Chem 3322 homework #7 solutions

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.

Solution:

$$0 = \int \psi_2 \psi_0^* = A_0 A_2 \int_{-\infty}^{\infty} (x^2 + c)e^{-2\alpha x^2} \tag{4}$$

which means that

$$\int_{-\infty}^{\infty} x^2 e^{-2\alpha x^2} = -c \int_{-\infty}^{\infty} e^{-2\alpha x^2} \tag{5}$$

Evaluating the integrals gives

$$c = -\frac{1}{4\alpha} \tag{6}$$

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

Solution:

The orthogonality integral is

$$\int_{-\infty}^{\infty} \psi_1^* \psi_2 = A_1 A_2 \int_{-\infty}^{\infty} x(x^2 + c)e^{-2\alpha x^2} \tag{7}$$

which is zero because the integrand is an odd function of x and the domain of integration is even (and because the integral from 0 to ∞ converges).

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

Solution:

We require that

$$1 = \int_{-\infty}^{\infty} A_0^2 e^{-2\alpha x^2} \tag{8}$$

Evaluating the integral, we find that

$$A_0 = \left(\frac{2\alpha}{\pi}\right)^{1/4} \tag{9}$$

Problem 2 – atomic orbitals

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

Solution:

See the "solutions to Chapter 6 practice problems" link at the bottom of the course web page

Problem 3 – atomic orbitals

Do problem 6-30 from your textbook.

Solution:

See the "solutions to Chapter 6 practice problems" link at the bottom of the course web page