

Exercise Sheet 2 due 23 April 2018

1. *integrating the radial Schrödinger equation for a spherically symmetric potential*
 - i. Plot the radial functions of hydrogen on a logarithmic mesh.
 - ii. Implement the Numerov integration for the radial Schrödinger equation on a logarithmic mesh for a general radial potential $V(r)$ given on the mesh.
 - 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 mesh 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. Compare the logarithmic derivatives of the two solutions at one of the classical turning points $V(r_M) = E$. Change E until they match. Count the nodes in the eigenfunction to find the principal quantum number.
 - vi. Plot the numerical eigenfunctions $u_{nl}(r)$ for $n = 1, 2, 3$ and $l = 0, 1, 2$ vs. r and on the logarithmic mesh and compare the numerical eigenvalues to the exact solutions. How does the accuracy depend on r_{\min} , r_{\max} , the spacing of mesh points and on how you initialize the wavefunctions?