

Lausanne HW #2

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This is your homework for the week.

Use the ABC of DFT to find any background material that you need to do these calculations. All can be done by hand, but most will be easiest using Mathematica or something similar.

1. Hydrogenic orbitals:

- (a) A Bohr atom has the electron-electron repulsion set to 0_+ . For $N = Z = 10$, plot r_s and s as a function of r , and comment on what values are relevant to functionals.
- (b) Apply LDA exchange to the hydrogen atom, both as a pure density functional, and then as a spin density functional. Calculate the exact answer, and comment on the errors in the approximation.

2. Functional derivatives:

- (a) Calculate the functional derivative of the the von Weisacker kinetic energy functional. Set this equal to $-v(r)$, and name the resulting equation. (Assume one electron).
- (b) Show that if N is kept fixed, then $\delta A/\delta n(\mathbf{r})$ is undetermined up to a constant.

3. Coordinate scaling and the coupling constant:

- (a) Prove $E_{xc}^\lambda[n] = \lambda^2 E_{xc}[n_{1/\lambda}]$.
- (b) Using the Wigner approximation to the LDA correlation energy, and an exponential approximation for the He atom density (determining the decay parameter variationally), plot the adiabatic connection curve for the He atom within LDA. What feature of true LDA is missed in this curve?