Name: KEY

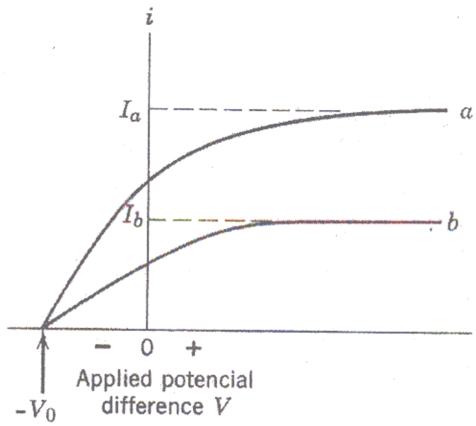
Chemistry 312
Test 1
February 28, 2008

Instructions before starting the test:

1. Write your name in the space above and on the backs of the other pages.
2. Your exam booklet should have **eight pages** total, with questions on Pages 2-7, and reference data on Page 8. Check to see you have eight pages now. If you do not, ask for another copy of the exam.
3. You may carefully remove Page 8 from your exam booklet.
4. You may fill both sides of an 8.5" x 11" sheet of paper with whatever information you would like, and refer to it during the exam.
5. You should always demonstrate your thought process in writing. You will be awarded credit only for work I can decipher.
6. You have a maximum of **2 hours and 30 minutes** to work on this exam.

Page (Possible Points)	Your Score
Page 2 (18)	
Page 3 (23)	
Page 4 (17)	
Page 5 (7)	
Page 6 (25)	
Page 7 (10)	
Total (100)	
Estimated Grade	

1. The figure at the right shows data from two photoelectric effect experiments (*a* and *b*) on the same metal. Specifically, the current *i* (not to be confused with $\sqrt{-1}$!) collected by the Faraday cup is plotted as a function of the voltage *V* applied to the cup. The figure indicates that in the limit of large positive *V*, the current in Experiment *a* is twice as large as the current in Experiment *b*. (Remember that current measures how many electrons are hitting the Faraday cup per unit time.)



(a) (6 points) How would you rationalize the experimental results at high positive V in terms of <u>Einstein's model</u> of light? Be concise, but specific.

The light in Exp a is 2x as intense; that is, 2x the # of photons hit the metal per unit time.

-4 Light has higher E_K/shorter λ in Exp a

-6 other

(b) (6 points) How would you rationalize the experimental results at high positive V in terms of the <u>19th century wave model</u> of light? Be concise, but specific.

The light in Exp a has twice the frequency / half the wavelength of the light in Exp b.

or the light in Exp. a has twice the intensity (ε^2)

Either characteristic would liberate e^-'s 2x as fast in Exp a

-5 used $E = hc/\lambda$ -3 didn't apply true principles specifically to data

-4 can't explain w/ 19th C physics

-6 no valid physical discussion

(c) (6 points) What does the quantity $-V_0$ (labeled in the above figure) tell us about the experiment? Be concise, but specific.

Stopping potential - ie the max E_K of the e^-'s generated.

$$E_{light} = \Phi + E_{K,e^-} = \Phi + (-e)(-V_0)$$

-3 tells us Φ ($-V_0$ does so only indirectly)

-4 true, but incomplete

-5 some discussion

2. Consider a one-dimensional harmonic oscillator governed by the potential $E_p = (1/2)kx^2$. The second excited state of this system is described by the energy eigenfunction $\psi = N_2(4y^2 - 2)e^{-y^2/2}$, where N_2 is the normalization constant and $y = x/\alpha$.

(a) (15 points) Find the value(s) of x at which a particle in the second excited state is most likely to be found. Express your answer(s) in terms of α.

Extrema (ie max in prob. density) where $\frac{d\psi}{dx} = 0$

Since y differs from x only by a constant, $\frac{d\psi}{dy} = 0$ at the same locations.

$$\frac{d\psi}{dy} = N_2\left[(4y^2-2)(-y)e^{-y^2/2} + 8ye^{-y^2/2}\right] = 0$$

$$N_2 e^{-y^2/2}\left[-4y^3 + 2y + 8y\right] = 0$$

$$10y - 4y^3 = 2y(5-2y^2) = 0$$

$$\Rightarrow y = 0 \quad \text{or} \quad 5 - 2y^2 = 0 \Rightarrow 2y^2 = 5 \Rightarrow y = \pm\sqrt{\frac{5}{2}}$$

$$\Downarrow \qquad\qquad \Downarrow$$

$$\boxed{x = \alpha y = 0} \qquad \boxed{x = \pm\sqrt{\frac{5}{2}}\,\alpha}$$

(2 got completely correct)

-4 1st error

-2 2nd error

→ Missed $x = 0$

→ Missed $x = -\sqrt{\frac{5}{2}}\alpha$

-2 Math error

→ Reported an extremum in $\frac{d(\psi^*\psi)}{dx} = 0$ {which is a minimum}

-9 set up correctly, but not solved (+1 for $x = 0$)

-13 some work

-9 correctly found $\langle x \rangle$

(b) (8 points) Is/are your answer(s) in part (a) consistent with the classical model of a one-dimensional harmonic oscillator? Explain. (Note: Answering <u>either</u> "yes" <u>or</u> "no" can earn you full credit, depending on how you justify your answer!)

