Physics 685 – Electronic Structure

Homework 16-17

Please read Martin, Electronic Structure, Chapter 7, especially sections 3-5. Read Martin, Chap 8.1 Come prepared to answer questions based on reading.

1. Problems 7.2 and 7.7 (or 7.8) in Martin.

2. One technical problem for solving the Kohn-Sham equation is solving for Poisson's equation – that is calculating the classical electronic potential (or Hartree potential) associated with a static charge density. Devise a numerical strategy for finding the Hartree potential of a spherical charge density based on fundamental electrostatic properties of spherical charge. This should entail an expression that can be easily integrated using the numerical trapezoid rule you have used, e.g., to calculate orbital normalizations. Added to the LDA models for exchange and correlation based on the LDA, one can use this to get a full DFT calculation for any spherical atom.

Exchange hole: real versus LDA

1. In a previous assignment, you calculated the exchange hole for a 2s2p configuration of spins, say in Boron, at two specific locations in the atom. Compare the exchange hole you obtained in "real-life" with the LDA hole based on the exchange hole (chapter 5) of an HEG at the same spin-density as that at the center of the exchange hole. How does this value compare to "reality"?