Homework for Lecture 4, Configuration Interaction

1. Multiply both sides of the CI Schrödinger equation on the left by $\langle \Phi_i^a |$ and simplify. What does the result tell you about the CI coefficients of different excitations? What can you infer about all higher order excitation coefficients?

2. Suppose you have a system with 6 electrons, and 20 basis functions. How many $\langle \Phi_m^e | H_c | \Phi_i^a \rangle$ matrix elements are there in the upper triangle of the full-CI matrix? What about the $\langle \Phi_{mn}^{ef} | H_c | \Phi_{ijkl}^{abcd} \rangle$ block?

3. Derive the CID coefficient equation from the notes using KM notation (time consuming)

4. Explain why computing a potential energy surface with CISD is a stupid idea. (hint: size consistency)