If at least one right answer in part (a), most earned full credit here

-2 if inconsistency

-5 if no discussion of particle location

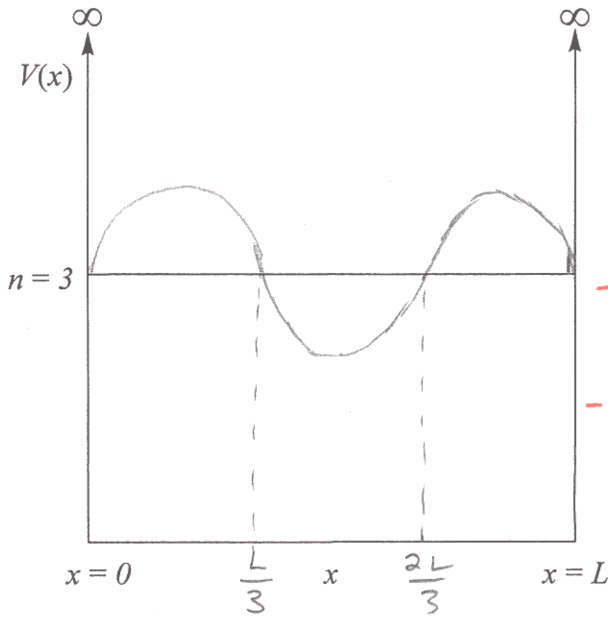
Same rubrics if nothing right in part (a)

-4 [illegible] some (incorrect) discussion of location

3. We have seen that pi electrons can be modeled as particles in a one-dimensional "box." Consider the potential energy function on the right with the $n = 3$ energy level labeled. The corresponding normalized eigenfunction for the $n = 3$ state is

$$\psi = \sqrt{\frac{2}{L}}\sin\left(\frac{3\pi x}{L}\right)$$

(a) (4 points) Sketch the energy eigenfunction on the diagram to the right. Take the $n = 3$ line as the line of zero amplitude.



-3 if unequal amplitudes
-2 if wrong phase
-4 if wrong λ

(b) (4 points) Draw the Lewis structure or line-angle structure of a molecule whose highest occupied pi molecular orbital is described by the $n = 3$ eigenfunction.

no partial credit

(c) (9 points) Verify that the given ψ satisfies the Schrodinger equation for the given potential, and derive a simplified expression for the energy of the given ψ.

$$\hat{H}\psi = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left[\sqrt{\frac{2}{L}}\sin\left(\frac{3\pi x}{L}\right)\right]$$

$$= \underbrace{-\frac{\hbar^2}{2m}\left(\frac{3\pi}{L}\right)^2(-1)}_{\text{real }\#}\underbrace{\left[\sqrt{\frac{2}{L}}\sin\left(\frac{3\pi x}{L}\right)\right]}_{\psi}$$

$\therefore$ ψ is an energy eigenfunction

and $E = -\frac{h^2}{4\pi^2}\left(\frac{1}{2m}\right)\left(\frac{9\pi^2}{L^2}\right)(-1) = \boxed{\frac{9h^2}{8mL^2}}$

-2 not fully simplified or math error
-5 wrong Hamiltonian
-5 no final expression for E

[Problem 3 continues on the next page.]

(d) (7 points) The function $\Gamma = \sqrt{\frac{2}{L}}\cos\left(\frac{3\pi x}{L}\right)$ is also a solution of the Schrodinger equation for a particle in a one-dimensional box. Briefly explain why, in spite of this fact, Γ is not an appropriate wavefunction for the potential energy function in this problem.

