PHY403 Atomic and Molecular Physics Aug-Dec 2019: Tutorial 4

Dr. Kavita Dorai, Department of Physics, IISERM, kavita@iisermohali.ac.in

- 1. Apply the variational techniques used to find the ground state of helium, to find the best upper bound on E_g for the case of H⁻ and Li⁺ ions. Each has two electrons like helium but with nuclear charges Z=1 and Z=3, respectively.
- 2. The operator S^2 is the square of the total spin angular momentum of two electrons $S^2 = (s_1 + s + 2)^2$. Given that $\alpha(i)$ and $\beta(i)$ are the eigenfunctions for spin up(down) state of each electron, show that $\alpha(1)\alpha(2)$ and $\beta(1)\beta(2)$ are each eigenfunctions of the operator S^2 . What is the eigenvalue in each case?
- 3. Consider a system with three spin-1/2 particles with individual spin states (up and down) $|\alpha\rangle$ and $|\beta\rangle$. Consider a state such as $|\alpha\rangle|\alpha\rangle|\beta\rangle$ (with two spins up and one spin down), which is totally symmetric under any exchange of spin. Write down three other such totally symmetric states. Show that it is not possible to construct a linear combination of products of individual spin states which is totally antisymmetric.
- 4. Write a Slater determinant for the $1s^22s^22p^1$ ground state of the Boron atom. Be very specific in your labels. Is your Slater determinant an eigenfunction for the exact Hamiltonian?
- 5. Briefly explain what is the term quantum defect used in the description of the alkali atom energy levels. The sodium atom has atomic number Z=11. Write down the complete configuration of the ground 3s level. Find the quantum defect of this level, given that the first ionization potential of sodium is 5.14 eV.