19F-CHEM20A-1 Exam 2

RYAN DALY

TOTAL POINTS

91 / 100

QUESTION 1

1 30 pts

1.1 1a **8 / 8**

✓ **+ 8 pts** **Correct, 13.6 eV**

+ **6 pts** \-13.6 eV
+ **4 pts** 122 eV
+ **3 pts** \-122 eV
+ **2 pts** $$ E_n = -\frac {Z^2}{n^2}R$$
- **2 pts** Math or unit error or incorrect answer or no work shown

1.2 1b **8 / 8**

✓ **+ 8 pts** **Correct, $$\psi_{100}$$, $$\psi_{200}$$, $$\psi_{210}$$, $$\psi_{211}$$,$$\psi_{21-1}$$, $$\psi_{300}$$**

+ **4 pts** At least 2 of the right wavefunctions
+ **1 pts** 1 correct wavefunction
+ **0 pts** incorrect answer

1.3 1c **10 / 14**

+ **14 pts** Correct, $$v_{3->1}=26.3*10^{15}Hz$$, $$v_{2->1}=22.2*10^{15}Hz$$, $$v_{3->2}=4.1*10^{15}Hz$$

✓ **+ 10 pts** **Two of the three frequencies correct**

+ **6 pts** One of the three frequencies correct
+ **2 pts** $$E=hv$$
- **2 pts** Math or unit error or incorrect answer

QUESTION 2

2 25 pts

2.1 2a **10 / 10**

✓ **+ 10 pts** **Correct**

+ **3 pts** $$\psi(x)$$ vs x
+ **3 pts** From $$-\frac {L}{2}$$ to $$\frac {L}{2}$$
+ **4 pts** Correct shape of curve
+ **0 pts** No plot

2.2 2b **10 / 10**

✓ **+ 10 pts** **Correct**

+ **3 pts** $$\psi^2(x)$$ vs x
+ **3 pts** From $$-\frac {L}{2}$$ to $$\frac {L}{2}$$
+ **4 pts** Correct shape of the curve
+ **0 pts** No plot

2.3 2c **5 / 5**

✓ **+ 5 pts** **Correct, most probable x = $$-\frac {3L}{8}$$, $$-\frac {L}{8}$$, $$\frac {L}{8}$$, $$\frac {3L}{8}$$; least probable x = $$-\frac {L}{2}$$, $$-\frac {L}{4}$$,0, $$\frac {L}{4}$$, $$\frac {L}{2}$$ (can ignore the walls)**

+ **3 pts** Got one of the two sets (most probable or least probable) correct
+ **0 pts** Click here to replace this description.
+ **0 pts** Wrong bounds, 0 to L instead of -L/2 to L/2.

QUESTION 3

3 3 **15 / 15**

✓ **+ 15 pts** **Correct, $$\frac {P_V(a_0,\pi/2,\pi/2)}{P_V(a_0,\pi/4,\pi/4)}=14$$ or $$\frac {P_V(a_0,\pi/4,\pi/4)}{P_V(a_0,\pi/2,\pi/2)}=\frac {1}{14}=0.07$$**

+ **5 pts** $$ P_{V,\, at \, r} = \int_{V,\, at \, r} (\psi_{2p_y}(r,\theta,\varphi))^2dV$$
+ **5 pts** $$ P_{V,\, at \, r} \approx (\psi_{2p_y}(r,\theta,\varphi))^2V$$
- **2 pts** Math or unit error
+ **8 pts** Only calculated one probability
+ **0 pts** Click here to replace this description.

