*Answer each question in the space provided; use back of page if extra space is needed. Answer questions so the grader can READILY understand your work; only work on the exam sheet will be considered. Write answers, where appropriate, with reasonable numbers of significant figures. You may use **only** the "Student Handbook," a calculator, and a straight edge.*

1. (15 points) The wave function for a one-dimensional harmonic oscillator has the form

$$\Psi_n(x) \;=\; A_n H_n\left(\frac{x}{\alpha}\right) exp(-x^2/2\alpha^2)$$

where $H_n\left(\frac{x}{\alpha}\right)$ is a Hermite polynomial, α is a characteristic length, and n is the quantum number. $x = (r - r_{eq})$, the position relative to the equilibrium position. Normalize the wave function with $= 2$.

Normalization requires the integral of the square of the wave function over all space to be unity:

$$\int_{-\infty}^{+\infty} \Psi_2^*(x)\,\Psi_2(x)\,dx \;=\; 1$$

The form of the wave function is found from Table 11.1 in the Handbook:

$$\Psi_2(x) \;=\; A_2\left(4\frac{x^2}{\alpha^2} - 2\right) exp\left(-\frac{x^2}{2\alpha^2}\right)$$

Substitution into the integral gives the following equation:

$$A_2^2 \int_{-\infty}^{+\infty}\left(4\frac{x^2}{\alpha^2} - 2\right)^2 exp\left(-\frac{x^2}{\alpha^2}\right)dx \;=\; 1$$

Expanding the integrand gives

$$A_2^2 \int_{-\infty}^{+\infty}\left[16\frac{x^4}{\alpha^4} - 16\frac{x^2}{\alpha^2} + 4\right] exp\left(-\frac{x^2}{\alpha^2}\right)dx \;=\; 1$$

Noting that this function is even, one may relate this integral to its half integral:

$$2A_2^2 \int_{0}^{+\infty}\left[16\frac{x^4}{\alpha^4} - 16\frac{x^2}{\alpha^2} + 4\right] exp\left(-\frac{x^2}{\alpha^2}\right)dx \;=\; 1$$

Changing variables to $y = x/\alpha$, we have

$$2A_2^2\alpha \int_{0}^{+\infty}[16y^4 - 16y^2 + 4]exp(-y^2)\,dy \;=\; 1$$

This integral is a sum of three integrals that can be found in the Handbook.

$$2A_2^2\alpha\left\{16\left(\frac{3\sqrt{\pi}}{8}\right) - 16\left(\frac{\sqrt{\pi}}{4}\right) + 4\left(\frac{\sqrt{\pi}}{2}\right)\right\} \;=\; 2A_2^2\alpha\sqrt{\pi}\{6 - 4 + 2\} \;=\; 2A_2^2\alpha\sqrt{\pi}\{4\} \;=\; 1$$

Rearranging this equation to find the value of A_2, presuming it is a real number, gives this result:

$$A_2 \;=\; \frac{1}{\sqrt{8\alpha}\,\sqrt[4]{\pi}} \;=\; \frac{1}{2\sqrt{2\alpha}\,\sqrt[4]{\pi}}$$

2. (10 points) Fill in the blanks with the proper word or phrase.

1)   The constant a in the following equation $(\hat{a}f(x) = af(x))$ is the **_eigenvalue_** of the operator $\hat{a}$.

2)   The equation $\psi(0) = \psi(a) = 0$ lists the **_boundary_conditions_** that any well-behaved wave function for the one-dimensional box of length a with infinite walls must satisfy.

3)   Unlike the quantum mechanical harmonic oscillator, the classical harmonic oscillator has a **_continuous_** energy spectrum.

4)   For the radial part of the hydrogen-atom system, one may describe it as subject to an effective potential consisting of two parts: the **_centrifugal_** potential (which varies as $1/r^2$) and the **_Coulomb_** potential, which varies as -1/r.

