FYS4480 Quantum mechanics for many-particle systems
— Project 1 —

Erlend Lima, Lasse Lorentz Braseth and Halvard Sutterud

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Abstract

Hei

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1 Introduction

2 Theory

2.1 Second quantization

We introduce the second quantization formalism to simplify the notation and calculations. Second quantization introduces creation and annihilation operators, which we will represent as $a_p^\dagger$ and a_p respectively. They work on a slater determinant in the following way,

$$\begin{aligned} a_p^\dagger |\alpha_1\alpha_2\dots\alpha_n\rangle &= |p\alpha_1\alpha_2\dots\alpha_n\rangle \\ a_p |p\alpha_1\alpha_2\dots\alpha_n\rangle &= |\alpha_1\alpha_2\dots\alpha_n\rangle . \end{aligned}$$

The $a_p^\dagger$ thus has the effect of creating a particle in the state p, and a_p to remove a particle from the same state. In addition, we have

$$\begin{aligned} a_p^\dagger |p\alpha_1\alpha_2\dots\alpha_n\rangle &= 0 \\ a_p |\alpha_1\alpha_2\dots\alpha_n\rangle &= 0, \end{aligned}$$

i.e. the creation operator cannot create a particle in an occupied state (the Pauli Exclusion principle), and in the second case the annihilation operator cannot remove a particle not present (common sense).

2.2 Wicks theorem

Wicks theorem states that a product of N operators can be expressed as the normal-ordered product of the operators plus the normal-ordered products of every possible permutation of one to $N/2$ contractions of the same operators.

only need to consider the sum over normal products of all contractions between two and two operators.

2.2.1 Generalized wicks theorem

When using the particle-hole formalism, we need to give a small reformulation of wicks theorem. Main changes: We consider

2.3 Part a (to be renamed)

Our basis in the second quantization are slater determinants consisting of s-wave ($l = 0$) hydrogen like single particle functions $R_{n0}(r)$, given by

$$R_{n0}(r) = \left(\frac{2Z}{n}\right)^{3/2} \sqrt{\frac{(n-1)!}{2n(n!)}} L_{n-1}^1\left(\frac{2Zr}{n}\right) \exp\left(-\frac{Zr}{n}\right), \quad (1)$$

where $L_{n-1}^1(r)$ are the so-called Laguerre polynomials. We then have a degeneracy for the states with quantum number n of 2, since we only consider s-waves.

We will be working with the helium atom. We define our single-particle Hilbert space to consist of the single-particle orbits $1s$, $2s$, and $3s$ with corresponding spin degeneracies, and consider that we will be working with a two-electron system. We will number the six possible single particle states $|nm_s\rangle$ as seen in table 1. The Fermi level is then defined to be $F = 2$. Our ansatz for the ground state $|c\rangle = |\Phi_0\rangle$ of the helium atom is then two electrons placed in the ground state with $n = 1$, with opposite spin values, which we can then represent as

$$|c\rangle = \prod_{i=1}^{F} a_i^\dagger |0\rangle = a_2^\dagger a_1^\dagger |0\rangle \tag{2}$$

Assuming that the total spin is projection of the possible states is $M_S = 0$, the possible one-particle-one-hole excitations are $|\Phi_i^a\rangle = a_a^\dagger a_i |c\rangle$ in these combinations,

$$\begin{aligned} |\Phi_1^3\rangle &= a_3^\dagger a_1 |c\rangle, & |\Phi_1^5\rangle &= a_5^\dagger a_1 |c\rangle \\ |\Phi_2^4\rangle &= a_4^\dagger a_2 |c\rangle, & |\Phi_2^6\rangle &= a_6^\dagger a_2 |c\rangle, \end{aligned}$$

while the possible two-particle-two-holes excitations are $|\Phi_{ij}^{ab}\rangle = a_b^\dagger a_a^\dagger a_j a_i |c\rangle$ in the following combinations,

$$\begin{aligned} |\Phi_{12}^{34}\rangle &= a_4^\dagger a_3^\dagger a_2 a_1 |c\rangle, & |\Phi_{12}^{56}\rangle &= a_6^\dagger a_5^\dagger a_2 a_1 |c\rangle \\ |\Phi_{12}^{36}\rangle &= a_6^\dagger a_3^\dagger a_2 a_1 |c\rangle, & |\Phi_{12}^{45}\rangle &= a_5^\dagger a_4^\dagger a_2 a_1 |c\rangle. \end{aligned}$$

Table 1: Here ↑ corresponds to magnetic spin quantum number $m_s = 1/2$, while ↓ corresponds to $m_s = -1/2$.

index	1	2	3	4	5	6
state	$\|1\uparrow\rangle$	$\|1\downarrow\rangle$	$\|2\uparrow\rangle$	$\|2\downarrow\rangle$	$\|3\uparrow\rangle$	$\|3\downarrow\rangle$

2.4 Part b (to be renamed)

The Hamiltonian in a second-quantized form is given as

$$\hat{H} = \sum_{pq} \langle p|\hat{h}|q\rangle a_p^\dagger a_q + \frac{1}{4} \sum pqrs \langle pq|\hat{v}|rs\rangle a_p^\dagger a_q^\dagger a_s a_r, \tag{3}$$

where the sums run both above and below the fermi surface. Splitting these sums give us the BLA BLA

Or maybe we should split it into non-interacting and interacting?

$$\hat{H}_0 = \sum_{pq>F} \langle p|h_0|q\rangle \tag{4}$$

3 Methods and implementation

4 Results

5 Discussion

6 Conclusions