

Exercise Sheet 2

1. *integrating the radial Schrödinger equation for a spherically symmetric potential*
 - i. Plot some of the radial functions $u_{nl}(r)$ of hydrogen and the corresponding $v_{nl}(x)$ on a logarithmic grid.
 - ii. Implement the Numerov integration for the radial Schrödinger equation on a logarithmic grid for a general radial potential $V(r)$ given on the grid.
 - iii. Assuming a hydrogen potential $V(r) = -1/r$, integrate the radial Schrödinger equation for a given l outwards for an exact eigenenergy $E_n = -1/2n^2$ and compare the wavefunction to the exact solution $u_{nl}(r)$. What is a good starting point r_{\min} for the integration and how do you initialize the first two points? How far should you integrate? What happens when you integrate too far? Why? How do accuracy and stability of the Numerov integration depend on the density of the grid points? Plot your solutions.
 - iv. Repeat the previous steps, but now integrate inwards from some r_{\max} .
 - v. For a given energy E , integrate from r_{\min} outwards and from r_{\max} inwards to some matching point r_M , e.g., close to a classical turning point, $V(r_M) = E$. Normalize the two solutions such that $u^{\leftarrow}(E; r)$ and $u^{\rightarrow}(E; r)$ such that they agree on the matching point. When E is not an eigenvalue the resulting continuous function $u(E; r)$ has a kink, i.e., a discontinuity in the first derivative, at r_M . Vary E until the kink disappears. Count the nodes in the eigenfunction to find the principal quantum number.