**Exchange-correlation potential**

*Make*[*programming module*](https://www.dsedu.org/courses/dft/xc)*for exchange-correlation potential .*

The exchange potential in local density approximation (LDA) has a form [[[1]](#endnote-1), see Ref. 1]

The correlation potential in LDA in the form of Ceperley-Alder with Perdew-Zunger parametrization for unpolarized case has a form [[[2]](#endnote-2), Ref. 2]:

where , , , , , , , .

The exchange-correlation potential .

1. Parr, R.G.; Yang, W. Density functional theory of atoms and molecules. Oxford University. Press, New York, 1989. [↑](#endnote-ref-1)
2. Perdew, J.P.; Zunger, A. Self-interaction correction to density-functional approximations for many-electron systems. *Phys. Rev. B* *23*, 5048, 1981. [↑](#endnote-ref-2)