

hydrogen atom: center-of-mass and relative

2-particle problem (electron & proton)

$$\left[-\frac{\hbar^2}{2m_e} \Delta_e - \frac{\hbar^2}{2m_p} \Delta_p + V(|\vec{r}_e - \vec{r}_p|) \right] \Psi(\vec{r}_e, \vec{r}_p) = E \Psi(\vec{r}_e, \vec{r}_p)$$

separation in center-of-mass and relative coordinates

$$\vec{R} = \frac{m_e \vec{r}_e + m_p \vec{r}_p}{m_e + m_p}$$

$$M = m_e + m_p$$

$$\vec{r} = \vec{r}_e - \vec{r}_p$$

$$\mu = \frac{m_e m_p}{m_e + m_p}$$

$$-\frac{\hbar^2}{2M} \Delta_R S(\vec{R}) = E_{\text{CM}} S(\vec{R}) \quad \left[-\frac{\hbar^2}{2\mu} \Delta_r + V(|\vec{r}|) \right] \psi(\vec{r}) = E_H \psi(\vec{r})$$

$$\Psi(\vec{r}_e, \vec{r}_p) = S(\vec{R}) \psi(\vec{r}) \quad \text{and} \quad E = E_{\text{CM}} + E_H$$

hydrogen atom: spherical separation

relative motion

$$\left[-\frac{\hbar^2}{2\mu} \Delta_r + V(|\vec{r}|) \right] \psi(\vec{r}) = E_H \psi(\vec{r})$$

spherical symmetry

$$\psi(\vec{r}) = \frac{u(r)}{r} Y_{l,m}(\theta, \phi)$$

$$\left(-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{\hbar^2}{2\mu} \frac{l(l+1)}{r^2} - \frac{e^2}{4\pi\epsilon_0 r} \right) u(r) = E_H u(r)$$

dimensionless units: $\rho = \kappa r$ with $\kappa^2 = 2m|E|/\hbar^2$ and $\rho_0 = 2me^2 / (4\pi\epsilon_0 \hbar^2 \kappa)$

$$\left(\frac{d^2}{d\rho^2} - \frac{l(l+1)}{\rho^2} + \frac{\rho_0}{\rho} - 1 \right) u(\rho) = 0$$

hydrogen atom: radial solution

ansatz (solve asymptotics)

$$u(\rho) = \rho^{l+1} w(\rho) e^{-\rho}$$

differential equation for $L(s)$:

$$\rho \frac{d^2 w}{d\rho^2} + 2(l+1-\rho) \frac{dw}{d\rho} + (\rho_0 - 2(l+1))w = 0$$

