10/28/16

QUANTUM MECHANICS (471)
PROJECT Atoms (hand in November 21)

Write a computer program using the diagonalization method that solves the differential equation for the radial wave function at negative energy for the effective potential an electron experiences in an atom. Use a smooth function to go from $-Z/r$ at small r to $-1/r$ at large r. Do this problem for the case $Z = 10$ (neutral Neon atom). Find the lowest eigenvalues of this potential consistent with the number of electrons that you are considering, *i.e.* you should find all the eigenvalues relevant for putting all the electrons in according to the Pauli principle. Be sure that you check whether your results are reasonably stable with respect to the grid step size and the total size of the grid.
Report the values of your single-particle energies and compare with the experimental ionization energies for neon. In fact, you might consider "optimizing" your interpolating function to get these numbers approximately right. Also, plot all the **normalized** wave functions of the occupied states and compare them on the same scale with the hydrogen-like wave functions. Comment on the differences. It may be wise to start this project by doing the helium atom first. You can do this project with a partner but I want to be informed about this before you start.