

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 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, $|\Psi_{CC}\rangle$, defined as

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

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

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

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

1. 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

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