Γ does not equal zero at $x = 0$ and $x = L$, which is necessary since $V = \infty$ at these points and no particle (even in QM!) can have ∞ energy.
(or make some point about ψ's needing to be a standing wave)

-3 no specific physical reason given why wavefunction ~~its~~ should be zero at boundaries
-6 Something

(e) (25 points) Calculate the uncertainty Δx in the location of an electron described by the wavefunction given at the start of the problem. Express your answer in term of L. You may avoid performing any integrations by invoking symmetry.

$$\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2}$$

By symmetry, $\langle x\rangle = \frac{L}{2}$ (i.e. in the middle of the box)
(if you don't believe me, see two pages ahead in the key)

$$\langle x^2\rangle = \int_0^L \psi^* x^2 \psi\, dx = \int_0^L x^2 \psi^2 dx = \frac{2}{L}\int_0^L x^2 \sin^2\left(\frac{3\pi x}{L}\right) dx$$

$$= \frac{2}{L}\left[\frac{x^3}{6} - \left(\frac{x^2}{4a} - \frac{1}{8a^3}\right)\sin 2ax - \frac{x\cos 2ax}{4a^2}\right]_0^L$$

and $\sin 2ax = \sin\left(\frac{6\pi x}{L}\right) = 0$ at $x = 0$

$= \sin\left(\frac{6\pi L}{L}\right) = \sin 6\pi = 0$ at $x = L$

and $\cos 2ax = \cos\left(\frac{6\pi x}{L}\right) = 1$ at $x = 0$ and $x = L$

$$\therefore \langle x^2\rangle = \frac{2}{L}\left[\frac{x^3}{6} - \frac{x}{4a^2}\right]_0^L$$

[More space for Problem 3e on the next page; see Page 7 for the last part of the problem!]

$$\langle x^2\rangle = \frac{2}{L}\left[\frac{L^3}{6} - \frac{L}{4}\left(\frac{L^2}{9\pi^2}\right) + 0 - 0\right] = \frac{L^2}{3} - \frac{L^2}{18\pi^2} \quad \left(\begin{matrix}\text{right}\\ \text{units!}\end{matrix}\right)$$

$$\text{So } \Delta X = \sqrt{\frac{L^2}{3} - \frac{L^2}{18\pi^2} - \frac{L^2}{4}} = L\sqrt{\frac{1}{3} - \frac{1}{4} - \frac{1}{18\pi^2}} = \boxed{L\sqrt{\frac{1}{12} - \frac{1}{18\pi^2}}}$$

2 people got this problem completely right.

(-6) $\langle x\rangle = 0$ by symmetry

(-2) math error (small)

(-5) error in evaluating antiderivative

(-4) problems with trig functions

only the single biggest mistake of these 3 counts against you

[Problem 3 concludes on the next page.]

or $\langle x \rangle = \int \psi^* \hat{x} \psi \, d\tau = \int_0^L x \psi^2 \, dx$

$= \int_0^L x \left(\frac{2}{L}\right) \sin^2\left(\frac{3\pi x}{L}\right) dx = \frac{2}{L} \int_0^L x \sin^2\left(\frac{3\pi x}{L}\right) dx$

$= \frac{2}{L} \left[\frac{x^2}{4} - \frac{x \sin 2ax}{4a} - \frac{\cos 2ax}{8a^2} \right]_0^L$

and $\sin 2ax = \sin\left(\frac{6\pi x}{L}\right) = 0$ at $x=0$ and $x=L$

and $\cos 2ax = \cos\left(\frac{6\pi x}{L}\right) = 1$ at $x=0$ and $x=L$

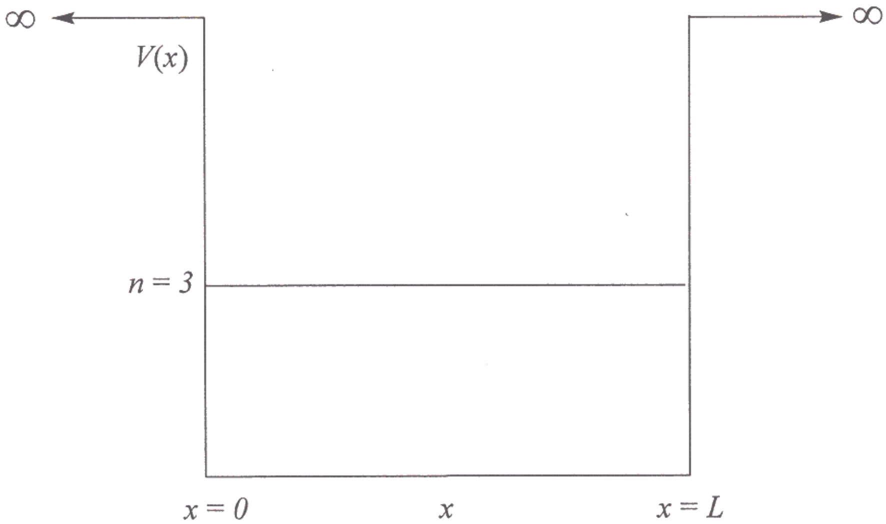
so $\langle x \rangle = \frac{2}{L} \left[\frac{x^2}{4} - \frac{1}{8a^2} \right]_0^L = \frac{2}{L} \left[\frac{x^2}{4} - \frac{1}{8} \frac{L^2}{9\pi^2} \right]_0^L$

