Problem 5 (Uniform coordinate scaling in 1D)

Consider a system of N non-interacting electrons in one dimension. A uniformly scaled wavefunction Ψ_γ is defined in terms of an unscaled one, Ψ, as:

$$\Psi_\gamma(x_1, x_2, \ldots, x_N) = \gamma^{N/2}\Psi(\gamma x_1, \gamma x_2, \ldots, \gamma x_N) \tag{1}$$

a) Show that Ψ_γ is normalized provided that the unscaled wavefunction Ψ is normalized. What is the relation between the scaled density $n_\gamma(x)$ (coming from Ψ_γ) and the unscaled density (coming from Ψ)?

b) How does the non-interacting kinetic energy $T_s[n]$ scale with γ?

c) Derive the LDA for $T_s[n]$ in 1D.

d) What is the proper reduced density gradient in 1D and what is the form of the gradient expansion for $T_s[n]$?

Problem 6 (Hellmann-Feynman theorem)

Let $\hat{H}(\lambda)$ be the time-independent Hamiltonian of a system which depends on some parameter λ. The corresponding stationary Schrödinger equation then reads

$$\hat{H}(\lambda)|\Psi^\lambda\rangle = E(\lambda)|\Psi^\lambda\rangle \tag{2}$$

where $|\Psi^\lambda\rangle$ is assumed to be normalized. Show that

$$\frac{\mathrm{d}E(\lambda)}{\mathrm{d}\lambda} = \left\langle \Psi^\lambda \middle| \frac{\partial \hat{H}(\lambda)}{\partial \lambda} \middle| \Psi^\lambda \right\rangle \tag{3}$$