

Exercise Sheet 5 due 28 May 20181. *Self-consistent Hartree calculation*

Perform a self-consistent Hartree calculation (i.e. assuming that there is no exchange-correlation potential) for a Helium atom ($Z = 2$) with two electrons (of opposite spin) in the $1s$ orbital.

- i. start with a potential $V(r) = -Z/r$
- ii. solve the radial Schrödinger equation for the occupied orbitals
- iii. calculate the Hartree potential $V_H(r)$ arising from the occupied orbitals
- iv. obtain the radial potential for the next iteration by linear mixing $V(r) \leftarrow (1 - \alpha)V(r) + \alpha(-Z/r + V_H(r))$, with $\alpha \approx 0.5$
- v. solve the radial Schrödinger equation with the new potential for the occupied orbitals and repeat until the potential does not change any more
- vi. what happens if you make $\alpha \in (0, 1]$ very small (very large)?