**Radial Kohn-Sham equation**

*Consider*[*radial KS equation*](https://www.dsedu.org/courses/dft/ks)*for H-like atom in 1s state.*

*Literature: Hartree, D.R. The calculation of atomic structures. Chapman & Hall, Ltd., London, 1957*

The radial Kohn-Sham (KS) equation for the H-like atom has a form [[[1]](#endnote-1), p.9, formula (8)]:



where  is the radial wave function,

whereas  is the KS potential,

** is the exchange-correlation potential,

the Coulomb potential from the nucleus



the electron-electron repulsion potential (the Hartree potential)



here is the electron density.

1. Hartree, D.R. The calculation of atomic structures. Chapman & Hall, Ltd., London, 1957 [↑](#endnote-ref-1)