Ground state energy of quantum dots using the coupled cluster method

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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.

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

We thus get the total Hamiltonian

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

Working in a basis of L single particle functions, $\{|p\rangle\}_{p=1}^{L}$. We define the reference Slater determinant as

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

i.e., a tensorproduct of the N first single particle functions, $|i\rangle$, of the system. We call these single particle functions *occupied* as they are contained in the Slater determinant. 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 $p, q, r, s, \cdots \in \{1, \ldots, L\}$. In terms of sets of basis functions we can write this as

$$\{|p\rangle\}_{p=1}^{L} = \{|i\rangle\}_{i=1}^{N} \cup \{|a\rangle\}_{a=N+1}^{L}, \tag{5}$$

i.e., the general indexed states consists of both occupied and virtual states.

A. 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

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

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

Note that the two-body matrix elements are not antisymmetric yet.

B. The coupled cluster approximation

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

$$|\Psi_{\text{CC}}\rangle \equiv e^T|\Phi_0\rangle = \left(\sum_{i=0}^{n} \frac{1}{n!}T^n\right)|\Phi_0\rangle, \tag{9}$$

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

$$T = T_1 + T_2 + \cdots + T_p \tag{10}$$

$$= \sum_{ia} t_i^a a_a^\dagger a_i + \left(\frac{1}{2!}\right)^2 \sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_i a_j + \ldots, \tag{11}$$

where $t_{i\ldots}^{a\cdots}$ We will be looking at the *doubles* approximation, that is

$$T = T_{\text{CCD}} \equiv T_2. \tag{12}$$

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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.

$$E = \langle \Psi_{\mathrm{CC}} | H | \Psi_{\mathrm{CC}} \rangle. \tag{13}$$

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.

$$H|\Psi_{\mathrm{CC}}\rangle = E|\Psi_{\mathrm{CC}}\rangle. \tag{14}$$

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

$$e^{-T}H|\Psi_{\mathrm{CC}}\rangle = e^{-T}E|\Psi_{\mathrm{CC}}\rangle = E|\Phi_0\rangle. \tag{15}$$

Projecting this equation on the reference state we get

$$E = \langle \Phi_0 | e^{-T} H | \Psi_{\mathrm{CC}} \rangle = \langle \Phi_0 | e^{-T} H e^{T} | \Phi_0 \rangle, \tag{16}$$

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

$$\bar{H} \equiv e^{-T} H e^{T}. \tag{17}$$

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[1]. The one-body part of the Hamiltonian thus becomes

$$h = \sum_{pq} h_q^p a_p^\dagger a_q = \sum_{pq} h_q^p \left(\{a_p^\dagger a_q\} + \{\overbrace{a_p^\dagger a_q}\} \right) \tag{18}$$

$$= h_N + \sum_{pq} \varepsilon_i. \tag{19}$$

The two-body part yields

$$v = \sum_{pqrs} w_{rs}^{pq} a_p^\dagger a_q^\dagger a_s a_r \tag{20}$$

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

$$H = H_N + \langle \Phi_0 | H | \Phi_0 \rangle. \tag{21}$$

The energy equation thus becomes

$$E = \langle \Phi_0 | \bar{H} | \Phi_0 \rangle = E_{\mathrm{ref}} + \langle \Phi_0 | e^{-T} H_N e^{T} | \Phi_0 \rangle. \tag{22}$$

[1] Fermi vacuum corresponds to the reference Slater.

In this equation the unknowns are the cluster amplitudes

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

$$\bar{H} = H + [H, T] + \frac{1}{2}\left[[H, T], T \right] + \ldots. \tag{23}$$