Homework #6

(due Wednesday, May 29, 2024)

1. (10 pts) Consider the Li atom.

   (a) Write down the Hamiltonian describing this system
   (b) Write down the wave function describing this system in terms of one-electron functions
   (c) What is the unperturbed energy?
   (d) If we are to use perturbation theory to calculate the energy correction, what direct integrals J and exchange integrals K describing Coulomb and exchange interactions would need to be taken into account?

2. Reading assignment: Chapter 10.1-10.4, 11.1-11.3 of B&J. Also take a look at the posted JCP 1933 –calculations of the energies (using different methods) for the hydrogen molecule !