SOUTH EASTERN KENYA UNIVERSITY

UNIVERSITY EXAMINATIONS 2016/2017

SECOND SEMESTER EXAMINATION FOR THE DEGREE OF BACHELOR OF SCIENCE(CHEMISTRY)

SCH 409: QUANTUM CHEMISTRY

DATE: 20TH APRIL, 2017 TIME: 10.30-12.30 P.M

INSTRUCTIONS TO CANDIDATES

(a) Answer question One and any other Two questions

(b) Question 1 carries 30 marks while the other questions carry 20 marks each

(c) Illustrate your answers with well label diagrams where applicable

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R = 8.3144598 J mol^{-1} k^{-1}

h = 6.626 X 10^{-34} JS

Me = 9.109 x 10^{-31} kg

e = 1.609 x 10^{-19} c

Question 1 (30 marks)

(a) Define the following terms(4 marks)

i. Quantization of Electronic Angular Momentum

ii. de Broglie law

iii. Photoelectric effect.

iv. Ultraviolet catastrophe.

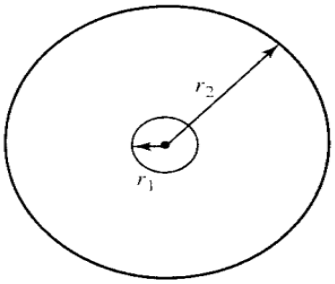
(b) Define wave particle duality (4 mrks)

(c) Compare and contrast classical and quantum theories(5marks)

(d) State Braggs law (3 marks)

(e) What was the important observation derived from Davisson and Gemer Experiment? (2 marks)

(f) Using the following diagram



Derive an expression for total Energy of an orbit using kinetic energy and columbic energy. What is the conclusion you can derive from this model? (4 marks)

(g) State the important step in Bohr model (2 marks)

(h) Using Bohr equation, de Broglie and force balance (columbic and centrifugal) relationship, derive expression for radii that stable Bohr orbit obey, velocities of electrons in the orbits and the sum of kinetic and coulomb potential energies (5 marks)

Question 2 (20 marks)

a.) Using Young's slit experiment, with illustraitions and equations, discuss wave particle duality (10 marks)

b.) i. Write the dispersion equation and discuss it's implications (2 marks)

ii. Write an expression for, A (x, y, t) for waves moving on the surface of a rectangular two-dimensional surface of lengths Lx and Ly. Why are the waves quantized in two-dimension? (2 marks)

iii. Rewrite the equation below using the de Broglie expression(2 marks)

$$\frac{d^2A}{dx^2} = -(\frac{2\pi}{\lambda})^2 A$$

iv. Derive the primitive Schrodinger equation from equation (b iii) above (4 marks)

Question3(20marks)

a) Discuss the classical Jean Rayleigh Law and its shortcomings(6marks)

b) Discuss thetwoapproximatemethodsofsolvingSchrodingerwaveequation?

(14marks)

Question4(20marks)

a) Whatis thesimilarityanddifferenceofSchrodingerandHeisenbergequation(3mark)

b) Startingwithone-dimensionalclassicalwavederivetime-independentSchrodingerwave equation?(15marks)

c) Statetheshortcomings oftime-independentSchrodingerwaveequation?(2marks)

Question5(20marks)

(a) DefineHeisenberg'suncertaintyprincipleanditsimportanceinquantummechanics? (3 marks)

(b) DerivetheHeisenbergs uncertaintyprinciple?How do you make Heisenbergs uncertainty principle real(8marks)

(c) State thetwoeffects of Hamiltonianneglects?(3marks)

(d) Discuss theBorn-OppenheimerApproximation(6marks)