

7. General principles of TDDFT

(2 points)

- a) Can more than one potential produce the same time-dependent density?
- b) If a system is subjected to a driving potential that, after a time, returns its density to its initial value, will the potential return to its initial value?
- c) Answer question b) for an adiabatic approximation.

8. Adiabatic LDA exchange

(2 points)

The LDA exchange functional in 3 dimensions is given as

$$E_x^{\text{LDA}}[\rho] = -\frac{3}{4} \left(\frac{3}{\pi}\right)^{1/3} \int d^3r \rho^{4/3}(\mathbf{r}).$$

- a) Calculate the adiabatic LDA exchange potential $v_x^{\text{ALDA}}(\mathbf{r}, t)$.
- b) Calculate the corresponding exchange kernel $f_x^{\text{ALDA}}(\mathbf{r}, \mathbf{r}', t, t')$.
- c) Which property of f_x^{ALDA} shows that the approximation is adiabatic? Which property shows that it is a local approximation?

9. Dipole moment

(2 points)

The dipole moment of a single particle in state $\phi(\mathbf{r}, t)$ is given as

$$\mathbf{D}(t) = \int d^3r \phi^*(\mathbf{r}, t) \mathbf{r} \phi(\mathbf{r}, t).$$

- a) Give the corresponding equation for the calculation of the dipole moment of N particles in state $\psi(\mathbf{r}_1 \dots \mathbf{r}_N, t)$.
- b) Show that one can rewrite the result of a) as

$$\mathbf{D}(t) = \int d^3r \mathbf{r} \rho(\mathbf{r}, t).$$