THE CATHOLIC UNIVERSITY OF EASTERN AFRICA

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MAIN EXAMINATION

SEPTEMBER – DECEMBER 2019 TRIMESTER

FACULTY OF SCIENCE

DEPARTMENT OF PHYSICS

REGULAR PROGRAMME

PHY 401: QUANTUM MECHANICS II

Date: DECEMBER 2019	**Duration: 2 Hours**
INSTRUCTIONS: Answer Question ONE and ANY other TWO Questions	

Speed of light in the vacuum, c = 3.00 × 10^{8} m s^{-1}

Planck's constant, h = 6.63 × 10^{-34} J s

s

Mass of the electron, m_e = 9.11 × 10^{-31} kg

Mass of a proton m_p = 1.66× 10^{-27} kg

1 eV = 1.6 × 10^{-19} J

1MeV = 10^{6} eV

1nm = 10^{-9} m.

$$\int \sin^2 bx \; dx = \frac{x}{2} - \frac{1}{4b}\sin(2bx)$$

$$\int x^{2n} e^{-bx^2} dx = \frac{1\times3\times\ldots\ldots\times(2n-1)}{2^{n+1}}\left(\frac{\pi}{b^{2n+1}}\right)^{\frac{1}{2}} \; ; \; n=1,\,2,\,3,\,\ldots\ldots\ldots$$

$$\sin^2 A = \frac{1}{2}[1-\cos 2A]$$

Q1. i) Write down the time-dependent Schrodinger equation for the wave function ψ (x, t) of a particle of mass m moving in one dimension x in the potential V (x). Also write down the time-independent

Schrodinger equation for the wave function ψ (x) of a particle of mass m moving in one dimension x in a potential V (x).

(4 marks)

ii) A particle on a line has a normalized wave function ψ (x). Write down a formula for the expectation value of x^2 .

(3 marks)

iii) Explain the physical meaning of the Heisenberg uncertainty relation. **(3 marks)**

iv) Explain what is meant by the orthogonality of two wavefunctions $\psi_1(x)$ and $\psi_2(x)$), in the quantum mechanics of a particle on a line $-\infty < x < \infty$

(3 marks)

v) The momentum operator is $\hat{p} = -i\hbar \frac{\partial}{\partial x}$ Calculate the momentum of a particle described by the wave function $\psi_k(x) = e^{ikx}$.

(3 marks)

vi) For a one – dimensional system, the momentum operator $\hat{p}$ is defined in (v) above and the position operator, $\hat{X} = x$. Show that [$\hat{p}$, $\hat{X}$] = $-i\hbar$ Can momentum and position of a given state be measured simultaneously ? **(4 marks)**

vii) Write down the normalization condition for the wave function ψ (x) of a particle which can move in the interval −a ¿ x ¿ a. Hence normalize the wave function $\psi(\varphi) = A\, e^{-ik\varphi}$ for $0 < \varphi < \pi$.

(3 marks)

viii) What is parity, and when would you expect a wave function to have a definite parity?

(2 marks)

ix) How does the energy of the n^{th} bound state for a particle confined by a finite quantum well compare to that of the same state in the infinite quantum well? Give reasons for your answers.

(2 marks)

x) Two copper conducting wires of uniform cross-sectional area are separated by an oxide layer of copper oxide. Treat the oxide layer as a square barrier of height 10 eV and estimate the transmission coefficient for penetration by 7 eV electrons if the layer thickness is 5.00 nm. **(6 marks)**

$$For\ \ E<V_0\ ;\ T=\frac{1}{\left[1+\dfrac{V_0^2\sinh^2\beta a}{4E\left(V_0-E\right)}\right]}\ \ ;\ For\ \ E>V_0\ ;\ T=\frac{1}{\left[1+\dfrac{V_0^2\sinh^2\beta a}{4E\left(E-V_0\right)}\right]}$$

$$where \qquad \beta^2=\frac{2m\left(V_0-E\right)}{\hbar^2}$$

Q2. The spin-orbit coupling of an electron of an angular momentum *l* and spin *s*=1/2 is described by the Hamiltonian
H=*λl*•*s*, where λ is the spin-orbit coupling parameter.

a) Write down the matrix *H* and diagonalize it to show that the state is split into two states with total angular momentum *j*=*l*±1/2. Find the energies. **(8 marks)**

b) Show that the eigenenergies can be determined using the relation *j*=*l*+*s* **(4 marks)**

c) Obtain the relativistic Hamiltonian for a Hydrogen atom starting from classical physics **(8 marks)**

Q3. a) Formulate the Hartree-Fock approximation in electronic structure theory **(6 marks)**

b) Derive the Hartree-Fock electronic energy in terms of the density matrix and the density for an electron wave function. **(5 marks)**

c) What is the Hohenberg-Kohn observation for the basis of density functional theory? **(4 marks)**

d) State the three fundamentals of properties of a Born-Oppenheimer model **(3 marks)**

e) What do you understand by LCAO approximation? **(2 marks)**

Q4. A particle of mass *m* moves along the x-axis, with a potential energy $U(x)=\frac{k\,x^2}{2}$

(i) Write down the time-independent Schrodinger equation for this particle. **(2 marks)**

(ii) The ground state wavefunction is of the form $\psi_1(x) = A_0\, e^{-a\,x^2}$. The parameter a is a function of k; m; $\hbar$ and A_0 is a normalisation constant. Calculate a and obtain the energy E of this state. **(6 marks)**

For parts (iii) and (iv) you may use the integral $\int_0^{\infty} e^{-a\,x^2} = \frac{1}{2}\sqrt{\frac{\pi}{a}}$

(iii) Determine the expectation values of x^2 and of the kinetic energy in the ground state. **(6 marks)**

(iv) The first excited state is $\psi_1(x) = A_1\, x\, e^{-a\,x^2}$. Calculate the expectation value of x^2 and the kinetic energy in the state $\psi_1(x)$.

(6 marks)

Q5. a) An electron is confined to move in the xy plane in a rectangle whose dimensions are L_x and L_y. That is, the electron is trapped in a 2D potential well having lengths L_x ans L_y. In this situation, the allowed energies of the electron depend on two quantum numbers nx and ny. The allowed energies are given by,

$E=h^2/8m_e(n_x^2/L_x^2+n_y^2/L_y^2)$.

i) Assuming that Lx=Ly=L, find the energies of the lowest four energy levels for the electron. **(8 marks)**

ii)

iii) Construct an energy level diagram for the electron and determine the energy difference between the second and the ground state **(3 marks)**

b) By considering angular momentum in spherical coordinates and choosing the common eigen functions of (L^2, L_z) for L=1 as our basis, show that for

$L_z = \begin{bmatrix} h & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -h \end{bmatrix}$

(9 marks)

END