ansatz: power series

$$w(\rho) = \sum_{k=0}^{\infty} a_k \rho^k$$

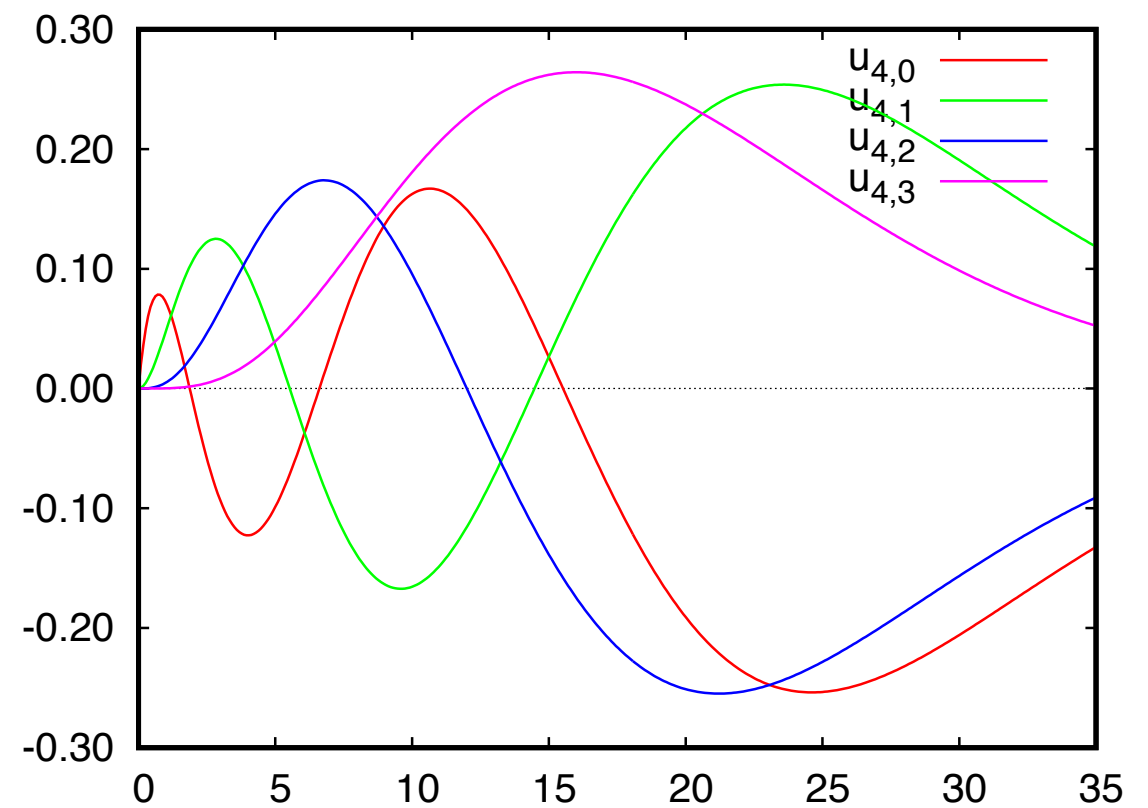
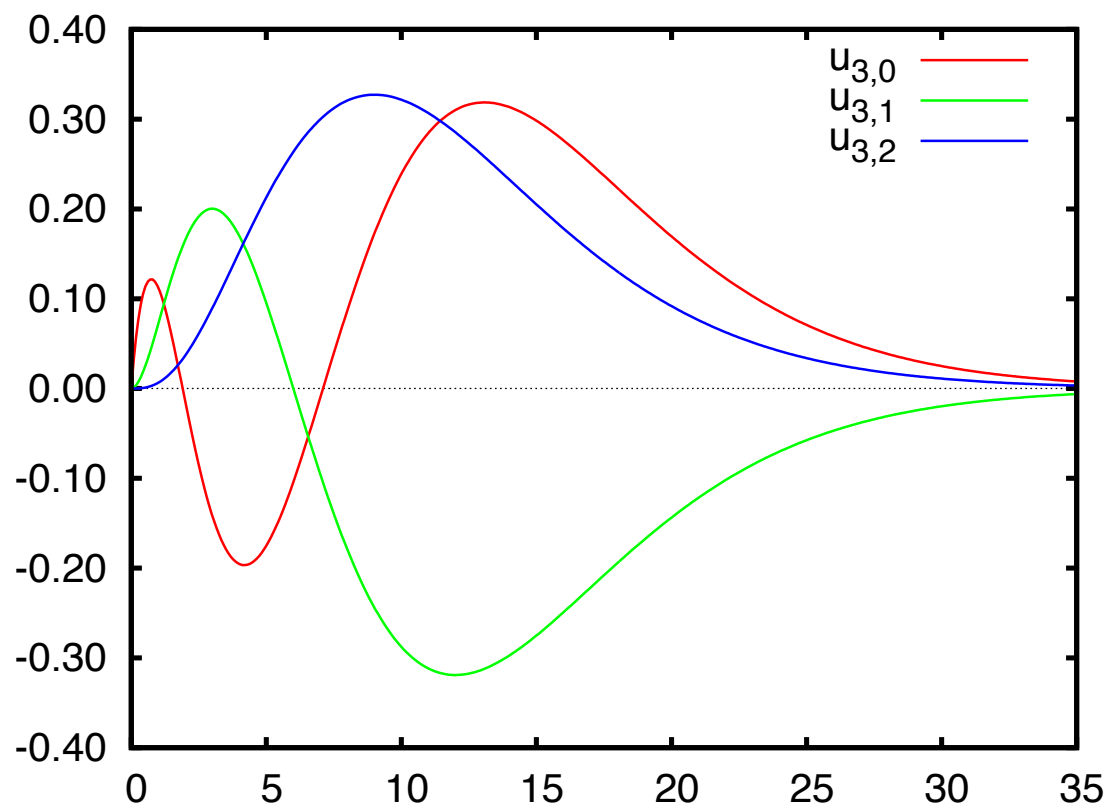
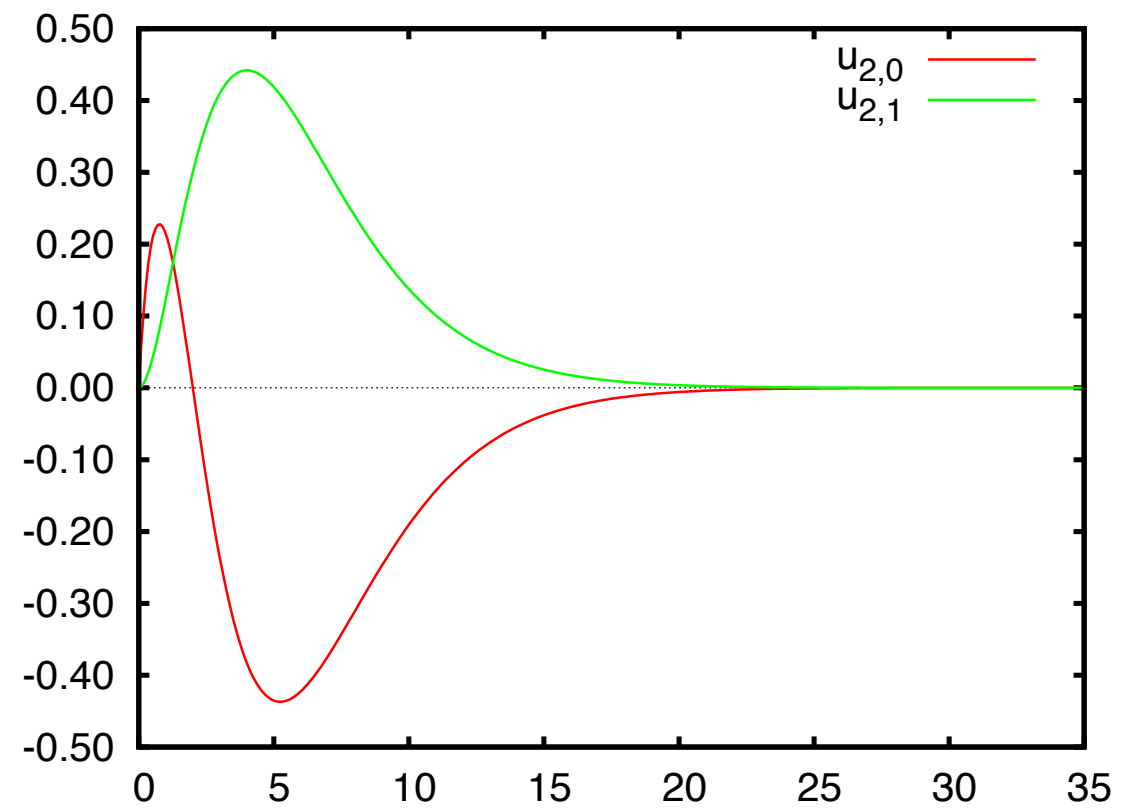
