

Exercise Sheet 8 due 2 July 2018

1. Spherical potential approximation

- i. Show that the charge density of a filled shell $n(\vec{r}) = \sum_{m=-l}^l |\phi_{nlm}(\vec{r})|^2$ 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.