QUESTION 4

4 30 pts

4.1 4a 3 / 3

✓ **+ 3 pts Correct, $$ \frac {kg}{s^2}$$, $$ \frac {N}{m}$$, $$ \frac {J}{m^2}$$**

+ **1 pts** kgm/s^2, N, kg/s, J/m, kg/s^2*m
+ **0 pts** wrong

4.2 4b 3 / 3

✓ **+ 3 pts Correct, $$\frac {1}{m^2}$$, $$ \frac {kg}{J*s^2}$$,**

+ **1 pts** 1/m
+ **0 pts** Blank/several errors in derivation
+ **1 pts** kg*m/Js^2 / other close value/forgot square root
+ **1 pts** confused m with meters, it is kg
+ **2 pts** correct setup but not fully simplified/minor error
+ **1 pts** h has units J*s

4.3 4c 6 / 6

✓ **+ 6 pts Correct, $$ [\psi]=m^{-1/2} $$, $$ [\psi^2]=m^{-1} $$, $$ [\psi^2dx]=unitless\,\, probability $$**

+ **2 pts** $$ [\psi]=m^{-1/2} $$
+ **2 pts** $$ [\psi^2]=m^{-1} $$
+ **2 pts** $$ [\psi^2dx]=unitless\,\, probability $$
+ **0 pts** wrong answer
+ **2 pts** e has no units

4.4 4d 7 / 9

+ **9 pts** Correct, $$ P_{x>o}=\int_0^{\infty} P_o(x)dx=\frac {1}{2}$$

✓ **+ 3 pts $$P= \int P_o(x)dx= \int \psi_o^2dx $$**

✓ **+ 4 pts $$ P_{x>o}=\int_0^{\infty} P_o(x)dx$$**

+ **2 pts** $$P_{x>0}=\frac {1}{2}$$
+ **5 pts** Integrate from 0 to x but squared waveform
+ **2 pts** Switched integration limits/did from -inf to inf
+ **0 pts** Blank

4.5 4e 6 / 9

+ **9 pts** Correct, $$ PE = \frac {1}{4}h(\frac {1}{2\pi} \sqrt{\frac {k}{m}})=\frac {1}{4}hv=\frac {1}{2}E$$

✓ **+ 3 pts $$PE=\int_{-\infty}^{\infty} (\frac {1}{2}kx^2)\psi_o^2dx$$**

✓ **+ 3 pts $$PE=\frac {1}{4}h(\frac {1}{2\pi} \sqrt{\frac {k}{m}})$$**

+ **3 pts** $$PE=\frac {1}{2}E$$
+ **0 pts** Wrong answer/blank
+ **2 pts** State PE is less than TE

November 19, 2019

Second Hour Test
Chem 20A
Fall 2019

Name Ryan Daly

UID 505-416-119

Problem	Points Possible	Points Scored
1	30	
2	25	
3	15	
4	30	
Total	100	

BE SURE TO SHOW ALL YOUR REASONING AND CALCULATIONS!

PLEASE WORK IN PEN AND **DO NOT WRITE ON THE BACK OF THE EXAM.** AN EXTRA PAGE HAS BEEN ADDED FOR EACH QUESTION

DEMONSTRATING CLEARLY HOW YOU ARRIVE AT YOUR ANSWER IS MORE IMPORTANT THAN THE NUMERICAL ANSWER ITSELF

AND PLEASE BE CAREFUL WITH UNITS:
NEVER GIVE A NUMERICAL ANSWER WITHOUT UNITS

CHECK THE FIRST PAGE FOR EQUATIONS AND CONSTANTS

PLEASE CROSS OUT ANY WORK YOU DO NOT WANT US TO GRADE

CIRCLE IF YOU USED NEXT PAGE, **DO NOT WRITE ON BACK**

1. (30 pts) (a) Use our simple model for Z_{eff} shown below to calculate the binding energy of the valence electron in the ground state of phosphorous (P).

$$Z_{eff} = Z - (number\ of\ e's\ in\ lower\ shells) - \frac{1}{2}(number\ of\ other\ e's\ in\ the\ same\ shell)$$

(b) Write the atomic orbitals in the form $\psi_{n,\ell,m}$ for each of the occupied atomic orbitals in magnesium (Mg).

(c) When a Li^{2+} electron is excited from its ground state to its n = 3 state, what are the emission frequencies observed as the ion radiates light to return to its n = 2 and n = 1 states?