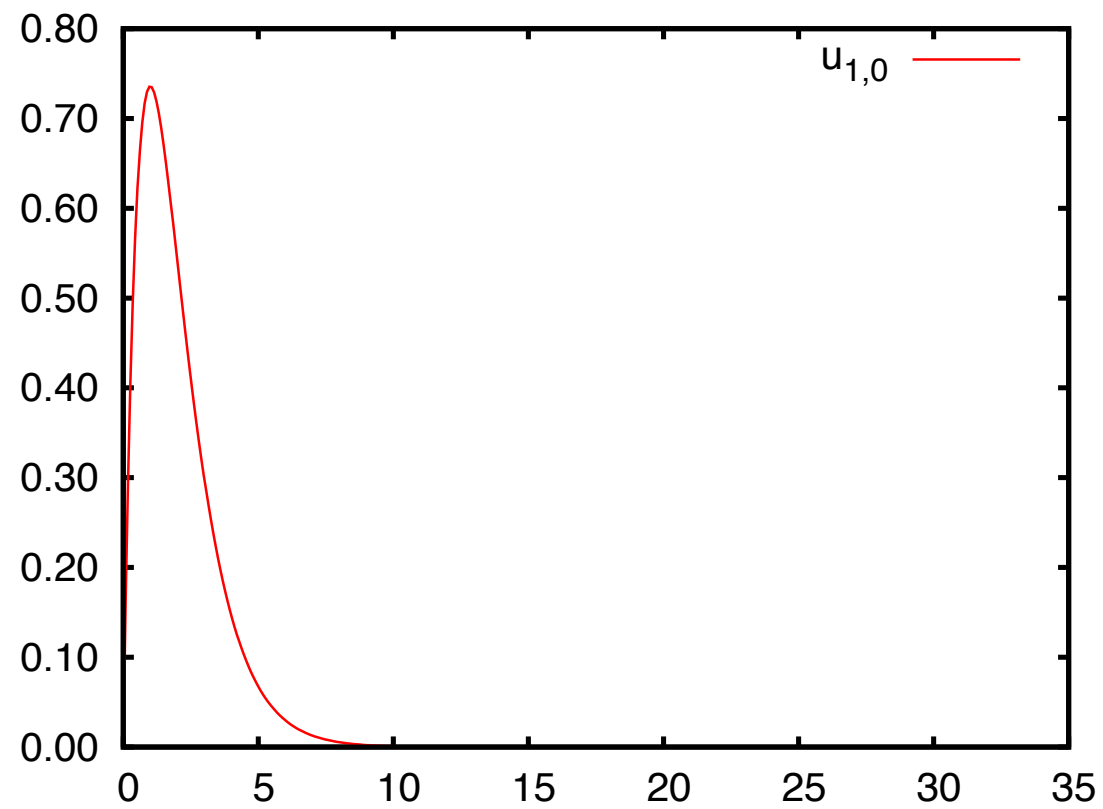
recursion for coefficients

