Exercise Sheet 4

1. *Hartree potential*

Calculate the electrostatic potential of a spherically symmetric charge distribution.

i. Write down the charge density of an electron in an s-orbital in terms of its radial function $u_{n,0}(r)$.

ii. Find the electric field strength generated by this spherically symmetric charge density as a function of r in terms of the charge $Q(r) = 4\pi \int_0^r \rho(r')\, r'^2 dr'$ inside a sphere of radius r.

iii. Show that the Hartree potential is given by

$$V_{\mathrm{H}}(r) = \int_r^\infty dr'\, \frac{Q(r')}{r'^2}\,,$$

Assume that $Q(r) = Q_{\mathrm{tot}}$ for $r > r_{\mathrm{max}}$. Show that for $r_> > r_{\mathrm{max}}$ we have the simple Coulomb potential: $V_{\mathrm{H}}(r_>) = Q_{\mathrm{tot}}/r_>$, where the total charge is given by the number of electrons N. For a radial functions given on a grid up to r_{max} we can thus write

$$V_{\mathrm{H}}(r) = \int_r^{r_{\mathrm{max}}} dr'\, \frac{Q(r')}{r'^2} + \frac{N}{r_{\mathrm{max}}}\,.$$

iv. Calculate the Hartree potential arising from an electron (in a hydrogen atom) with $n = 1, 2, 3$ and $l = 0$ (1s, 2s, and 3s).

v. Write a routine that calculates from a radial function $u(r)$ given on a logarithmic grid the spherically averaged Hartree potential.