}^\dagger c_{q-} c_{q+}. \quad (3)$$

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

$$|\Phi\rangle = c_{1+}^\dagger c_{1-}^\dagger \dots c_{N/2+}^\dagger c_{N/2-}^\dagger |\Phi\rangle. \quad (4)$$

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

$$\hat{P}_p^\dagger \equiv c_{p+}^\dagger c_{p-}^\dagger, \quad \hat{P}_p \equiv c_{p-} c_{p+} \quad (5)$$

$$\hat{n}_p \equiv \sum_{\sigma} c_{p\sigma}^\dagger c_{p\sigma} \quad (6)$$

$$\hat{P} = \sum_p \hat{P}_p^\dagger \hat{P}_p \quad (7)$$

and finally

$$\hat{S}_z = \frac{1}{2} \sum_{p\sigma} \sigma c_{p\sigma}^\dagger c_{p\sigma}. \quad (8)$$

2.1 Exercise 1A

2.2 Exercise 1B

2.3 Exercise 1C

2.4 Exercise 1D

$$[\hat{P}_p, \hat{P}_q^\dagger] = \hat{P}_p \hat{P}_q^\dagger - \hat{P}_q^\dagger \hat{P}_p \quad (9)$$

Will only include terms which contribute, and we obtain

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

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:

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

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:

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

2.5 e

We have $N = 4$, thus

$$|\Phi\rangle = c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger |-\rangle \quad (13)$$

$$= \hat{P}_1^\dagger \hat{P}_2^\dagger |-\rangle. \quad (14)$$

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

$$\hat{P} = \sum_{p=1}^M \hat{P}_p^\dagger \hat{P}_p \quad (15)$$

$$= \hat{P}_1^\dagger \hat{P}_1 + \hat{P}_2^\dagger \hat{P}_2 + \hat{P}_3^\dagger \hat{P}_3 + \hat{P}_4^\dagger \hat{P}_4 \quad (16)$$

since $M = 4$.

$$\hat{P}|\Phi\rangle = (\hat{P}_1^\dagger \hat{P}_1 \hat{P}_1^\dagger \hat{P}_2^\dagger + \hat{P}_2^\dagger \hat{P}_2 \hat{P}_1^\dagger \hat{P}_2^\dagger + \dots) |-\rangle \quad (17)$$

$$= (\delta_{11} \hat{P}_1^\dagger \hat{P}_2^\dagger + \delta_{22} \hat{P}_1^\dagger \hat{P}_2^\dagger) |-\rangle \quad (18)$$

$$= 2|\Phi\rangle \quad (19)$$

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

$$\hat{S}_z = \frac{1}{2} \sum_{p\sigma} \sigma c_{p\sigma}^\dagger c_{p\sigma} \quad (20)$$

$$= \frac{1}{2} \left(c_{1+}^\dagger c_{1+} - c_{1-}^\dagger c_{1-} + c_{2+}^\dagger c_{2+} - c_{2-}^\dagger c_{2-} + c_{3+}^\dagger c_{3+} - c_{3-}^\dagger c_{3-} + c_{4+}^\dagger c_{4+} - c_{4-}^\dagger c_{4-} \right) |-\rangle \quad (21)$$

$$\hat{S}_z|\Phi\rangle = \frac{1}{2} \left(c_{1+}^\dagger c_{1+} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger - c_{1-}^\dagger c_{1-} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger + c_{2+}^\dagger c_{2+} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger - c_{2-}^\dagger c_{2-} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger \right) |-\rangle \quad (22)$$

$$= \frac{1}{2} \left(c_{1+}^\dagger \overline{c_{1+}^\dagger c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger} - c_{1-}^\dagger \overline{c_{1-}^\dagger c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger} + c_{2+}^\dagger \overline{c_{2+}^\dagger c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger} - c_{2-}^\dagger \overline{c_{2-}^\dagger c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger} \right) |-\rangle \quad (23)$$

$$= \frac{1}{2} \left(\delta_{1+1+} c_{1+}^\dagger c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger - \delta_{1-1-} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger + \delta_{2+2+} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger - \delta_{2-2-} c_{1+}^\dagger c_{1-}^\dagger c_{2+}^\dagger c_{2-}^\dagger \right) |-\rangle \quad (24)$$

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

$$= 0 |\Phi\rangle \quad (26)$$

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

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

2.7 g

2.8 h

$$\hat{H} = \hat{H}_0 + \hat{V} \quad (28)$$

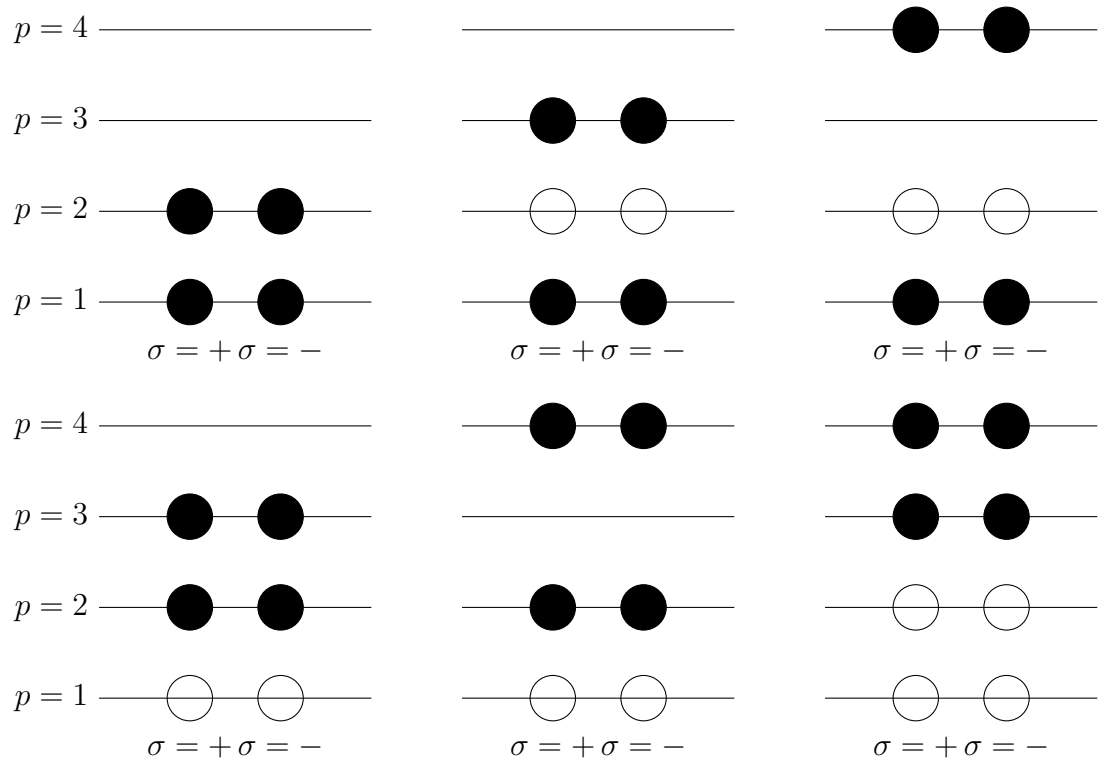


Figure 1: Need good caption here.

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

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

Similarly we get

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

Thus we end up with

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

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