$$a_{k+1} = \frac{2(k+l+1) - \rho_0}{(k+1)(k+2l+2)} a_k$$

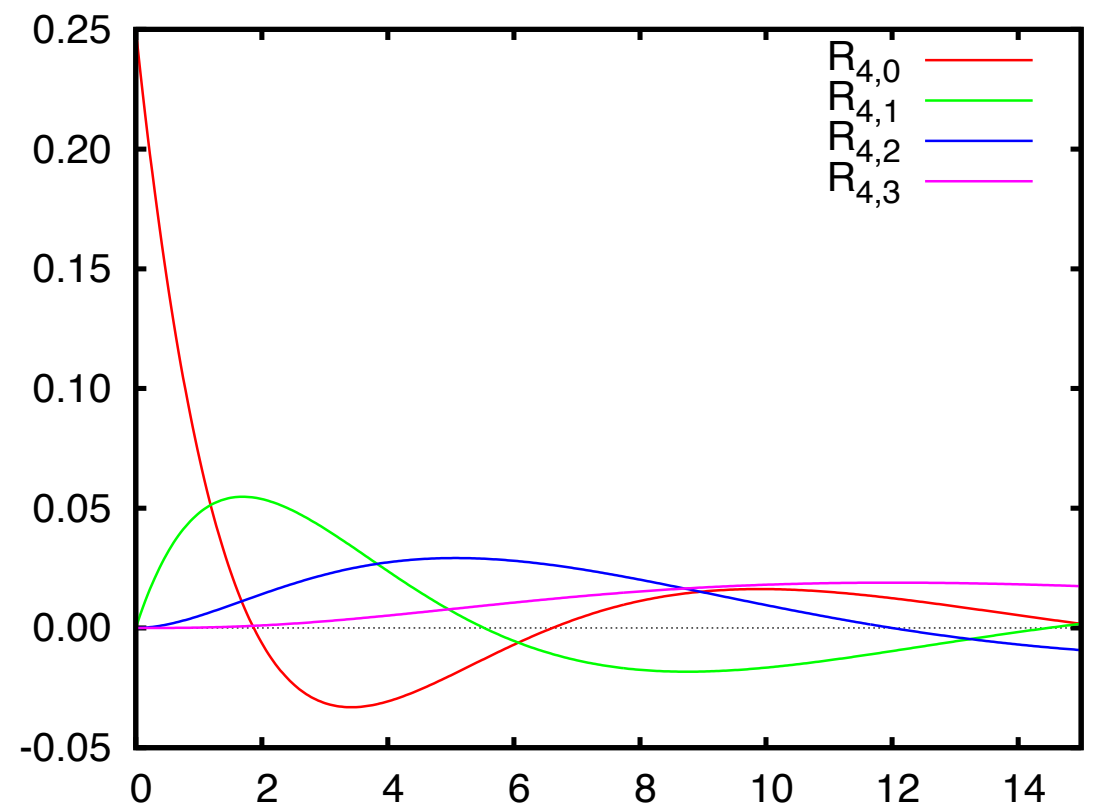