5)   The **_variational theorem_** states that in a quantum mechanical system, no matter what approximate wave function is substituted for the ground state eigenfunction in the following equation:

$$E = \frac{\int_{all\,space} \phi^* H \phi\, d\tau}{\int_{all\,space} \phi^* \phi\, d\tau},$$

the approximate energy is always greater than or equal to the true energy.

Score for Page

3. (15 points) Find the simplest form for the commutator of the following operators. (Put answer in the space provided; show work below the equation.

(a) $\frac{d^2}{dx^2}$ *and* x

$$\left[\frac{d^2}{dx^2},x\right]f(x) = \frac{d^2}{dx^2}(xf(x)) - x\frac{d^2f(x)}{dx^2} = \frac{d}{dx}\left(f(x) + x\frac{df(x)}{dx}\right) - x\frac{d^2f(x)}{dx^2}$$

$$= \frac{df(x)}{dx} + \frac{df(x)}{dx} + x\frac{d^2f(x)}{dx^2} - x\frac{d^2f(x)}{dx^2} = 2\frac{df(x)}{dx}$$

Thus, $\left[\frac{d^2}{dx^2},x\right] = 2\frac{d}{dx}$

(b) $\frac{d^3}{dx^3}$ *and* x

$$\left[\frac{d^3}{dx^3},x\right]f(x) = \frac{d^3}{dx^3}(xf(x)) - x\frac{d^3f(x)}{dx^3} = \frac{d^2}{dx^2}\left(f(x) + x\frac{df(x)}{dx}\right) - x\frac{d^3f(x)}{dx^3}$$

$$= \frac{d}{dx}\left(\frac{df(x)}{dx} + \frac{df(x)}{dx} + x\frac{d^2f(x)}{dx^2}\right) - x\frac{d^3f(x)}{dx^3} = 2\frac{d^2f(x)}{dx^2} + \frac{d^2f(x)}{dx^2} + x\frac{d^3f(x)}{dx^3} - x\frac{d^3f(x)}{dx^3}$$

$$= 3\frac{d^2f(x)}{dx^2}$$

Thus, $\left[\frac{d^3}{dx^3},x\right] = 3\frac{d^2}{dx^2}$

(c) $\frac{d^4}{dx^4}$ *and* y

$$\left[\frac{d^4}{dx^4},y\right]f(x,y) = \frac{d^4}{dx^4}(yf(x,y)) - y\frac{d^4f(x,y)}{dx^4} = y\frac{d^4f(x,y)}{dx^4} - y\frac{d^4f(x,y)}{dx^4} = 0$$

These two operators commute (they work on two different variables), so the simplest commutator is <u>multiplication by zero</u>.

Score for Page

4. (10 points) From the statements in column B, select the best match for each phrase in column A and put its letter in the adjacent blank. There is only one best match for each phrase.

Column A	Column B
1. If a particle can escape through a barrier of finite height, even if it does not have sufficient energy to go over the barrier, such a process is called ___m____ 2. Since the outcomes of quantum mechanical measurements have to yield real numbers, all quantum mechanical operators have to be ____e___, meaning they must have real eigenvalues. 3. The quantum mechanical model system used in the class to represent exclusively rotational motion is referred to as the ___j___. 4. In the lowest energy state of the quantum mechanical harmonic oscillator model, the probability function describing the system at zero displacement has a _____h____. 5. The function $R_{nl}^2 r^2$ describing a hydrogen atom-like molecule is called the _____g____.	a) Helmholtzian b) Radial function c) Minimum d) Holumpian e) Hermitian f) Borrowing g) Radial distribution function h) Maximum i) Rotor j) Rigid rotor k) Flex l) Transitioning m) Tunneling n) True o) Zero p) Radial component of the hydrogen wavefunciton q) Lorentzian

Score for Page

5. (15 points) For a hydrogen atom, determine <u>all distances</u> from the nucleus at which the radial distribution function for a 2s orbital is at the minimum value of zero. [You may express the result in bohrs, a_0.]

