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Computational Quantum Physics
Exercise 7

FS 09
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Problem 7.1 DFT for Helium (part 1)

We want to treat the Helium atom in density functional theory. In this exercise, you will write a Schrödinger solver as well as a Poisson solver. In the following exercise, you will apply these to Helium and create a self-consistent procedure.

- First, solve the radial equation in the $l = 0$ sector for the hydrogen atom

$$\left[-\frac{1}{2}\nabla^2 - \frac{1}{r}\right] u(r) = Eu(r) \tag{1}$$

  where $u(r) = rR(r)$, $R(r)$ being the radial wave function. Use the Numerov algorithm to find the ground-state wave function and energy and compare your result with the analytical solution $E = 0.5$ a.u. and $u(r) \propto r\exp(-r)$.

- Then, implement a solver for the Poisson equation

$$\nabla^2 V_H(\mathbf{r}) = -4\pi n_S(\mathbf{r}),$$

$$\frac{d^2}{dr^2}U(r) = -\frac{u^2(r)}{r} \tag{2}$$

  where $V_H = U(r)/r$ is the Hartree potential generated by the charge distribution from the wave function and n_S denotes the density of a single orbital. A convenient choice for this integration task is the Verlet algorithm.

- Combine these parts and check the correctness by using the hydrogen atom again. Compare your numerical solution for the potential with the analytical result

$$U(r) = -(r+1)\exp(-2r) + 1 \tag{3}$$