**Supplement 4: Chemistry 6854**

**Physical Chemistry Alfred State College**

**The Quantum Harmonic Oscillator Summarized**

**Schrodinger equation:**

 ħ 2 d2 ϕ + (E-½ kx2) ϕ = 0

2μ dx2 m1 k m2

reduced mass=μ =

m1+m2 Lo = distance between m1,m2 with no tension

m1m2 x1 x2

x= (x2-x1-Lo)

Solution to equation is not straightforward because of x2 ( a non-constant coefficient). Requires

`Hermite’ polynomial and use of series solutions. ( The equation d2 ϕ - **x2** ϕ = -**λ** ϕ is actually solved)

 (**x**=αx α =[ kμ/ ħ 2 ]1/2 λ=2E) d**x2**

**Key results**

En = ħω(n + ½) , n=0,1,2… wi**t**h ω = (k/μ)1/2 an evenly spaced set of levels wiht ħω steps

[En cannot be zero otherwise x is fixed at 0 and there is no motion=>p=0, so ½ factor arises directly from Uncertainty principle since ΔxΔp > h]

ϕn = NnHn (√α\*x) exp (-αx2/2)

α =[ kμ/ ħ 2 ]1/2

Nn = normalization constant = (1/2nn!)1/2 (α/π)1/4

Hn (√α\*x) = hermite polynomial of nth order

Selection rule Δn = 1 given induced or permanent dipole

 Some hermite polynomials (z= (√α\*x)) )

 n Hn(z)

 0 1

 1 2z

 2 4z2 -2

 3 8z3 -12z

 4 16z4 -48z2 +12

 5 32z5 -16z3 +120z

The Hermite solution has several distinct properties where it is observed that the derivative of an odd function is even and the derivative of an even function is odd, and, that:

**A A**

∫ even = finite ∫ odd = 0

-A -A

a) ϕn = NnHn (√α\*x) exp (-αx2/2) alternates from even to odd function as n alternates from even to odd

b) the foregoing means that; average x= <ϕ|x|ϕ> = 0 since the product x\*ϕ2 will always be an odd function (odd\* odd= even; even\* even= even so x\*even = odd)

c) similarly average p = <ϕ|-i ħ ∂/∂x|ϕ> = 0 since the derivative of an odd is even and the derivative of an even is odd, so that we always have from the derivative operator, a product of even\*odd in the integral.