

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 $L \rightarrow \infty$ 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. Exact exchange

(2 points)

The exact exchange (EXX) functional is given as a functional of the Kohn-Sham orbitals $\varphi_{j\sigma}$ which reads

$$E_{xc}^{\text{EXX}}[\{\varphi_{j\sigma}\}] = -\frac{1}{2} \sum_{\sigma=\uparrow,\downarrow} \sum_{j,k=1}^{N_\sigma} \iint d^3r d^3r' \frac{\varphi_{j\sigma}(\mathbf{r})\varphi_{j\sigma}^*(\mathbf{r}')\varphi_{k\sigma}(\mathbf{r}')\varphi_{k\sigma}^*(\mathbf{r})}{|\mathbf{r} - \mathbf{r}'|}$$

Show that for two electrons in a singlet ground-state this energy is equal to $-1/2E_H$. Hint: Consider which Kohn-Sham orbitals are actually occupied for this specific state.

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?