UNIVERSITY OF SWAZILAND

MAIN EXAMINATION 2017/2018

TITLE OF PAPER: INTRODUCTION TO QUANTUM MECHANICS

COURSE NUMBER: CHE343

TIME: THREE (3) HOURS

INSTRUCTIONS:

This paper consists of two sections; Section A and B. **Answer all question in section A and any two (2) questions in section B.**

NB: Each question should start on a new page.

A data sheet and a periodic table are attached

A non-programmable electronic calculator may be used

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SECTION A [50 MARKS]

a) Outline four differences between classical and quantum mechanics [4]

b) What is the experimental evidence that showed that the existence of photons is not only a suggestion and that photons can behave as particles [5]

c) State four properties of an acceptable wavefunction assuming that the potential energy is smoothly well behaved [4]

d) The lowest energy electrons of a carbon nanotube can be described by the normalized wavefunction $\psi = \left(\frac{2}{L}\right)^{\frac{1}{2}} \sin\left(\frac{\pi x}{L}\right)$, where L is the length of nanotube. What is the probability of finding the electron between x= L\4 and x=L/2? [5]

e) Determine which of the following functions are eigenfunction of the inversion operator $\hat{i}$ which has the effect of making the replacement x →-x.

i. $x^3 - kx$ [2]

ii. Cos kx [2]

iii. $x^2 + 3x - 1$ [2]

State the eigenvalue where possible.

f) Use the Heisenberg uncertainty principle and properties of acceptable wavefunctions to explain the physical origin of the zero point energy of a particle in a box [4]

g) Given that $\langle x^2 \rangle = \left(v + \frac{1}{2}\right)\frac{\hbar}{(mk_f)^{\frac{1}{2}}}$, show that the mean potential energy is given by $\langle V \rangle = \frac{1}{2}\left(v + \frac{1}{2}\right)\hbar\omega$ [4]

h) Starting with the classical definition of angular momentum, $J_z = \pm pr$, and also given that $\lambda = \frac{h}{p}$, derive the origin of quantized rotation [5]

i) The energy levels of a hydrogenic atom are given by the following equation:

$E_n = -\frac{R_H hcZ^2}{n^2}$, where R_H is the Rydberg constant, Z is the nuclear charge and n = 1, 2, 3,....

i. Calculate the wavelength of a photon emitted when an electron goes from n = 3 to n = 2 in the hydrogenic atom He^+ [4]

ii. What is the wavenumber of the first line in the Lyman series of He^+? (For Lyman series, $n_2 \rightarrow n_l$, with $n_l = 1$, $n_2 = 2, 3...$ [3]

j) The wave function for a 2s orbital of a hydrogen atom is

$\psi_{2s} = N(2 - r/a_0)e^{-\frac{r}{2a_0}}$. Determine the normalization constant N. [6]

SECTION B

QUESTION 1 (25 MARKS)

a) Consider a particle of mass m confined in a cubic box of edge L. The potential energy inside the box is zero and infinity outside the box.

i. Write the Hamiltonian for the particle inside the box [1]

ii. Write the Schrodinger equation for this system [1]

iii. Without doing any calculations, use the solutions of the particle in a one dimensional box (given below) to write the solutions for the above Schrodinger equation and the expression for energy of the system. [4]

iv. What is the degeneracy of the energy level $\frac{18h^2}{8mL^2}$? [4]

NB: For a particle in a one dimensional box of length L, $\psi(x) = \left(\frac{2}{L}\right)^{\frac{1}{2}} \sin\left(\frac{n\pi x}{L}\right)$

where n= 1, 2, 3,... and $E_n = \frac{n^2h^2}{8mL^2}$

b) The harmonic oscillator may be used for a model for molecular vibrations, considering the masses connected by spring-like bonds. The molecule vibrates like a harmonic oscillator with mass equal to the reduced mass of the atoms of the molecule.

i. Calculate the reduced mass of an HBr molecule (atomic masses are 1.0078 u and 79.90 u for H and Br, respectively. [3]

ii. The vibrational frequency of the HBr molecule is $v = 7.944 \times 10^{13}\ s^{-1}$. Find the bond force constant k_f. [4]

c) Find the most probable value(s) of x for a harmonic oscillator in its ground state, $\psi_0 = Ne^{-ax^2}$, a is a constant. [3]

d) The wavefunction of a particle rotating on a ring is given by $\psi(\phi) = \frac{1}{\sqrt{2\pi}} e^{-im_l\phi}$, $m_l = 0, \pm1, \pm 2, \ldots$ Calculate the expectation value of ϕ. [5]

QUESTION 2 (25 MARKS)

(a) Briefly explain the relationship between the Heisenberg uncertainty principle and the commutation of operators. [5]

(b) Given that $\hat{A} = \frac{d}{dx}$ and $\hat{B} = x^2$ find the commutator $[\hat{A}, \hat{B}]$. [5]

