Exercise Sheet 6 due 18 June

1. *Exchange-correlation potential*

Read the article *Parameterised local spin density exchange-correlation energies and potentials for electronic structure calculations I: Zero temperature formalism* by J.M. MacLaren, D.P. Clougherty, M.E. McHenry, and M.M. Donovan in Computer Physics Communications **66**, 383 (1991) [`http://doi.org/10.1016/0010-4655(91)90084-X`] and implement the Vosko-Wilk-Nusair parametrization for the correlation potential assuming $n_\uparrow = n/2 = n_\downarrow$ (paramagnetic electron density).

2. *LDA calculations with spherical potentials*

In the spherical-potential approximation we assume that the charge density coming from orbitals with $l > 0$ are spherically symmetric (as those with $l = 0$ are). Using this assumption, perform a self-consistent LDA calculation for iron in the configuration [Ar] $3d^6\ 4s^2$.