1. Functional derivatives (3 points)

Calculate the functional derivatives of the following functionals

a) $F[\varphi] = \varphi(x_0)^n$

b) $F[\varphi] = f(\varphi(x_0))$, where f is a Taylor-expandable function

c) $F[\varphi] = \int dx\ \varphi(x)^n$

d) $F[\varphi] = \int dx\ f(\varphi(x))$, where f is a Taylor-expandable function

e) $F[\varphi] = \int dx\ f(\nabla\varphi(x))$, where f is a Taylor-expandable function

2. Hartree potential (1 point)

Show that the functional derivative of the Hartree energy

$$E_H[\rho] = \frac{1}{2}\iint d^3r d^3r' \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$$

w.r.t. the density ρ equals the Hartree potential

$$v_H(\mathbf{r}) = \int d^3r' \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}.$$

3. Local kinetic energy (3 points)

Consider a system of non-interacting spinless fermions (i.e. each level can be occupied by maximum one particle) moving in an external potential

$$v(x) = \begin{cases} 0 & 0 \le x \le L \\ \infty & \text{otherwise.} \end{cases}$$

The single-particle eigenfunctions are then given as

$$\phi_j(x) = \sqrt{\frac{2}{L}} \sin k_j x, \quad j = 1, 2, ...$$

with $k_j = j\pi/L$ and $\epsilon_j = k_j^2/2$.

a) Calculate the density for $N = 1$, 2, 5, and 10 particles. Plot the densities for $L = 5$.

b) Calculate the total kinetic energy T for each case as a function of L (the potential energy is zero).

c) The local kinetic density approximation reads

$$T_{loc}[\rho] = 1.645 \int_{-\infty}^{\infty} dx\ \rho^3(x).$$

Calculate T_{loc} as a function of L and the relative error

$$\delta T = \frac{T - T_{loc}}{T}$$

for each case.