Session 1 - Background check. This session is intended to be a reminder of topics you should already be comfortable with.

1. Consider an electron in a central Coulomb potential, i.e. a hydrogen like atom, with the following hamiltonian:

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{Ze^2}{r} = -\frac{\hbar^2}{2m}\frac{1}{r}\partial_r^2 r + \frac{\hat{L}^2}{2mr^2} - \frac{Ze^2}{r} \tag{1}$$

with $Z = 1$ for a single proton.
a) Show that eigenvalue equation can be separated into radial and angular parts: $\Psi(r, \theta, \phi) = \Phi(r)Y(\theta, \phi)$. Rewrite the radial equation in a more compact form by scaling the solution with r: $\Phi(r) = u(r)/r$.
b) Transform the radial equation so that it is dimensionless by defining a unit of length r_0 and unit of energy E_0. What is the asymptotic behavior of the radial function?
c) The eigenfunctions of the above hamiltonian are what we call the orbitals of the hydrogen-like atom. What are the degeneracies of this hamiltonian?
d) Assume an electron in the ground state orbital. Comment on the symmetry of this orbital. How about the first excited state? What is the energy required to excite the electron into the first excited state in the units of E_0?
e) Assume a hydrogen-like atom with $Z = 7$, with seven bound, non-interacting electrons with spin, i.e. a hydrogen-like nitrogen. What is the ground state wavefunction? Comment on the symmetry and degeneracy of the ground state wavefunction. How does it compare with the real nitrogen atom? How can you modify your non-interacting electron hamiltonian to reflect better the experimental situation ?

2. Assume two identical hydrogen-like atoms, with one electron each, at finite distance R apart, i.e. a hydrogen-like-atom-dimer, with non-interacting electrons.
a) Write a parametrized hamiltonian in the basis of the single-atom ground state orbitals. Solve the eigenvalue equation of this hamiltonian and sketch the eigenfunctions.
b) Comment on how the eigenvalues depend on the interatomic distance. Comment on how the hybridization of the single atom orbitals per site depend on the parameters of the hamiltonian.
c) Does this hamiltonian commute with the angular momentum operator? Does it commute with the parity operator?

3. Let us now assume a hydrogen-like-nitrogen dimer, each atom with 7 electrons.
a) What are the assumptions in this problem that allows us to reduce the problem such that we only consider the "valance" electrons? (Let us define the valance electrons as the ones that occupy the 2s and 2p levels)
b) Write the parametrized hamiltonian for the valance electrons in the basis of the single atom orbitals. Solve the eigenvalue equation.

4. Consider an equally spaced triangular configuration of three hydrogen-like atoms: the hydrogen trimer.
a) Write the parametrized hamiltonian in the basis of single atom orbitals. Comment on the degeneracies of the system.

b) Using the symmetry of the system, i.e. the commutation of the hamiltonian with the symmetry operator, find the eigenvalues and eigenfunctions of the trimer.
c) The hamiltonian of this system corresponds to the one of 3-hydrogen-chain with periodic boundary conditions. In this picture, show that the eigenfunctions can be written in the form of travelling/standing waves.

5. Generalize the solution of the trimer to an N-hydrogen ring with d interatomic distance.
   a) What is the general form of this hamiltonian?
   b) What is the symmetry operator that commutes with the hamiltonian?
   c) What is the spectrum of the eigenvalues? What is the degeneracy?
   d) Sketch the eigenfunctions of this hamiltonian.
   e) Consider the N-atom-ring as the N-atom-chain with periodic boundary conditions. Show that the eigenfunctions can be written in the form of travelling/standing waves. Plot the energy as a function of the wavenumber k.
   f) Consider the limit where $N \to \infty$ for the fixed interatomic distance. Determine the eigenvalues and eigenfunctions of the hamiltonian. How does your solution relate to the Bloch Theorem?

The End.