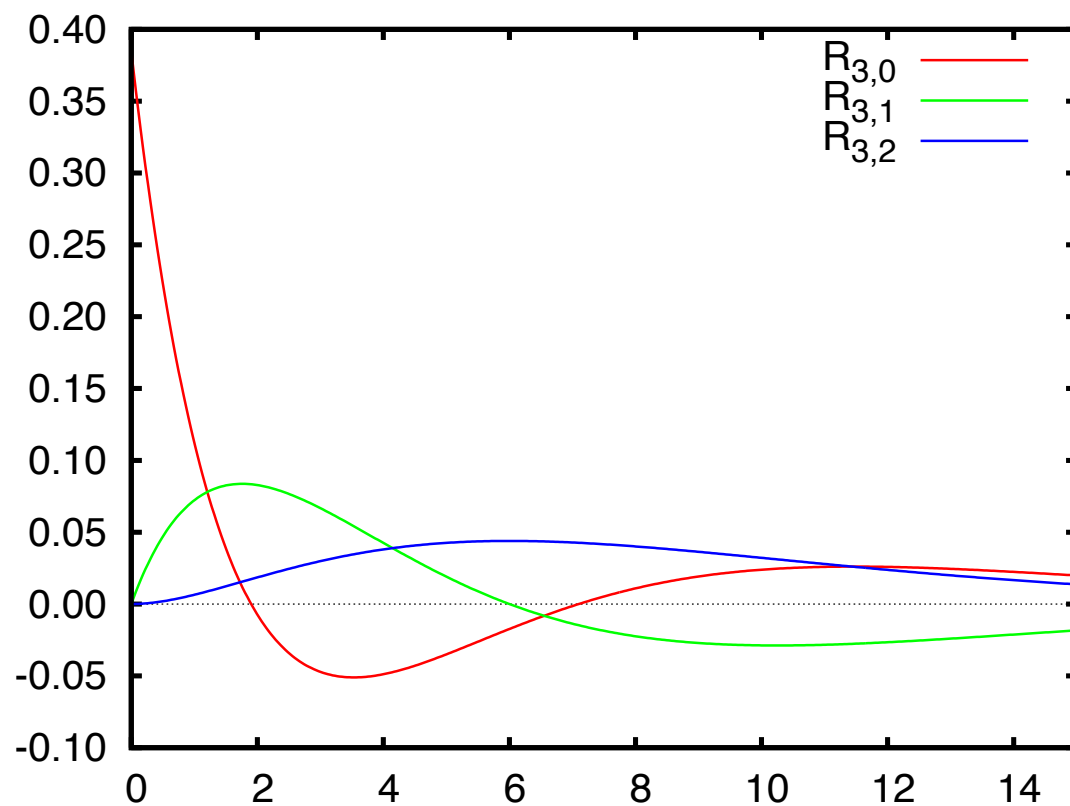
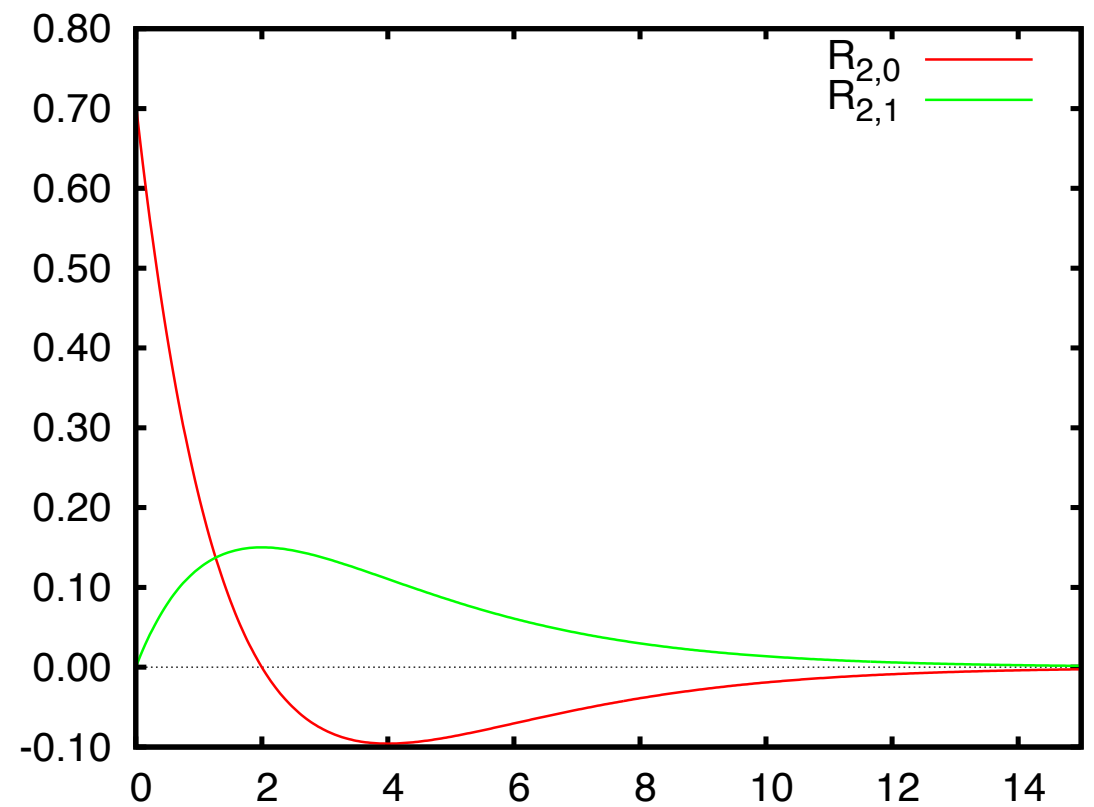
