# **Total energy of the system**

*Write expression for*[*total energy*](https://www.dsedu.org/courses/dft/tot_energy)*of the system in DFT approach (how  depends on ).*

*Literature: Parr, R.G.; Yang, W. Density functional theory of atoms and molecules. Oxford University Press, New York, 1989*

The total energy of the system has a form (see formula (7.2.10) from [1])



where  and  are electron-electron repulsion and exchange-correlation potentials, and  in the exchange-correlation energy.

The exchange-correlation energy is the integral of energy density (see formula (7.4.1) from [1])



where



The exchange density has a form (see formula (7.4.5) from [1])



and the correlation energy density is (see [2])



References:

[1] Parr, R.G.; Yang, W. Density functional theory of atoms and molecules. Oxford University. Press, New York, 1989.

[2] Perdew, J.P.; Zunger, A. Self-interaction correction to density-functional approximations for many-electron systems. *Phys. Rev. B* *23*, 5048 (1981).