Homework3: Bound states in the central potential I

Compute energies of the bound states in central potential of the nucleus with charge Z.

Verify that your algorithm can compute energies of bound states of any atom found in nature. For example, lawrencium with $Z = 103$ has the following configuration of electrons: $Rn\ 5f^{14}\ 7s^2\ 7p^1$. You have to find energy of $5f$, $7s$ and $7p$ oribitals (use $Z = 1$ when computing bound states since large nucleous charge Z is always screened by electros in inner shells).

The implementation might follow these steps (fell free to do it in your own way):

- call SciPy routine `integrate.odeint` to integrate the one-electron Schroedinger equation

$$-u''(r) + \left(\frac{l(l+1)}{r^2} - \frac{2Z}{r}\right) u(r) = \varepsilon u(r). \tag{1}$$

  Here $\psi_{lm}(\vec{r}) = \frac{u(r)}{r} Y_{lm}(\hat{r})$, distance is measured in units of bohr radius and energy

units is Rydberg ($1Ry = 13.6058...eV$)

- The boundary conditions are $u(0) = 0$ and $u(\infty) = 0$. Use shooting method to obtain wave functions:
  - Use logarithmic mesh of radial points for integration. Start integrating from a large distance ($R_{max} \sim 100$). At R_{max} choose $u = 0$ and some nonzero (not too large) derivative.
  - Integrate the Schroedinger equation down to $r = 0$. If your choice for the energy ε corresponds to the bound state, the wave function at $u(r = 0)$ will be zero.
- Start searching for the first bound state at sufficiently negative energy (for example $\sim -1.2Z^2$) and increase energy in sufficiently small steps to bracket all necessary bound states. Ones the wave function at $r = 0$ changes sign, use root finding routine (for example `optimize.brentq`) to compute zero to very high precision. Store the index and the energy of the bound state for further processing.
- Ones bound state energies are found, recompute $u(r)$ for all bound states. Normalize $u(r)$ and plot them.
- Compute electron density for various atoms (for example He, Li, ..) neglecting Coulomb

repulsion:

– Populate first Z lowest laying electron states and compute $\rho = \sum_{lm \in occupied} u_{lm}^2(r)/(4\pi r^2)$. Each state with quantum number l can take $2(2l+1)$ electrons. Be carefull, if atom is not one of the Nobel gases (He, Ne, ...) the last orbital is only partially filled.