CHEM 372 Rybolt Spring 2009 Exam 1 NAME KEY

Draw a CIRCLE around your final answer if math or derivation done. Clearly identify the quantity you are reporting and include the units if it is a numerical answer. Present your work neatly and in order beneath each question. Staple the requested homework sheets (in order) to the back of this exam in the extreme left hand corner. Be sure to answer only the specific question that is asked.

R = 8.31 (J/ K mol) R= 0.08206 (L atm/ K mol) N_A=6.02x10^{23} h= 6.63x10^{-34} J s c=3.0x10^{8} m/s

k= 1.38x10^{-23} 1 atm = 760 torr = 1.01 x 10^5 (N/ m^2) = 1.01 bar = 101 kPa

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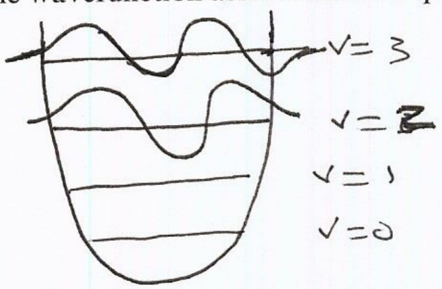
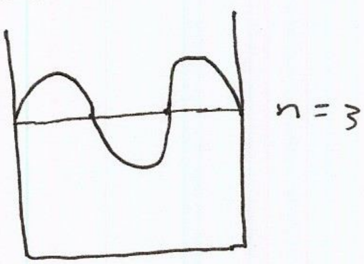
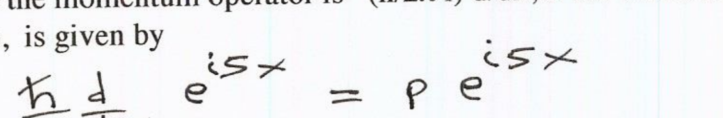
1) Draw the potential energy curve for a simple harmonic oscillator. Now within the potential energy curve draw a plot of the wavefunction associated with quantum number v=3.



2) Draw the potential energy curve for a particle in a one-dimensional box with a potential of V=0 but walls of V=infinity. Now within the potential energy curve draw a plot of the wavefunction associated with quantum number n=3



3) Consider rotational motion around a circle, where the circle is represented by a straight line and the potential is V=0. Draw the wavefunction along this straight line (representing a circle) where m_l =3.



4) Given that the momentum operator is (h/2π i) d/dx, if the wavefunction is Ψ= e^{i5x} then the momentum, p, is given by

$$\frac{\hbar}{i}\frac{d}{dx} e^{i5x} = p\, e^{i5x}$$

$$\frac{\hbar}{i}(i5)e^{i5x} = p\, e^{i5x} \Rightarrow \boxed{5\hbar = p}$$

5) Write the Schrodinger equation for a particle in 1 dimensional free space with a potential field of V=0 and solve for E. Let $\Psi = e^{ikx}$. Recall that the kinetic energy operator is $(-h^2/8\pi^2 m)d^2/dx^2$. Solve for E

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}e^{ikx} = E\, e^{ikx}$$

$$-\frac{\hbar^2}{2m}\, ik \frac{d}{dx} e^{ikx}$$

$$-\frac{\hbar^2 (ik)(ik) e^{ikx}}{2m} = E\, e^{ikx}$$

$$-\frac{i^2 \hbar^2 k^2}{2m} = E$$

$$\frac{\hbar^2 k^2}{2m} = E \quad \text{or} \quad \frac{h^2 k^2}{8\pi^2 m} = E$$

6) A photon of visible light has a wavelength = 682nm. The energy(J) of this single photon is

$\lambda \nu = c \qquad E = h\nu \Rightarrow E = hc/\lambda$

$\nu = c/\lambda$

$$E = \frac{(6.63\times10^{-34}\ \mathrm{Js})(3.0\times10^{8}\ \mathrm{m/s})}{(682\ \mathrm{nm})\left(\frac{10^{-9}\mathrm{m}}{\mathrm{nm}}\right)}$$

E=

$$E = 2.92\times10^{-19}\ \mathrm{J}$$

7) According to Einstein's theory of the photoelectric effect, if the work function to eject an electron from a metal exceeded the energy of an individual photon of light by a factor of 3.5 then striking the surface with 28 of these photons of light should cause the ejection of how many electrons?

0 none

photon has to have minimum energy equal to work function Φ to eject electron

8) In the solution to the particle in a one-dimensional box we find at one point a general solution of $\Psi(x) = A \sin(kx) + B \cos(kx)$. Using just the boundary condition where $\Psi(0) = 0$, show how the solution is simplified be specific and show the relevant math (don't answer more than what is asked)

$$\Psi(0) = 0 = A \sin(k\cdot 0) + B\cos(k\cdot 0)$$

$$0 = A\sin(0) + B\cos(0)$$

$$0 = A\cdot 0 + B\cdot 1$$

$$0 = B \Rightarrow \Psi(x) = A\sin(kx)$$

9) To insure that a wavefunction is normalized in three dimensional space requires a triple integral in spherical polar coordinates. Write the proper limits of each of the integrals below and the write the value on the right side of the equation

$$\int_0^{\infty}\int_0^{2\pi}\int_0^{\pi} \Psi(r,\theta,\phi)\ \Psi(r,\theta,\phi)\ r^2\,dr\ \sin\theta\,d\theta\ d\phi = \underline{\ 1\ }$$

10) Write the full electronic configuration for Cd.