Final answer for (a):	Final answer for (b):	Final answer for (c):
13.6eV $= 2.2 \times 10^{-18}$ J	ψ_{100} ψ_{200} ψ_{21-1} ψ_{210} ψ_{211} ψ_{300}	4.1×10^{15} Hz and 2.6×10^{16} Hz

$$Z_{eff} = 15 - \frac{1}{2}(4) - 10 = 3$$

$$IE(P) = 0 - \left(-\frac{3^2}{3^2}R\right) = R = 13.6\text{eV}$$

3 to 2 $$\Delta E_1 = -\frac{3^2}{2^2}R - \left(-\frac{3^2}{3^2}R\right) = -1.25R = -17\text{eV} = 2.7 \times 10^{-18}\text{J}$$

$$\nu = \frac{E}{h} = \frac{2.7 \times 10^{-18}}{h} = 4.1 \times 10^{15}\text{ Hz}$$

3 to 1 $$\Delta E = -\frac{3^2}{1}R - \left(-\frac{3^2}{3^2}R\right) = -8R = -108.8\text{eV} = 1.7 \times 10^{-17}\text{J}$$

$$\nu = \frac{E}{h} = \frac{1.7 \times 10^{-17}}{h} = 2.6 \times 10^{16}\text{ Hz}$$

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2. (25 pts) Consider a mass m confined in a one-dimensional (*1D*) box of length L, centered at x = 0. (NOTE: this system is identical to the one we considered at length in class, except for the allowed x-values ranging from $-\frac{L}{2}$ to $\frac{L}{2}$, rather than from 0 to L). The allowed wavefunctions and energies are identified by finding solutions to the Schrodinger equation

$-\frac{h^2}{8\pi^2 m}\frac{d^2\psi(x)}{dx^2} = E\psi(x)$ that satisfy the boundary conditions, i.e., $\psi(x)$ must vanish at the boundaries of the box.

(a) The wavefunction corresponding to the 4th-lowest allowed energy of this system has the form $\psi_4(x) = A_4 sin(\frac{4\pi x}{L})$, where A_4 is the normalization constant. Plot $\psi_4(x)$, labeling the x-values where $\psi_4(x)$ vanishes, and where it has extrema (maxima and minima).

(b) Plot $(\psi_4(x))^2$, labeling the x-values where it vanishes, and where it has extrema.

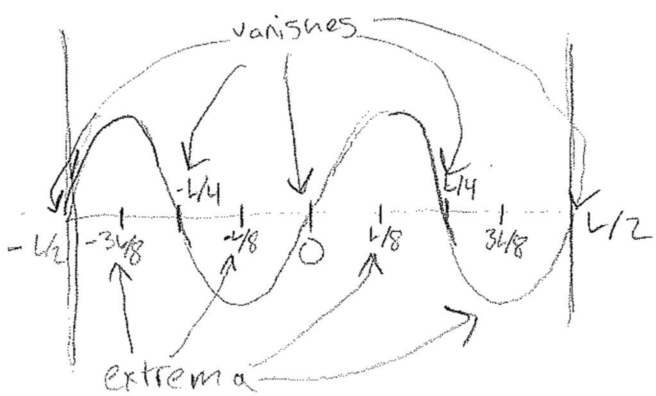
(c) What are the most probable positions? And the least probable?

Final answer for (c):

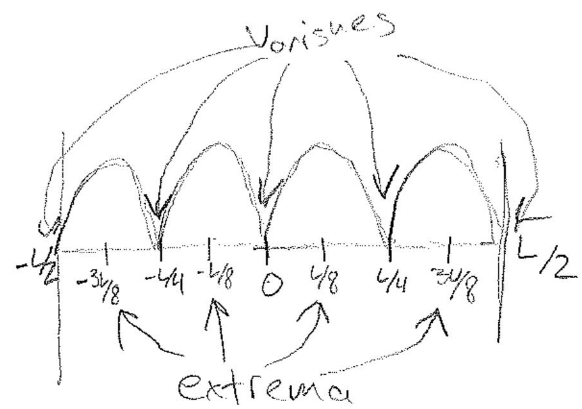
most probable: $-3L/8, -L/8, L/8, 3L/8$

least probable: $-L/2, -L/4, 0, L/4, L/2$

a)



b)



