Hello hello

Håkon Kvernmoen

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Abstract

Heiie

1 Introduction

[Hastie et al., 2001]

$$F = ma \tag{1}$$

Eq. 1

2 Theory

2.1 Mathematical framework and notation

Define shortly

$$N, L, R \tag{2}$$

creation and annihilation, anitcommutators, normal order, Hamiltonian, normal order Hamiltonian,

2.2 Coupled Cluster

The exact solution $|\Psi\rangle$ is approximated by an exponential ansatz $|\Psi_{\mathrm{CC}}\rangle$

$$|\Psi\rangle \approx |\Psi_{\mathrm{CC}}\rangle \equiv e^{\hat{T}} |\Phi_0\rangle . \tag{3}$$

The operators $\hat{T} = \hat{T}_1 + \hat{T}_2 + \ldots$ acting on the ground state ansatz $|\Phi_0\rangle$ are the so-called *cluster operators* defined as

$$\hat{T}_m = \frac{1}{(m!)^2} \sum_{\substack{ab\ldots \\ ij\ldots}} t_{ij\ldots}^{ab\ldots} \{\hat{a}^\dagger \hat{i} \hat{b}^\dagger \hat{j} \ldots\} \tag{4}$$

where $m \leq N$. The scalars $t_{ij\ldots}^{ab\cdots}$ are unknown expansion coefficients called *amplitudes*, which we need to solve for. All the creation and annihilation operators of Eq. 4 anticommute, giving the restriction that

$$t_{\hat{P}'(ij\ldots)}^{\hat{P}(ab\ldots)} = (-1)^{\sigma(\hat{P}) + \sigma(\hat{P}')} t_{ij\ldots}^{ab\ldots}. \tag{5}$$

Here P and P' permutes $\sigma(P)$ and $\sigma(P')$ indices respectively. This is the reason for the prefactor of Eq. 4, since we have $m!$ ways to independently permute particle and hole indices. Instead of having $(L-N)^m N^m$ independent unknowns, we reduce this number by a factor of $(m!)^2$.

2.3 Doubles truncation

Considering N cluster operators in the exponential ansatz of Eq. 3 is not computationally feasible for realistic systems. The common practice is to include one or more $\hat{T}_m$ operators, making a truncation on $|\Psi_{\mathrm{CC}}\rangle$ as well. In the following we will include only the double excitation operator $\hat{T}_2$, know as the CCD approximation. This gives us

$$|\Psi\rangle \approx |\Psi_{\mathrm{CC}}\rangle \approx |\Psi_{\mathrm{CCD}}\rangle \equiv e^{\hat{T}_2} |\Phi_0\rangle , \tag{6}$$

$$\hat{T}_2 = \frac{1}{4} \sum_{abij} t_{ij}^{ab} \{\hat{a}^\dagger \hat{i} \hat{b}^\dagger \hat{j}\}, \tag{7}$$

with the four-fold amplitude permutation symmetry [1].

$$t_{ij}^{ab} = -t_{ij}^{ba} = -t_{ji}^{ab} = t_{ji}^{ba} \tag{8}$$

3 Method

4 Results

5 Discussion

6 Concluding remarks

[1] For double amplitudes, the index permutation symmetry is equal to that of antisymmetrized two-body matrix elements $\langle pq||rs\rangle$.

References

Trevor Hastie, Robert Tibshirani, and Jerome Friedman. *The Elements of Statistical Learning*. Springer Series in Statistics. Springer New York Inc., 2001.