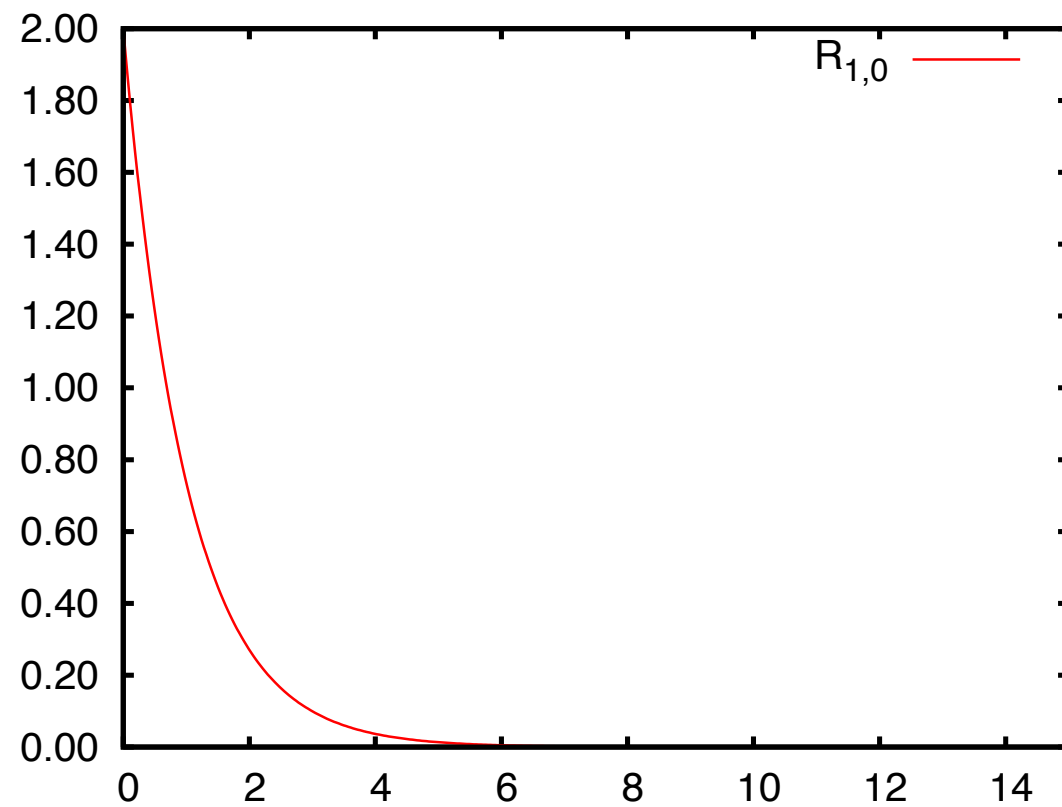
normalizability: recurrence must terminate at some finite k

