Exercise Sheet 5

1. *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 ($1s^2$ configuration).

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)?