Ground state energy of quantum dots using the coupled cluster method

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(Dated: April 9, 2018)

Something about coupled-cluster... Preferably doubles.

CONTENTS

I. INTRODUCTION

In this project we will study the ground state energy of quantum dots.

II. THEORY

In this project we will study a system of N interacting electrons. We will be looking at a Hamiltonian consisting of a one-body and a two-body part. The one-body part is given by

$$h(\mathbf{r}_i) = -\frac{1}{2}\nabla_i^2 + \frac{1}{2}\omega^2\mathbf{r}_i^2, \tag{1}$$

where we use natural units $\hbar = c = e = 1$ and set the mass to unity. The two-body part is the Coulomb interaction potential.

$$v(\mathbf{r}_i, \mathbf{r}_j) = \frac{1}{\left|\mathbf{r}_i - \mathbf{r}_j\right|}. \tag{2}$$

We thus get the total Hamiltonian

$$H = \sum_{i=1}^{N} h(\mathbf{r}_i) + \sum_{i<j}^{N} v(\mathbf{r}_i, \mathbf{r}_j). \tag{3}$$

Next we define the reference Slater determinant as

$$|\Phi_0\rangle \equiv |1, 2, \ldots, N\rangle, \tag{4}$$

where $|p\rangle$ are the single particle functions that satisfies the equation

$$h|p\rangle = \varepsilon_p|p\rangle. \tag{5}$$

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[*] Project code: https://github.com/Schoyen/FYS4411

They are the eigenfunctions to the one-body part of the Hamiltonian and are thus harmonic oscillator functions. Note that $|\Phi_0\rangle$ consists of the N first occupied single particle functions. We will denote the occupied indices with $i, j, k, l, \cdots \in \{1, \ldots, N\}$, the virtual states with $a, b, c, d, \cdots \in \{N+1, \ldots, L\}$ and general indices with $p, q, r, s, \cdots \in \{1, \ldots, L\}$.

A. Second quantization

We now move over to a use second quantization. Employing the creation operators, $a_p^\dagger$, and the destruction operators, a_p, we can write the Hamiltonian as

$$H = \sum_{pq} h_q^p a_p^\dagger a_q + \sum_{pqrs} w_{rs}^{pq} a_p^\dagger a_q^\dagger a_s a_r, \tag{6}$$

where the sums are general indices over all L basis states and the matrix elements are defined as

$$h_q^p \equiv \langle p|h|q\rangle, \tag{7}$$

$$w_{rs}^{pq} \equiv \langle pq|v|rs\rangle. \tag{8}$$

In the case of the eigenstates we have that the one-body operator reduces to a diagonal matrix.

$$h_q^p = \langle p|h|q\rangle = \varepsilon_q\langle p|q\rangle = \varepsilon_q\delta_{pq}, \tag{9}$$

where δ_{pq} is the Kronecker-Delta.

B. The coupled cluster approximation

We approximate the true wavefunction, $|\Psi\rangle$, of the system by the coupled cluster wavefunction, $|\Psi_{\mathrm{CC}}\rangle$, defined as

$$|\Psi_{\mathrm{CC}}\rangle \equiv e^T|\Phi_0\rangle. \tag{10}$$