UNIVERSITY OF JOHANNESBURG

FACULTY OF SCIENCE

DEPARTMENT OF CHEMICAL SCIENCES

MODULE: **CEM8X05**
(Quantum Chemistry and Spectroscopy)

CAMPUS: **APK**

EXAM **Supplimentary Exam (2019)**

DATE: 07 JAN 2020	**SESSION: 8:00 – 11:00 AM**
ASSESSOR:	**Prof. Kaushik Mallick**
ASSESSOR:	**Dr. Sanyasi Sitha**
MODERATOR:	**Prof. Sekhar C. Ray**
DURATION: 3 Hours	**Total Marks: 100**

NUMBER OF PAGES: 4 Pages (Including this page)

INSTRUCTIONS: Answer all the questions.
Indicate the correct question number for your answer.
Using of a non-graphing scientific calculator is allowed.

Physical Constants and trigonometric identities:

Trigonometric identities:	$Sin^2\theta = \frac{1-cos2\theta}{2}$ $sin(\alpha + \beta) = sin(\alpha)cos(\beta) + cos(\alpha)sin(\beta)$	$\sin 2\theta = 2 \sin\theta \,.\, \cos\theta$ 2SinA.SinB = Cos(A-B) – Cos(A+B)

Planck's Constant	h	6.626×10^{-34} J.S , 6.626×10^{-34} kg.m^2.S^{-1}

SECTION A: Quantum Chemistry (*Dr. S. Sitha*) *Total marks = 70*

Question 1: **(5+5 = 10 marks)**

The function $\psi = Ax(1-x)$ is a well-behaved wave function in the interval $0 \le x \le 1$. Calculate

(i) the normalization constant (A), and
(ii) the average value of a series of measurements of x (find the expectation value: $\langle x \rangle$).

Question 2: **(3+3 = 6 marks)**

For a particle in a one-dimensional box $(0 \le x \le a)$, we used eigenfunctions of the form $\psi = A\sin(kx)$. Explain why we could not use

(i) $\psi = Ae^{kx}$

(ii) $\psi = A\cos(kx)$

Question 3: **(5+10+5 = 20 marks)**

The potential for a particle in one dimensional box problem, is

$V(x) = 0$ for $0 < x < L$ $V(x) = \infty$ for $x \le 0$ or $x \ge L$

The wavefunctions that are solutions to the time independent Schrodinger's equation for this system and the corresponding energy levels are:

$\psi_n(x) = (2/L)^{1/2} \sin(n\pi x/L)$ inside the box $E_n = n^2h^2/8mL^2$

$\psi_n(x) = 0$ outside the box $n = 1, 2, 3, \ldots$

a) Find P(L/4 < x < L/2), i.e., the probability of finding the particle between the region L/4 and L/2, for the n = 2 state.

b) Show that the n = 2 and n = 3 states are **orthonormal**, that is, show the following

$$\int \sin(mx)\sin(nx)\,dx = \frac{\sin(m-n)x}{2(m-n)} - \frac{\sin(m+n)x}{2(m+n)} \quad \text{(where, } m \neq n\text{)}$$

c) Is $f(x) = e^{ikx}$, where k is a positive constant, an eigenfunction of the Hamiltonian for the particle in a box for the region where V = 0? If so, is it an acceptable solution to the time independent Schrodinger's equation for the system? Justify your answer.

Question 4: **(8+5 = 14 marks)**

(a) Find the result of operating with the operator $\hat{O} = \frac{1}{r^2}\left(\frac{d}{dr}\right)r^2\left(\frac{d}{dr}\right) + \frac{2}{r}$ on the function $\psi = Ae^{-br}$. What values must the constants (A, b) have for ψ to be an eigenfunction of $\hat{O}$, and in that case what will be the eigenvalue ?

(b) Show that the wave function $\psi = (\sin\theta)(e^{i\phi})$ is an eigenfunction of $\hat{L}_z$. What is the eigenvalue?

Question 5: **(4+5 = 9 marks)**

(i) Write the general expression for the energy of a harmonic oscillator.

(ii) Calculate the zero-point energy of a harmonic oscillator consisting of a particle of mass 2.33×10^{-26} kg and force constant 155 N/m. [*Hint*: Planck's constant, *h*,is 6.626 $\times 10^{-34}$ J s.]

Question 6: **(3+8 = 11marks)**

(a) What is the main assumption of the Born-Oppenheimer approximation?

(b) Using the Born-Oppenheimer approximation, write the Hamiltonian for the H_2 molecule (two electrons and two nucleus system).

<u>SECTION B: Solid State Electronics</u> (***Prof. K. Mallick***) *Total marks = 30*

<u>Question 7:</u> **(3+2+5=10 marks)**

(a) Explain the difference between Intrinsic and Doped semiconductor.

(b) Give the examples of (III-V) and (II-VI) semiconductor.

(c) Show the correlation between the interatomic spacing and the electrical properties of the group (IV) A elements.

<u>Question 8:</u> **(5+5=10 marks)**

(a) Schematically explain the mechanism of current flow in an intrinsic semiconductor under electric field.

(b) Explain the concept of the Band Theory of Solids (for insulator, semiconductor and metal) in the light of Fermi level.

<u>Question 9:</u> **(2+2+2+2+2=10 marks)**

(a) What are the differences in the energy band configurations between conductors, insulators, and semiconductors?

(b) What is a p-n junction? What is a transistor?

(c) What kind of transition leads to the production of light in a semiconductor p-n junction?

(d) Describe what a semiconductor laser is and how it operates.

(e) Give a few examples of the uses and advantages of semiconductor lasers.