4. 1 dimensional homogeneous electron gas (1 point)

The Kohn-Sham orbitals for the 1D homogeneous electron gas are plane waves in one dimension, i.e.

$$\varphi(x) = \frac{1}{\sqrt{L}} \exp(ikx)$$

with L being the size of the box (the limit $L \to \infty$ is taken at the end). The Kohn-Sham energies are given as $k^2/2$.

a) Calculate the number of particles N as a function of the Fermi vector k_F and the box size L.

b) Calculate the kinetic energy per particle t_s as a function of the density $\rho = N/L$.

c) Construct the local density approximation for the kinetic energy and compare it to the functional used in problem 3 of the last problem set.

5. Fourier transformation (2 points)

The Fourier transformation of the change in the density is defined as

$$\delta\tilde{\rho}(\mathbf{k}) = \int d^3r \exp(i\mathbf{kr})\delta\rho(\mathbf{r})$$

and the inverse transformation is given as

$$\delta\rho(\mathbf{r}) = \int \frac{d^3k}{(2\pi)^3} \exp(-i\mathbf{kr})\delta\tilde{\rho}(\mathbf{k}).$$

Show that

a) $\displaystyle\int \frac{d^3k}{(2\pi)^3} k^2 \delta\tilde{\rho}(\mathbf{k})\delta\tilde{\rho}(-\mathbf{k}) = \int d^3r \left(\nabla\delta\rho(\mathbf{r})\right)^2$

b) $\displaystyle\int \frac{d^3k}{(2\pi)^3} k^4 \delta\tilde{\rho}(\mathbf{k})\delta\tilde{\rho}(-\mathbf{k}) = \int d^3r \left(\nabla^2\delta\rho(\mathbf{r})\right)^2$

Hint: $\int \frac{d^3r}{(2\pi)^3} \exp(i\mathbf{kr}) = \delta(\mathbf{k})$

6. Coordinate scaling in 1D (3 points)

When scaling a coordinate one replaces x with γx, where γ is a positive constant. Consider a system with one electron. For the wave function to remain normalized it has to scale like

$$\Phi_\gamma(x) = \gamma^{1/2}\Phi(\gamma x).$$

a) Show that $\Phi_\gamma(x)$ is indeed normalized to 1, if the original wave function Φ is normalized. How does the density scale with γ, i.e. how is $\rho_\gamma(x)$ related to $\rho(\gamma x)$?

b) How does the kinetic energy scale with γ, i.e. how is $T[\Phi_\gamma]$ related to $T[\Phi]$?

c) Comparing the results from a) and b), what does this imply for a local approximation of T as a functional of the density in one dimension?