$$n \geq l+1$$

radial functions $u_{nl}(r) = r R_{nl}(r)$



radial functions $R_{nl}(r)$



A simplified periodic table diagram. The first column (Hydrogen) is a single yellow square. The second column (Helium) is a single yellow square. The next 10 columns (Lithium to Neon) are green. The next 10 columns (Sodium to Argon) are red. The final 10 columns (Potassium to Xenon) are blue. The blue block is arranged in a way that suggests the noble gas configuration, with the last column having 18 elements (Potassium to Xenon) and the previous columns having 10 elements (Sodium to Argon).

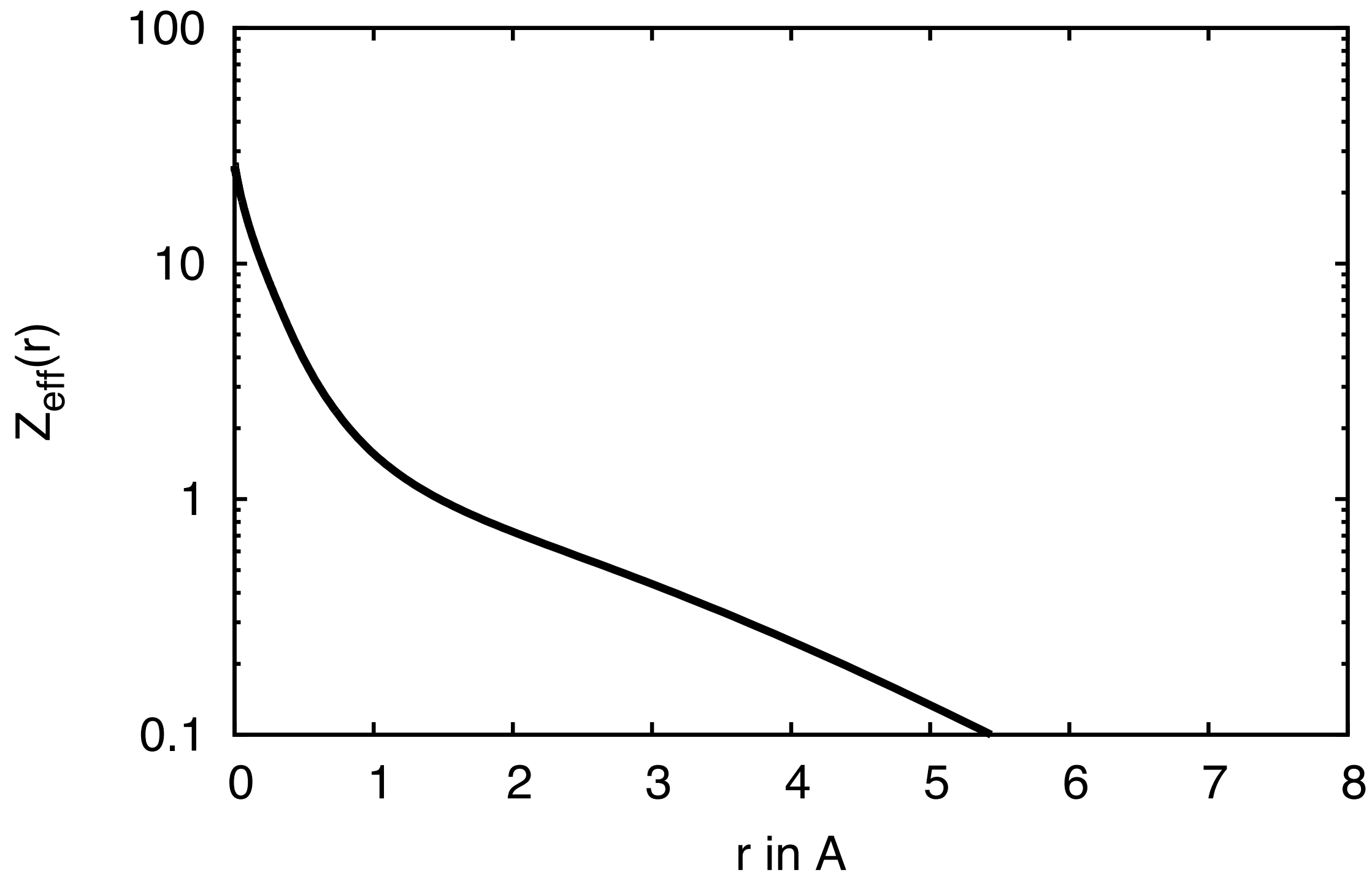
The diagram illustrates the relative sizes and shapes of atomic orbitals for principal quantum numbers $n = 1$ through $n = 7$. The orbitals are color-coded: yellow for s orbitals, red for d orbitals, blue for p orbitals, and green for f orbitals. The orbitals are arranged in a grid, with the principal quantum number n indicated on the left and right sides. The orbitals are labeled as follows:

- s orbitals (yellow):** 1s, 2s, 3s, 4s, 5s, 6s, 7s. The size increases significantly with n . The 6s and 7s orbitals are shown with a single black dot at the center, indicating the nucleus.
- p orbitals (blue):** 2p, 3p, 4p, 5p, 6p. The size increases with n . The 2p orbitals are shown as three dumbbell-shaped lobes.
- d orbitals (red):** 3d, 4d, 5d, 6d. The size increases with n . The 3d orbitals are shown as five cloverleaf-shaped lobes.
- f orbitals (green):** 4f, 5f. The size increases with n . The 4f orbitals are shown as complex, multi-lobed shapes.

The diagram shows that the size of the orbitals increases rapidly with the principal quantum number n . The s orbitals are spherical, while the p, d, and f orbitals have more complex, directional shapes. The 6s and 7s orbitals are shown with a single black dot at the center, indicating the nucleus.

atom in spherical mean-field approximation

Fe : [Ar] 3d⁶ 4s² 4p⁰



Atom- und Hybrid-Orbitale

