Chem 3322 homework #7, due March 22, 2024

Problem 1 – harmonic oscillator wavefunctions

In class, we found that the stationary states of the 1d harmonic oscillator have the form

$$\psi_n = A_n \times \text{n}^{\text{th}} \text{ order polynomial} \times e^{-\alpha x^2} \tag{1}$$

where A_n is a normalization constant, and where

$$\alpha = \frac{m\omega}{2\hbar} \tag{2}$$

We did not derive a general formula for the polynomials, although we noted that each polynomial contains only even, or only odd, powers of x. These *could*, although its not very practical, be determined by *orthogonality*. For all of this question, express all your answers and do all your work in terms of the parameter α only. (You will need to use integral tables)

a) In particular, the second excited state ψ_2 has the form

$$\psi_2 = A_2(x^2 + c)e^{-\alpha x^2} \tag{3}$$

Find the constant c by requiring that ψ_2 be orthogonal to the ground state ψ_0.

b) ψ_2 is also orthogonal to the first excited state ψ_1. Why? (hint: symmetry)

c) Determine the normalization constant A_0 for the ground state.

Problem 2 – atomic orbitals

Do problem 6-21 from your textbook. Use Table 6.5 and the Jacobian (equation D.3).

Problem 3 – atomic orbitals

Do problem 6-30 from your textbook.