Return by tue 12.10. by 2 pm.

1. Calculate the total energies of hydrogen and helium atoms by using a) Thomas-Fermi (TF), b) Thomas-Fermi-Dirac (TFD), c) Hartree (HA) and d) Kohn-Sham (KS) approximations. Assume that the radial wavefunction is

$$\psi(r) = \sqrt{\frac{\alpha^3}{\pi}} e^{-\alpha r}, \tag{1}$$

where α is a variational parameter and the density is $n(r) = Z|\psi(r)|^2$, ($Z = 1$ for H and $Z = 2$ for He). Minimize the energy with respect to parameter α. Use atomic units where $\hbar = e = m = 4\pi\epsilon_0 = 1$. The unit of energy is Hartree (Ha = 27.2116 eV = 2 Ry) and the unit of lenght is Bohr radius ($a_0 = 0.529 \cdot 10^{-10}$ m). The TFD energy functional is given by Marder's equation (9.74). You will obtain the TF functional by simply omitting the exchange energy term from TFD. The Hartree energy functional is obtained by omitting the exchange energy term from KS functional. The KS functional can be obtained from TFD functional by replacing the kinetic energy by

$$T_s[n] = Z \int \psi^*(r)(-\frac{\hbar^2}{2m}\nabla^2)\psi(r)\mathrm{d}^3r.$$

Note that the external potential is $U(r) = 1/r$ in the functionals.
Compare your energies with the exact ones, H: -0.5 Ha and He: -2.8617 Ha.
Hints:

$$\int_0^\infty r^n \exp(-\alpha r)\mathrm{d}r = \frac{n!}{\alpha^{n+1}}.$$

The Laplacian for a radial function $f(r)$ is

$$\nabla^2 f(r) = \frac{\partial^2}{\partial r^2} f(r) + \frac{2}{r}\frac{\partial}{\partial r} f(r).$$

(4 points)

2. Consider a homogenous electron gas (jellium) in Hartree-Fock approximation. How does the total energy of a homogenous electron gas (jellium) change if the electron gas is completely polarized (the z-component of the spin of all the electrons is the same, say, $s_z = \hbar/2$). The total energy in Hartree-Fock approximation for a unpolarized jellium is given by Marder's equation (9.49). Calculate the density at which the electron gas would polarize spontaneously (the energy of the polarized gas is smaller than that of the unpolarized gas). Write your result in terms of density parameter r_s. This result shows that the Hartree-Fock theory fails to describe the jellium correcty at low densities. If the correlation energy is included, the electron gas stays unpolarized at all densities.

(2 points)