Study Plan for Thesis

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1 Chapter 1

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2 Chapter 2

2.1 Model Hamiltonian

- HDvV Hamiltonian
- Spin Hamiltonian
  - Focus on Zeeman
  - Study other stuff

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3 Chapter 3

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4 Chapter 4

- Mention how this study demonstrated that computational chemistry is about finding balance between accuray and computational cost.

4.1 BS DFT

4.2 CASSCF

- Pipek-Mezey localization scheme for double-shell orbs.

4.3 DDCI

- know the difference between DDCI1, DDCI2 and DDCI3.
- read about T_{sel} parameter.

4.4 BS Coupled Cluster

- Need to read on the CC ansatz and how it works.
- Know the difference between CCSD and CCSD(T).
- Read local methods and how they work.
- difference between LPNO and DLPNO.
- difference between all the parameters in LPNO approx: T_{CutPNO}, T_{CutPair} and the 3rd one. (see ORCA docs)

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5   Chapter 5

6   Chapter 6