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3. (15 pts) Consider an electron in the $2p_y$ state of He^+. Calculate the probability of finding it in a small volume $V = (10^{-14}m)^3$, centered at the point $(r, \theta, \varphi) = (a_0, \pi/2, \pi/2)$, **relative to** the probability of finding it in a small volume $V = (10^{-14}m)^3$, centered at the point $(r, \theta, \varphi) = (a_0/4, \pi/4, \pi/4)$.

$$\psi_{2p_y}(r,\theta,\varphi) = \left(\frac{3}{4\pi}\right)^{1/2} sin\theta sin\varphi \frac{1}{2\sqrt{6}}\left(\frac{Z}{a_0}\right)^{3/2}\frac{Zr}{a_0}e^{-\frac{Zr}{2a_0}}$$

Final answer:

$$\boxed{14}$$

$$\psi_{2py}^2 = \frac{3}{4\pi}\sin^2\theta\sin^2\varphi\frac{1}{4(6)}\frac{Z^3}{a_0^3}\frac{Z^2r^2}{a_0^2}e^{-\frac{2r}{a_0}} = \frac{Z^5r^2}{32\pi a_0^5}e^{-2r/a_0}\sin^2\theta\sin^2\varphi$$

for $(r,\theta,\varphi) = (a_0, \pi/2, \pi/2)$

$$P \approx \frac{2^5(a_0)^2}{32\pi a_0^5}e^{-2a_0/a_0}\sin^2(\pi/2)\sin^2(\pi/2)(10^{-14})^3 = 2.9\times10^{-13}$$

for $(r,\theta,\varphi) = a_0/4, \pi/4, \pi/4$

$$P \approx \frac{2^5(a_0/4)^2}{32\pi a_0^5}e^{-2(a_0/4)/a_0}\sin^2(\pi/4)\sin^2(\pi/4)(10^{-14})^3 = 2.0\times10^{-14}$$

$$\frac{P(a_0, \pi/2, \pi/2)}{P(a_0/4, \pi/4, \pi/4)} = 14.3$$

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4. (30 pts) The figure below is a plot of the lowest-energy, normalized, allowed wavefunction, $\psi_o(x) = (\frac{\alpha}{\pi})^{1/4} e^{-\frac{\alpha x^2}{2}}$, of a mass m moving in one-dimension (x) under the influence of a force $F = -kx$. Here x is the displacement of the particle from its origin, and $\alpha = \frac{2\pi}{h}(km)^{1/2}$. Note that the force $F = -kx$ corresponds to the potential energy $\frac{1}{2}kx^2$.

(a) What are the dimensions (or, if you prefer, SI units) of k?

$J = kx^2 \quad k = J/m^2 = J \cdot m^{-2}$

(b) What are the dimensions (units) of α?

(c) What are the dimensions (units) of $\psi_o(x)$? And of $(\psi_o(x))^2$? And of $(\psi_o(x))^2 dx$?

(d) What is the probability of finding a positive value for x? Write an explicit expression for this probability as a definite integral over x.

(e) Using the fact that $\int_{-\infty}^{\infty} x^2 e^{-\alpha x^2} dx = \frac{\sqrt{\pi}}{2}\frac{1}{\alpha^{3/2}}$, calculate the average potential energy in the lowest allowed state, $(\frac{1}{2}kx^2)_{average,\, in\, ground\, state} = \int_{-\infty}^{\infty} (\frac{1}{2}kx^2)\psi_o^2(x)dx$, and compare it to the total energy, $\frac{1}{2}h\nu = \frac{1}{2}h(\frac{1}{2\pi}\sqrt{\frac{k}{m}})$.