The radial part of the 2s orbital of a hydrogen atom is $R_{20}(r) \ = \ A_{20}\left(2 - \frac{r}{a_0}\right)exp(-r/2a_0)$. The radial distribution function is given by

$$D_{20}(r) \ = \ R_{20}^2\, r^2 \ = \ A_{20}^2\left[\left(2 - \frac{r}{a_0}\right)^2 exp(-r/a_0)\right]r^2$$

This function is never negative, hence the minimum value it has is zero. So, we seek all those points at which

$$D_{20}(r) \ = \ 0$$

Substitution of the exact form of the radial distribution function gives this equation

$$A_{20}^2\left[\left(2 - \frac{r}{a_0}\right)^2 exp(-r/a_0)\right]r^2 \ = \ 0$$

There are several ways this equation can be zero. The function is naturally factored, and if any of the factors is zero for a particular value of r, then this function will be zero.

The first factor that could make the function zero is if

$$r^2 \ = \ 0.$$

So, one place where the distribution function is zero is at the origin,

$$r \ = \ 0.$$

Another factor that could be zero is

$$exp(-r/a_0) \ = \ 0.$$

The exponential function is a positive function that continually decreases. It becomes identically zero when the variable $\frac{r}{a_0} \ = \ +\infty$. Thus, another point is at

$$r \ = \ +\infty.$$

The third possibility is when the remaining factor becomes zero:

$$\left(2 - \frac{r}{a_0}\right)^2 \ = \ 0$$

This is only true if

$$2 - \frac{r}{a_0} \ = \ 0$$

That gives the final place for a zero of the function

$$r \ = \ 2a_0$$

Score for Page

6. (13 points) A particle in a one-dimensional box is known to be in a superposition state, given by the following normalized wave function:

$$\Psi(x) \;=\; \frac{1}{2}\{\Psi_1(x) + \sqrt{3}\,\Psi_3(x)\} \;=\; \frac{1}{2}\left\{\sqrt{\frac{2}{a}}\,\sin\left(\frac{\pi x}{a}\right) + \sqrt{3}\sqrt{\frac{2}{a}}\,\sin\left(\frac{3\pi x}{a}\right)\right\}$$

where a is the width of the box that stretches from 0 to a. What is the expectation value of the energy when the system is in this state?

The expectation value of the energy is

$$<\hat{H}> \;=\; \int\limits_{\substack{all\\space}} \Psi^*(x)\hat{H}\,\Psi(x)dx \;=\; \frac{1}{2^2}\int\limits_{\substack{all\\space}} (\Psi_1^* + \sqrt{3}\,\Psi_3^*)\hat{H}(\Psi_1 + \sqrt{3}\,\Psi_3)dx$$

Expansion of the product gives

$$<\hat{H}> \;=\; \frac{1}{4}\left\{\int_0^a \Psi_1^*\hat{H}\,\Psi_1 dx + \sqrt{3}\int_0^a \Psi_1^*\hat{H}\,\Psi_3 dx + \sqrt{3}\int_0^a \Psi_3^*\hat{H}\,\Psi_1 dx + 3\int_0^a \Psi_3^*\hat{H}\,\Psi_3 dx\right\}$$

Knowing that each of the functions is a normalized eigenfunction of the Hamiltonian operator, this can be simplified to

$$<\hat{H}> \;=\; \frac{1}{4}\left\{E_1\int_0^a \Psi_1^*\,\Psi_1 dx + \sqrt{3}E_3\int_0^a \Psi_1^*\,\Psi_3 dx + \sqrt{3}E_1\int_0^a \Psi_3^*\,\Psi_1 dx + 3\,E_3\int_0^a \Psi_3^*\,\Psi_3 dx\right\}$$

