

# Ground state energy of quantum dots using the coupled cluster method

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Something about coupled-cluster... Preferably doubles.

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## 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

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

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

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

We thus get the total Hamiltonian

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

Next we define the reference Slater determinant as

$$|\Phi_0\rangle \equiv |1, 2, \dots, N\rangle, \quad (4)$$

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

$$h|p\rangle = \varepsilon_p|p\rangle. \quad (5)$$

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  $i, j, k, l, \dots \in \{1, \dots, N\}$ , the virtual states with  $a, b, c, d, \dots \in \{N+1, \dots, L\}$  and general indices with  $p, q, r, s, \dots \in \{1, \dots, L\}$ .

### 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

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

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

$$h_q^p \equiv \langle p|h|q\rangle, \quad (7)$$

$$w_{rs}^{pq} \equiv \langle pq|v|rs\rangle. \quad (8)$$

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

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

where  $\delta_{pq}$  is the Kronecker-Delta.

### B. The coupled cluster approximation

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

$$|\Psi_{CC}\rangle \equiv e^T |\Phi_0\rangle = \left( \sum_{i=0}^n \frac{1}{n!} T^n \right) |\Phi_0\rangle, \quad (10)$$

where the *cluster operator*,  $T$ , is given by a sum of  $p$ -excitation operators

$$T = T_1 + T_2 + \dots \quad (11)$$

$$= \sum_{ia} t_i^a a_a^\dagger a_i + \left( \frac{1}{2!} \right)^2 \sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_i a_j + \dots \quad (12)$$

We will be looking at the *doubles* approximation, that is

$$T = T_{CCD} \equiv T_2. \quad (13)$$

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\* Project code: <https://github.com/Schoyen/FYS4411>

### C. Energy of the coupled cluster approximation

When we're going to compute the energy of a system using the coupled cluster approximation we would ideally want to find the expectation value of the energy using the coupled cluster wavefunction.

$$E = \langle \Psi_{CC} | H | \Psi_{CC} \rangle. \quad (14)$$

As it turns out, this is an uncomfortable way of finding the energy as  $T \neq T^\dagger$ . Instead we will define what we call the *similarity transformed Hamiltonian*. We plug the coupled cluster wavefunction into the Schrödinger equation.

$$H | \Psi_{CC} \rangle = E | \Psi_{CC} \rangle. \quad (15)$$

Next, we left multiply with the inverse of the cluster expansion, i.e.,

$$e^{-T} H | \Psi_{CC} \rangle = e^{-T} E | \Psi_{CC} \rangle = E | \Phi_0 \rangle. \quad (16)$$

Projecting this equation on the reference state we get

$$E = \langle \Phi_0 | e^{-T} H | \Psi_{CC} \rangle = \langle \Phi_0 | e^{-T} H e^T | \Phi_0 \rangle, \quad (17)$$

where in the latter inner-product we have located the similarity transformed Hamiltonian defined by

$$\bar{H} \equiv e^{-T} H e^T. \quad (18)$$

#### 1. Normal ordered Hamiltonian

To get to the coupled cluster equations we need to write the Hamiltonian on a normal ordered form. We

use Wick's theorem on the Fermi vacuum<sup>1</sup>. The one-body part of the Hamiltonian thus becomes

$$h = \sum_{pq} h_q^p a_p^\dagger a_q = \sum_{pq} h_q^p \left( \{a_p^\dagger a_q\} + \{\bar{a}_p^\dagger a_q\} \right) \quad (19)$$

$$= h_N + \sum_{pq} \varepsilon_i. \quad (20)$$

The two-body part yields

$$v = \sum_{pqrs} w_{rs}^{pq} a_p^\dagger a_q^\dagger a_s a_r \quad (21)$$

We can then write the Hamiltonian in terms of the reference energy and the normal ordered Hamiltonian.

$$H = H_N + \langle \Phi_0 | H | \Phi_0 \rangle. \quad (22)$$

The energy equation thus becomes

$$E = \langle \Phi_0 | \bar{H} | \Phi_0 \rangle = E_{\text{ref}} + \langle \Phi_0 | e^{-T} H_N e^T | \Phi_0 \rangle. \quad (23)$$

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<sup>1</sup> Fermi vacuum corresponds to the reference Slater.

By expanding the exponentials the similarity transformed Hamiltonian and recognizing the commutators we get the Baker-Campbell-Hausdorff expansion.

$$\bar{H} = H + [H, T] + \frac{1}{2} [[H, T], T] + \dots \quad (24)$$