CHM 6480 – Take home exam 1
Due date: Wednesday, October 21st (by 11:59pm)
Do all of the following problems. Show your work.

1) Consider two operators A and B. Show that if

$$[A,B] = i\hbar \tag{1.1}$$

then it follows that

$$[A,B^2] = 2i\hbar B \tag{1.2}$$

2) As discussed in class, there is a recursion relationship that can be used to find the Hermite polynomials that are part of the solution to the harmonic oscillator TISE.

$$H_{n+1}(\gamma) = 2\gamma\, H_n(\gamma) - 2n\, H_{n-1}(\gamma) \qquad \gamma = \alpha^{1/2}\, x \qquad \alpha = \frac{2\pi m\nu}{\hbar} \tag{2.1}$$

and $H_n(\gamma)$ is the n^{th} Hermite polynomial (with the restriction n = 0, 1, 2, …).

a) Using the expressions for $H_2(\gamma)$ and $H_3(\gamma)$

$$H_2(\gamma) = 4\gamma^2 - 2 \tag{2.2}$$

$$H_3(\gamma) = 8\gamma^3 - 12\gamma \tag{2.3}$$

find the expressions for $H_4(\gamma)$ and $H_5(\gamma)$.

b) Using the fact that $H_0(\gamma) = 1$ is an even function in γ, and $H_1(\gamma) = 2\gamma$ is an odd function in γ, prove that for any Hermite polynomial $H_n(\gamma)$ the polynomial is even if n is an even number, and the polynomial is odd if n is an odd number. Note that a consequence of this result is that the wavefunctions that are solutions to the TISE for the harmonic oscillator also divide into even and odd functions.

3) In some applications of the harmonic oscillator (such as in perturbation theory calculations) it is of interest to evaluate integrals of the general form

$$\langle j|x^n|i\rangle \tag{3.1}$$

where $|i\rangle$ and $|j\rangle$ are harmonic oscillator wavefunctions.

Using the properties of the raising and lowering operators a^+ and a, find general expressions for the following

a) $\langle n+1|x|n\rangle$ (3.2)

b) $\langle n+3|x|n\rangle$ (3.3)

c) $\langle n+2|x^2|n\rangle$ (3.4)

4) Derive the following commutator relationship

$$[L_x,L_y] = i\hbar L_z \tag{4.1}$$

where L_x, L_y, and L_z are the operators for the components of the angular momentum vector. (Hint: It is easier to derive this result in Cartesian coordinates).

5) The time independent Schrodinger equation for a two dimensional system, in polar coordinates, may be written as

$$H\ \psi(r,\phi) = E\ \psi(r,\phi) \qquad (5.1)$$

where H = T + V, and

$$T = -\ (\hbar^2/2m)\ [\ \partial^2/\partial r^2 + (1/r)\ \partial/\partial r + (1/r^2)\ \partial^2/\partial\phi^2\ ] \qquad (5.2)$$

Show that for any potential where $V = V(r)$ (that is, for a potential whose value depends only on r and is independent of ϕ) the corresponding TISE equation can be separated into two equations, one in terms of r and the other in terms of ϕ. Give (but do not solve) the separate r and ϕ equations that are obtained.

6) Consider the following angular wavefunction for a three dimensional system with spherical symmetry

$$f(\theta,\phi) = B\ \sin\theta\ \cos\theta\ \cos\phi \qquad (6.1)$$

a) Find the value for B that makes the above function normalized.

b) Is $f(\theta,\phi)$ an eigenfunction of L_z? If your answer is yes, give the corresponding eigenvalue.

c) Is $f(\theta,\phi)$ an eigenfunction of L^2? If your answer is yes, give the corresponding eigenvalue.

7) Consider the following radial wavefunction for an electron in a hydrogen-like atom

$$R(r) = A\ [\ 1 - (r/r_0)\ ]\ \exp(-br) \qquad (7.1)$$

where A, b, and r_0 are constants.

a) Find the value of A that makes R(r) a normalized radial wavefunction.

b) Find $\langle r \rangle$, the average (expectation value) for r. You may leave your final answer in terms of A.

c) Find r_{mp}, the most probable value for the distance between the electron and the nucleus of the atom.