$\alpha = (km)^{\frac{1}{2}}\left(\frac{1}{h}\right)$

$= (kg \cdot kg/s^2)^{\frac{1}{2}}\left(\frac{1}{J \cdot s}\right)$

$= (kg^2/s^2)^{\frac{1}{2}}\left(\frac{1}{J \cdot s}\right)$

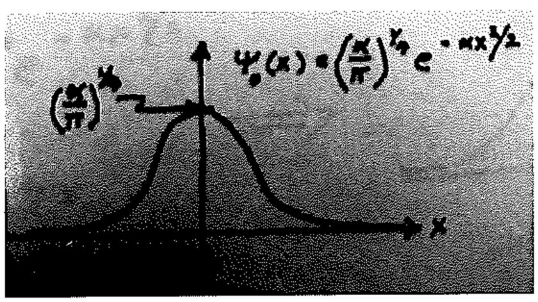
$= \frac{kg}{Js^2}$

$F = kg\, m/s^2$

$k = \frac{F}{X} = \frac{kg\, m/s^2}{m} = kg/s^2$

$\psi_o = (kg\, J^{-1} s^{-2})^{\frac{1}{4}} e^{(kg J^{-1} s^{-2} \cdot m^2)}$

$= (kg\, J^{-1} s^{-2})^{\frac{1}{4}} e^{kg\, m^2 J^{-1} s^{-2}}$



$(\psi_o(x))^2 dx$ is a probability no units

Final answer for (a):

kg/s^2 or $kg \cdot s^{-2}$

Final answer for (b):

$kg / J \cdot s^2$ or $kg \cdot J^{-1} \cdot s^{-2}$

Final answer for (c): $(\psi_o(x))^2 = \frac{(\psi_o(x))^2 dx}{dx} = \frac{1}{m} = m^{-1}$

$\psi_o(x) = \sqrt{(\psi_o(x))^2} = \sqrt{m^{-1}} = m^{-1/2}$

$\psi_o(x) = m^{-1/2}$

$(\psi_o(x))^2$ units: m^{-1}

$(\psi_o(x))^2 dx$ has no units

Final answer for (d):

$\int_0^{\infty} \psi_o^2(x)\, dx$

$\int_0^{\infty} (\frac{\alpha}{\pi})^{\frac{1}{2}} e^{-\alpha x^2} dx$

Final answer for (e):

$\frac{k}{4\alpha}$

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$$\int_{-\infty}^{\infty} x^2 e^{-\alpha x^2} dx = \frac{\sqrt{\pi}}{2} \frac{1}{\alpha^{3/2}}$$

Calculate $PE_{avg} = \int_{-\infty}^{\infty} \left(\frac{1}{2} kx^2\right) \psi_0^2(x)\, dx$

$$= \frac{1}{2} k \int_{-\infty}^{\infty} x^2 \left(\frac{\alpha}{\pi}\right)^{\frac{1}{2}} e^{-\alpha x^2} dx = \frac{1}{2} k \left(\frac{\alpha}{\pi}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} x^2 e^{-\alpha x^2} dx$$

$$= \frac{1}{2} k \left(\frac{\alpha}{\pi}\right)^{\frac{1}{2}} \left(\frac{\sqrt{\pi}}{2} \frac{1}{\alpha^{3/2}}\right) = \frac{k}{2} \frac{\sqrt{\alpha} \cdot \sqrt{\pi}}{\sqrt{\pi} \quad 2} \frac{1}{(\sqrt{\alpha})^3}$$

$$= \frac{k}{4(\sqrt{\alpha})^2} = \frac{k}{4\alpha}$$

$$\int_{-\infty}^{\infty} \frac{1}{2} k x^2 \left(\frac{\alpha}{\pi}\right)^{\frac{1}{2}} e^{-\alpha x^2} \qquad \frac{1}{2} k \left(\frac{\alpha}{\pi}\right)^{\frac{1}{2}} \frac{\sqrt{\pi}}{2} \frac{1}{\alpha^{3/2}} - \frac{k}{2 \cdot 2 \alpha} = \frac{k}{4\alpha}$$

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