

**Exercise Sheet 4** due 14 May1. *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

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

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

$$V_H(r) = \int_r^{r_{\text{max}}} dr' \frac{Q(r')}{r'^2} + \frac{N}{r_{\text{max}}}.$$

- 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 mesh the spherically averaged Hartree potential.