Physics 685 – Electronic Structure

Homework 6-7

Please read Martin, Electronic Structure, Chapter 5, sections intro-1. Also for the homework, look over Datta, Chapter 2. Come prepared to answer questions based on reading.

1. Martin 5.1 – playing with the definition of r_s and its value in real crystals.

2. (a) Martin 5.2 – carry out all the way through to get r_s for the valence electrons of the Silicon crystal in the diamond structure.
   (b) Get r_s for valence electrons of the sodium crystal.

3. Coding project for numerical Hydrogen atom using finite differences and shooting algorithm. For now, we want a subroutine to return $f(r_i)$ given

   - grid r_i defined somehow.
   - some guess at energy E
   - an external potential defined in terms of nuclear charge Z and optionally angular momentum l.
   - some finite size to the system L.

   It should return

   - the integrated function f_i for the system.
   - this should be normalized – for a uniform grid with $r_i - r_{i-1} = h$ we should have:
   $$\left(\sum f_i^2\right) h = 1$$
   - an estimate of the error of matching the $r = L$ boundary condition, as discussed before, being
   $$\text{error} = f_{last} - f(L) = f_{last}$$

4. Time permitting, a look at Martin 5.3, showing how the scaled version of the heg Hamiltonian arises from taking units
   $$\begin{aligned} [L] &= \frac{a_B}{r_s} \\ [E] &= \frac{\text{hartree}}{r_s^2} \end{aligned}$$
   for length and energy in the HEG Hamiltonian we discussed earlier:
   $$H = \sum_i \left\{ -\frac{\hbar^2 \nabla_i}{2m} - \frac{e^2 n}{2} \int \frac{d^3 r}{r} \right\} + \frac{e^2}{2} \sum_i \sum_{j \neq i} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}. \tag{1}$$