

22.2.2: ii. Exercises

1. In quantum chemistry it is quite common to use combinations of more familiar and easy-to-handle "basis functions" to approximate atomic orbitals. Two common types of basis functions are the Slater type orbitals (STO's) and gaussian type orbitals (GTO's). STO's have the normalized form:

$$\left(\frac{2\xi}{a_0}\right)^{n+\frac{1}{2}} \left(\frac{1}{(2n)!}\right)^{\frac{1}{2}} r^{n-1} e^{\left(\frac{-\xi r}{a_0}\right)} Y_{l,m}(\theta, \phi),$$

whereas GTO's have the form:

$$N r^1 e^{(-\xi r^2)} Y_{l,m}(\theta, \phi).$$

Orthogonalize (using Löwdin (symmetric) orthogonalization) the following 1s (core), 2s (valence), and 3s (Rydberg) STO's for the Li atom given:

$$Li_{1s}\xi = 2.6906$$

$$Li_{2s}\xi = 0.6396$$

$$Li_{3s}\xi = 0.1503.$$

Express the three resultant orthonormal orbitals as linear combinations of these three normalized STO's.

2. Calculate the expectation value of r for each of the orthogonalized 1s, 2s, and 3s Li orbitals found in Exercise 1.
3. Draw a plot of the radial probability density (e.g., $r^2 [R_{nl}(r)]^2$ with R referring to the radial portion of the STO) versus r for each of the orthonormal Li s orbitals found in Exercise 1.

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