Cd $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10}$

11) A researcher decides to repeat the Stern and Gerlock experiment in which silver atoms were passed through a magnetic field and found to half curve up and half curve down. The researcher figures how different can two elements be that are next to each other in the periodic table and so he uses element 48 cadmium. What did he observe?

No unpaired electrons so all Cd straight line - no deflection

12) A student is looking at electronic transitions for excited cadmium Cd* and is disappointed to find that she does not observe any 6s to 5s transitions. What property of photons of light (EM radiation) would make this transition not be allowed.

Photons have angular momentum of $\ell = 1$ so transition between electron levels must have $\Delta\ell = 1$

13) The term symbol $^3F_4$ what is S= 1 L= 3 J= 4

$\ell=3$ (L=3 F)
$\ell=2$ L=2 D
$\ell=1$ L=1 P
$\ell=0$ L=0 S

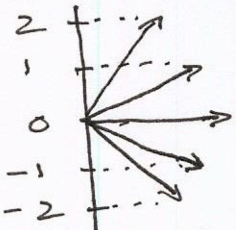
$2S+1=3$
$2S=2$
(S=1)

L+S=J max

14) The hydrogenic solution to the Schrodinger Equation for n=5 gives a number of degenerate orbitals. Indicate the number of each of the following types of orbitals

__1__ 5s __3__ 5p __5__ 5d __7__ 5f __9__ 5g __25__ total number of n=5 orbitals

15) Show the possible orientations of the vector that represents angular momentum for the 5d orbitals which when projected on to the z axis generate m_l values.



16) Recall that F = - dV/dx. If the force of a vibrating mass does not follow Hooke's law but instead is given by F= - k x^3 then the potential energy operator in the Schrodinger equation will be given by V =

$-kx^3 = -dV/dx$

$kx^3 dx = dV$

$\int dV = \int kx^3 dx$

$V = \frac{k}{4}x^4$

17) A biological quantum company called "See Spot Inc." is working on a new product line of quantum dots that have energy gaps in the ultraviolet region of EM radiation. Their current ones are in the visible region and they are having trouble figuring out how to change the ΔE to achieve the desired gap in the UV region. Considering the quantum dots to be like a one-dimensional particle in a box you realize the solution is obvious and suggest they if they want to double the ΔE they should just take the old length L and change it so the new length of quantum dot is =

$\Delta E = \frac{h^2 n^2}{8mL^2}$

2L   L/2 $(2)^{1/2}$ L   (L/ $(2)^{1/2}$)

smaller box makes bigger ΔE

18) The "See Spot Inc." quantum dot company CEO had Physical Chemistry many years ago and she has written a number of different equations on the board. She says, "if we were to consider our new flat quantum dots as two-dimensional objects and wanted to use the method of separation of variables to solve the Schrodinger Equation which of these equation would we use?" You step to the whiteboard and confidently circle one of the following:

$E_{total} = E_x E_y$ ($E_{total} = E_x + E_y$) $\Psi = \Psi(x) + \Psi(y)$ $E_x - \Psi(x) = 0$

19) An isotopic identification of a Mo atom attached to a fixed surface is based on the vibrational motion of the Mo atom. The value of the vibrational frequency of ^{92}Mo is X so therefore the vibrational frequency of ^{100}Mo would should be   heavier mass slower vibration √ factor

(92/100)X   (100/92)X   ($(92/100)^{1/2}$ X) $(100/92)^{1/2}$ X

20) C_2 has been observed by spectroscopy in the gas phase. Fill in the MO diagram below and then indicate the expected bond order for this diatomic molecule.

σ*2p$_x$

π*2p$_z$ π*2p$_y$

σ2p$_x$ 1↓

π2p$_z$ 1↓   π2p$_y$ 1↓

σ*2s 1↓

σ2s 1↓

σ*1s 1↓

σ1s 1↓

C_2

2(6e) = 12e

Bonds = $\frac{8-4}{2}$

(Bonds = 2)

$\Delta E^* = \frac{h^2 n^2}{8m\left(\frac{L}{\sqrt{2}}\right)^2}$

$\Delta E^* = \left(\frac{\sqrt{2}}{L}\right)^2 \frac{h^2 n^2}{8m}$

$\Delta E^* = 2 \frac{h^2 n^2}{8mL^2}$

so $\Delta E^* = 2\Delta E$

if

$L^* = \frac{L}{\sqrt{2}}$

21) Attach Homework
22) Attach Homework
23) Attach Homework
24) Attach Homework