Assignment number 4 CD100 October 17, 2007 SKH

(1) The Force constant of $^{79}Br^{79}Br$ is 240N m^{-1} , Calculate the fundamental vibration frequency and zero point energy for $^{79}Br^{79}Br$.

(2) Prove that the product of two even function is even, that the product of two odd function is even, and that the product of the even and odd function is odd.

(3) Prove that the derivative of the (even) odd function is (odd) even.

(4) For harmonic oscillator show that ψ_0 and ψ_1 are orthogonal to each other.

(5) Estimate the probability of finding the oscillator out side the box for its (a) ground state (b) first excited and (c) second excited state. What will be the value when $v \rightarrow \infty$.

(6) Plot the wave functions and probability densities for the harmonic oscillator from v=0 to v=7. Comments on number on nodes as a function of v

(7) Using chain rule and trigonometric relationship among (x,y,z) and (r, θ,ϕ) express the Laplacian, $\nabla^2 = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)$ into polar co-ordinate. For clues, please refer Problem 10 (pp246) in Mcquarrie, Q.Chem.