**In class, no-calculations part of exam 2: Chem 6854 Spring 2013**

Your name: \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ \_\_\_/34 pts

2 pts/problem

1. **If φ = Ceikx, express <φ\*|φ> as an integral over all space from 0🡪L. (Don’t evaluate: just set up)**
2. **If we were to `normalize φ above, what must the expression above be set equal to ??**
3. **Which expression below represents the reduced mass μ, for two masses m1 and m2 in a two-body problem ?**
4. μ= (m1+ m2)/m1m2 b) μ = (m1+ m2)2/m2 c) μ= m1m2/(m1 +m2) d) μ= m1m2/(m1+m2)2
5. **Briefly explain why spherical (r, θ,φ) rather than Cartesian (x,y,z) coordinates are used to solve the**

**Hydrogen atom Schrödinger equation.**

***If we stay with Cartesian coordinates, the potential 1/r term in the electrostatic field between proton and***

***electron requires expression as 1/(x2 +y2+z2)1/2 which is not separable, making solution of any differential equation requiring an eigen solution basically impossible. The spherical coordinates allow for expression of the field as ~ 1/r which makes separability possible.***

1. **The energy of an H atom is proportional to:**
2. -n2 b) -L(L+1)/n2 c) –mL2(L)(L+1)/n2 d) -L2/n2 e) -1/n2
3. **If = kinetic energy operator and +½ kx2 = the potential operator for a harmonic oscillator system, E = the eigen energy and ψ the wave function write down the basic form of the Schrödinger eigenvalue problem we need to solve.**

**ψ +½ kx2ψ = Eψ**

1. **The concept of a stationary wave function ψ(x) is posited in the first of the quantum postulates.**
2. **What are 2 basic requirements for the function ?**
3. continuous
4. differentiable
5. satisfies boundary conditions
6. normalizable
7. **ψhas been termed the `source code’ for all quantum systems by the instructor. In your own words briefly explain what is meant by this .**

**All physical quantities can be extracted by appropriate manipulation of ψ using the quantum operators in postulate 2**

**e.g. if you want linear momentum, you compute p = <ψ\*|ψ> = -i<ψ\*|d/dx|ψ>. Thus, ψ is a function allowing designation of the complete description of the state of a quantum system.**

1. **In your own words explain what the product ψ\*(x)ψ(x) dx represents**

**ψ\*(x)ψ(x) dx ~ the probability of a system to be at x ± dx**

**10a) The quantum equation <ψ\*(x)|ψ(x)> expresses what ? (1 pt)**

The average energy (eigen value) of the system, or just the eigen energy

**10b) For a given ψk, the above expression takes on what form when computed (1 pt)**

1. a function in x ii) a function in t iii) a constant for all k iv) a constant that changes with k

**remember that any system has several energies differentiated by a quantum number (or numbers) k**

**(for H k=n, for the rigid rotor k=J, for the harmonic oscillator, k =n etc.)**

1. **The quantum energy of a rigid rotor varies with:**
2. J(J+1) b) 1/J c) J d) J2/(1+J) e) J-1
3. **The correct expression for the energy of a quantum harmonic oscillator is:**
4. En = hωn b)En = hω(n +1) c) En = h(n + ½ )/ω d) En = hω(n + ½) e) En = μr2n(n+1)
5. **What is not true about the wave functions ψnLm (φ,θ,r) of H?**

**a)**They are all orthogonal to each other b) They are all normalized c) They all contain a function of r

d) They are composed of three separate terms: Rn(r) PL(θ)Φm (φ) e) They have alternative cos φ/sinφ and eiφ forms

(partial credit for circling (d) since ns orbits are really only functions of Rn(r) )

f) They provide exact energy solutions for all of H’s electronic states g) a-f are all true

1. **All atoms except H show a complex dependence in energy on all 4 quantum numbers, n,L,mL and ms.**

**What unique property of H allows its energy to depend only a single quantum number, n ?**

***The key property H has is that the single electron has complete and perfect centrosymmetry, whereas with just one more electron, that symmetry is destroyed, thereby lifting the degeneracy of the L and m pieces of the eigen energies for all the other elements***.

1. **Which is the correct expression for the spherical coordinate differential volume dV ?**

a)dV=r2 sin θ dφdθ dr b) dV=r sin φ dφdθdr c) dV= dx dy dz d) dV= r2 dφdθ dr e) dV= r2 sin θ cos φdφdθ dr

1. **Given that n=2 for an H atom, what are possible values of L ?**
2. **2,1,0 b) 2,1,0,-1,2 c) 1,0 d)1,0,-1 e) 2**
3. **If L= 1, what are the possible values of mL ?**
4. **1,0 b) 1,0,-1 c) 2,1,0 d) 0,-1 e) 0**