ETH
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Computational Quantum Physics
Exercise 8

FS 09
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Submitting the fourth block: We would like to ask you to hand in the solutions to exercises 7.1 and 8.1 by May 13th, 2009.

Problem 8.1 DFT for Helium (part 2)

In the last exercise, you have programmed a solver for the radial Schrödinger and Poisson equations.

- Apply these to the Helium atom, i.e. change the nuclear potential appropriately and add the Hartree potential term. Furthermore, include the following parameterization of the exchange potential

$$V_x(r) = -\left(\frac{3u^2(r)}{4\pi^2 r^2}\right)^{\frac{1}{3}}. \tag{1}$$

  Repeat these steps iteratively until you reach a self-consistent solution.

- You should obtain the following eigenvalue and energy respectively:

$$\epsilon = -0.52\, a.u. \tag{2}$$
$$E = -2.72\, a.u. \tag{3}$$

  where the relationship between these two reads

$$E = 2\epsilon - \int dr \left(V_H(r)u^2(r) + \frac{1}{2}u^2(r)V_x(r)\right). \tag{4}$$

  Decrease your step size and/or increase the cutoff radius to check where your results are not heavily depending on these constants any more.

- In this simple case, you should not encounter convergence problems when using sensible values for step sizes, cutoff radius, etc. However, if it doesn't converge, you can damp your solution by using the following potential update

$$u_{n+1} = \delta\, u_n + (1-\delta)\, v_n, \tag{5}$$

  where u_n is the effective potential in the n-th step and v_n denotes the solution of the Poisson equation.