$= \frac{2}{L} \left[\frac{L^2}{4} - \cancel{\frac{1}{8} \frac{L^2}{9\pi^2}} - 0 + \cancel{\frac{1}{8} \frac{L^2}{9\pi^2}} \right]$

$= \frac{2}{\cancel{L}} \left[\frac{L^{\cancel{2}}}{\cancel{4}_{2}} \right]$

$\boxed{\langle x \rangle = \frac{L}{2}}$

(f) (10 points) Say we modified our potential energy function as shown below:



For an electron in the $n = 3$ state of this modified potential, the uncertainty in its position is

less than **equal to** **greater than**

the uncertainty calculated in part (e).

Circle the correct answer above and justify your answer <u>qualitatively</u> below.

With finite potential barriers, tunneling by the particle into $x < 0$ and $x > L$ is allowed. ∴ the location of the particle is less certain.

-2 incorrect statement

-5 correct answer, but no specific mention of "tunneling" or "penetration"

-5 incorrect answer in spite of correct picture

-7 wrong answer, incorrect discussion

Possibly Useful Information

$$\int_0^\infty x^n e^{-ax}dx = \frac{n!}{a^{n+1}} \qquad \int_0^\infty e^{-a^2x^2}dx = \frac{\sqrt{\pi}}{2a} \qquad \int_0^\infty x^{2n}e^{-ax^2}dx = \frac{1\cdot 3\cdot 5\cdot(2n-1)}{2^{n+1}a^n}\sqrt{\frac{\pi}{a}}$$

$$\int \sin^2 ax\,dx = \frac{1}{2}x - \frac{1}{4a}\sin 2ax \qquad \int x(\sin^2 ax)dx = \frac{x^2}{4} - \frac{x\sin 2ax}{4a} - \frac{\cos 2ax}{8a^2}$$

$$\int x^2(\sin^2 ax)dx = \frac{x^3}{6} - \left(\frac{x^2}{4a} - \frac{1}{8a^3}\right)\sin 2ax - \frac{x\cos 2ax}{4a^2}$$

$$\cos^2 x + \sin^2 x = 1 \qquad \Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2}$$

1 H 1.0079																	2 He 4.0026
3 Li 6.941	4 Be 9.0122											5 B 10.81	6 C 12.011	7 N 14.007	8 O 15.999	9 F 18.998	10 Ne 20.179
11 Na 22.990	12 Mg 24.305											13 Al 26.982	14 Si 28.086	15 P 30.974	16 S 32.06	17 Cl 35.453	18 Ar 39.948
19 K 39.098	20 Ca 40.08	21 Sc 44.956	22 Ti 47.88	23 V 50.942	24 Cr 51.996	25 Mn 54.938	26 Fe 55.847	27 Co 58.933	28 Ni 58.69	29 Cu 63.546	30 Zn 65.38	31 Ga 69.72	32 Ge 72.59	33 As 74.922	34 Se 78.96	35 Br 79.904	36 Kr 83.80
37 Rb 85.468	38 Sr 87.62	39 Y 88.906	40 Zr 91.22	41 Nb 92.906	42 Mo 95.94	43 Tc (98)	44 Ru 101.07	45 Rh 102.91	46 Pd 106.42	47 Ag 107.87	48 Cd 112.41	49 In 114.82	50 Sn 118.69	51 Sb 121.75	52 Te 127.60	53 I 126.90	54 Xe 131.29
55 Cs 132.91	56 Ba 137.33	57 *La 138.91	72 Hf 178.49	73 Ta 180.95	74 W 183.85	75 Re 186.21	76 Os 190.2	77 Ir 192.22	78 Pt 195.08	79 Au 196.97	80 Hg 200.59	81 Tl 204.38	82 Pb 207.2	83 Bi 208.98	84 Po (209)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra 226.03	89 †Ac 227.03															

*	58 Ce 140.12	59 Pr 140.91	60 Nd 144.24	61 Pm (145)	62 Sm 150.36	63 Eu 151.96	64 Gd 157.25	65 Tb 158.93	66 Dy 162.50	67 Ho 164.93	68 Er 167.26	69 Tm 168.93	70 Yb 173.04	71 Lu 174.97
†	90 Th 232.04	91 Pa 231.04	92 U 238.03	93 Np 237.05	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (260)