But the eigenfunctions are an orthonormal set, The integrals of a cross product is automatically zero, and the integral of the square of any function is normalized. Using this fact, one finds the expectation value of the energy when the system is in this state:

$$<\hat{H}> \;=\; \frac{1}{4}\{E_1 + 3\,E_3\} \;=\; \frac{h^2}{32ma^2}\{1 + 3\times 9\} = \frac{28h^2}{32ma^2} = \frac{7h^2}{8ma^2}$$

Score for Page

7. (10 points) For the hydrogen atom, the quantization of the energy levels is well known. The transitions among these energy levels form a series, with each succeeding transition being closer to the one before it in the series. Because of this feature, each series is said to tend toward a limit. The Balmer series of transitions puts the electron in the state with n = 2 after emission, and the series of lines is in the visible region of the spectrum. Find the energy of that limit (in cm^{-1}) for the Balmer series.

First, the Balmer series is a set of lines, all of which end with the system in the state with $n = 2$ after emission. Hence, the energy of each transition is of the form:

$$\Delta E = R \left(\frac{1}{2^2} - \frac{1}{n^2} \right)$$

where R is Rydberg's constant and n is the quantum number of the state from which the transition originates in emission. All of the values of n are numbers larger than 2. As n increases the transition energy gets larger, until its limit is reached when n is infinity. Thus, the limit of the series is

$$\Delta E_{limit} = \frac{R}{2^2} = \frac{R}{4}$$

From Table 1.5 of the Handbook, one finds Rydberg's constant, so one gets

$$\Delta E_{limit} = \frac{10973731.568525 \ m^{-1}}{4} = 2.74343288 \times 10^6 \ m^{-1}$$

This formula gives the energy of the photon in m^{-1}, but the problem asks for the energy in cm^{-1}. We perform a unit transformation:

$$\Delta E = (\Delta E_{limit}) \frac{1 \ m}{100 \ cm} = 2.74343288 \times 10^6 \times 10^{-2} cm^{-1} = 2.74343288 \times 10^4 \ cm^{-1}$$

Score for Page

8. (12 points) For each formula in column A, find the name of a researcher (in column B) behind this formula. Insert its letter in the blank next to the formula.

Column A		Column B
1. $E = h\nu$	__h__	a. **Bohr**
2. $[x, p_x] \neq 0$	__e__	b. **de Broglie**
3. $E_n = -\left(\frac{Z^2 E_h}{2}\right)\frac{1}{n^2}$	__a__	c. **Euler**
4. $-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$	__i__	d. **Gerlach**
5. $\lambda = \frac{h}{p}$	__b__	e. **Heisenberg**
6. $re^{\pm i\Theta} = r\cos\Theta \pm ir\sin\Theta$	__c__	f. **Hermite**
		g. **Lagrange**
		h. **Planck**
		i. **Schrödinger**
		j. **Stern**

Score for Page

9. (5 points, extra credit) A particle in a n-dimensional universe is placed into an n-dimensional box with infinite potential walls and all the walls equal in length (a "cubic" n-dimensional box). What are the degeneracies of the two lowest energy levels of this system.

The energy of such a system will be (by analogy with 3D)

$$E_n = \frac{h^2}{8ma^2}\left(n_x^2 + n_y^2 + n_z^2 + \cdots + n_n^2\right)$$

In all cases and all dimensions n=1 produces the lowest possible energy level, and the degeneracy is 1. It has the energy

$$E_{lowest} = \frac{h^2}{8ma^2}n$$

The next lowest possible energy level has one of the quantum numbers (in one of the dimensions) equal to 2 and all the others will be 1. It has the energy

$$E_{secibd\ lowest} = \frac{h^2}{8ma^2}(n + 3)$$

There are a total of n such states by interchange of which quantum number is 2 (the rest having quantum number of 1). Thus, the degeneracy of the second lowest energy level in an n-dimensional box with equal sides is n.

Score for Page