

Homework2: 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 $7p$ orbitals (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

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

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. Once 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.
- Once 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.