

Homework-2

Consider the lithium atom, with atomic number 3. You have at your disposal the following basis functions: 1s, 2s and 2p (consider only one component of the 2p orbital, for example 2p_x)

1. How many spin orbitals can you generate with these three basic functions?
2. How many determinants can you generate in total?
3. Write down one Slater determinant for each possible spin multiplicity that you can generate with three electrons and write down their energy in terms of one-electron energy, Coulomb and exchange integrals.