

COMPUTATIONAL CHEMISTRY II EXAMINATION
ATTEMPT ALL QUESTIONS. TIME: THREE HOURS

Question 1. (20 Marks)

Set up KS equations for a) He ground state, b) H atom ground state.

Question 2. (20 Marks)

. How would you proceed to calculate the electron-nucleus spin coupling constant in the Li atom (ground state)?

Question 3. (20 Marks)

For two electron atoms with closed shell ground state, obtain the expression for $E^{(2)}$.

Question 4. (20 Marks)

How would you proceed to calculate the electron-nucleus spin coupling constant in the Li atom (ground state)?

Question 5. (20 Marks)

Set up MCSCF equation for a two electron two orbital problem, assuming a singlet ground state.