Evaluation of Electric and Magnetic Molecular Properties using Canonical Coupled Cluster Method (First-year Study Note)

Hang Xu

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This note is in no way complete since I just list all topics I think I should cover then keep filling in blanks.

Rough Guide

Theoretical Aspect:

- Get familiar with the notation and formulation which already exists in ORCA
- Derive the basic HF, CC theory with these ansatz
- Density formulation of HF and CC
- $\mathbf{\Lambda}$-equations
- Z-vector ansatz
- Construct the CC Lagrangian and impose stationary conditions
- Learn about molecular properties, especially electromagnetic properties
- Current goal: evaluate the NMR shielding tensor with canonical CC ansatz

Computational Aspect:

- Read ORCA codes (CPSCF, Canonical CC and CC gradient)

0.0.1 Need a tutorial on Frozen-core Approximation

Contents