Exercise Sheet 8 due 2 July

1. *Spherical potential approximation*
   i. Show that the charge density of a filled shell $n(\vec{r}) = \sum_{m=-l}^{l} |\varphi_{nlm}(\vec{r})|^2$ is spherically symmetric.

   ii. Calculate the spherical average of the charge density of an open shell with quantum numbers (n, l), $n(r) = 1/4\pi \int_0^{2\pi} d\varphi \int_0^{\pi} \sin\vartheta \, d\vartheta \, n(\vec{r})$, in terms of the radial function $u_{nl}(r)$. How does it depend on the number of electrons in the shell?

2. *Slater-Condon parameters*
   i. Calculate the Slater-Condon parameters

$$F_{nl}^{(k)} = \int_0^\infty dr_1 \, u_{nl}^2(r_1) \left(\frac{1}{r_1^{k+1}} \int_0^{r_1} dr_2 \, u_{nl}^2(r_2) \, r_2^k + r_1^k \int_{r_1}^\infty dr_2 \, u_{nl}^2(r_2) \, \frac{1}{r_2^{k+1}} \right)$$

   for the $3s$ (only $k = 0$), $3p$ ($k = 0, 2$) and $3d$ ($k = 0, 2, 4$) functions of hydrogen. Give the resulting energies in Rydbergs and in eV. For a given shell (n,l), calculate the ratio of the Parameters $F^{(k')}/F^{(k)}$.

   ii. Write a routine that returns for a given radial function $u_{nl}(r)$ the Slater-Condon Parameters. Test your routine with the hydrogen wave-functions from above. Run a self-consistent calculation for iron (Fe) and compare the ratio $F^{(4)}/F^{(2)}$ for the self-consistent $3d$-orbital to that obtained for a hydrogen $3d$-function.