QUANTUM MECHANICS II (524)
PROJECT Hartree-"Fock" (hand in May 1)


Start by writing a computer program 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.
Note that you can either use the Numerov method (see below) or use the diagonalization procedure used earlier. Because of the long range of the Coulomb potential, there is some issue concerning the size of the grid that you need to explore in the diagonalization (for a more appropriate strategy see secs 10.2.3 and 10.2.4 of my book in the library). When using the Numerov method, you can still integrate the wave functions outward as for scattering (but now for negative energy). You will have to consider an appropriate boundary condition in the domain where the potential becomes negligible. Some relevant material was discussed earlier in the course and can also be found in the Gottfried book Ch.3.6b. In practice, this means that when you integrate the wave function out for a certain **chosen** (negative) energy, the wave function will usually go to either plus or minus infinity for large distances. That chosen energy will **not** be an eigenvalue, since the eigenfunctions must be localized and normalizable. Vary the energy until the wave function changes to the opposite behavior, $i.e.$ if it went to plus infinity before, it now goes to minus infinity. Somewhere between the two last considered energies will be the energy of the bound state. You can make this more precise by continuing this process. So finding the eigenvalues requires a search for the energies that allow the boundary condition to be fulfilled in turn leading to a discrete set of bound-state energies. 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.
In the next step of this project, use the above wave functions to generate a new

Hartree potential (see class slides) for each occupied orbit. Make a orbit dependent correction to simulate the Pauli principle that would be incorporated when the Fock term is included. Solve for the new wave functions and repeat this process until the results are self-consistent. Compare the wave functions with the plot in the slides and report the energies of the occupied levels.

It may be wise to start this project by doing the helium atom first.