(c) A particle is in a state described by the function $\psi(x) = 0.632e^{2ix} + 0.775e^{-2ix}$. What is the probability that the particle will be found with momentum $2\hbar$? [4]

(d) Consider the function $f(x) = xe^{-x^2/2}$ $\quad -\infty \leq x \leq \infty$

i. Normalize f(x) [6]

ii. Find the average value of x [5]

QUESTION 3 [25 MARKS]

a) For a monatomic gas, one measure of the average speed of the atoms is the root mean speed, $v_{rms} = \langle v^2 \rangle^{1/2} = \left(\frac{3kT}{m}\right)^{\frac{1}{2}}$, in which m is the mass of the gas atom and k is the Boltzmann constant. Use this formula and any other information to calculate the de Broglie wavelength for the xenon atoms at 100K and 500K. [6]

b) The following data were observed in an experiment on the photoelectric effect from Potassium:

Kinetic Energy $x10^{9}J$	4.49	3.09	1.89	1.34	0.700	0.311
Wavelength, nm	250	300	350	400	450	500

Use the above information to determine the value of Planck's constant, work-function and the threshold frequency of potassium. [8]

c) In an experiment, the position of an electron can be measured with an accuracy of ±0.005nm.

   i. What will be the accuracy in measuring the momentum of the electron [3]

   ii. What will be the accuracy in measuring the speed of the electron? [3]

d) The work-function of Pd is 4.98eV

   i. What is the maximum kinetic energy of photons ejected from Pd when irradiated with UV light of 200nm wavelength? [2]

   ii. What is the wavelength associated with the electron travelling at this velocity [3]

Total Marks /100/

Useful Integrals

1. $\int x^2 e^{-x^2} dx = \frac{\sqrt{\pi}}{2}$
2. $\int x^3 e^{-x^2} dx = 0$
3. $\int_0 x^n e^{-ax} dx = \frac{n!}{a^{n+1}}$
4. $\int sin\theta d\theta = -cos\theta + constant$
5. $d\tau = r^2 sin\theta dr d\theta d\phi$
6. $\int x^n dx = \frac{1}{a^{n+1}} \qquad n \neq -1$
7. $\int_0^{2\pi} cos^2\theta sin\theta d\theta = \frac{2}{3}$

General data and fundamental constants

Quantity	Symbol	Value
Speed of light	c	$2.997\,924\,58 \times 10^{8}$ m s^{-1}
Elementary charge	e	$1.602\,177 \times 10^{-19}$ C
Faraday constant	$F = N_A e$	9.6485×10^{4} C mol^{-1}
Boltzmann constant	k	$1.380\,66 \times 10^{-23}$ J K^{-1}
Gas constant	$R = N_A k$	$8.314\,51$ J K^{-1} mol^{-1}
		$8.205\,78 \times 10^{-2}$ dm^{3} atm K^{-1} mol^{-1}
		6.2364×10 L Torr K^{-1} mol^{-1}
Planck constant	h	$6.626\,08 \times 10^{-34}$ J s
	$\hbar = h/2\pi$	$1.054\,57 \times 10^{-34}$ J s
Avogadro constant	N_A	$6.022\,14 \times 10^{23}$ mol^{-1}
Atomic mass unit	u	$1.660\,54 \times 10^{-27}$ Kg
Mass		
electron	m_e	$9.109\,39 \times 10^{-31}$ Kg
proton	m_p	$1.672\,62 \times 10^{-27}$ Kg
neutron	m_n	$1.674\,93 \times 10^{-27}$ Kg
Vacuum permittivity	$\varepsilon_0 = 1/c^2\mu_0$	$8.854\,19 \times 10^{-12}$ J^{-1} C^{2} m^{-1}
	$4\pi\varepsilon_0$	$1.112\,65 \times 10^{-10}$ J^{-1} C^{2} m^{-1}
Vacuum permeability	μ_0	$4\pi \times 10^{-7}$ J s^{2} C^{-2} m^{-1}
		$4\pi \times 10^{-7}$ T^{2} J^{-1} m^{3}
Magneton		
Bohr	$\mu_B = e\hbar/2m_e$	$9.274\,02 \times 10^{-24}$ J T^{-1}
nuclear	$\mu_N = e\hbar/2m_p$	$5.050\,79 \times 10^{-27}$ J T^{-1}
g value	g_e	2.002 32
Bohr radius	$a_0 = 4\pi\varepsilon_0\hbar/m_e e^2$	$5.291\,77 \times 10^{-11}$ m
Fine-structure constant	$\alpha = \mu_0 e^2 c/2h$	$7.297\,35 \times 10^{-3}$
Rydberg constant	$R_\infty = m_e e^4/8h^3 c\varepsilon_0^{\,2}$	$1.097\,37 \times 10^{7}$ m^{-1}
Standard acceleration of free fall	g	$9.806\,65$ m s^{-2}
Gravitational constant	G	$6.672\,59 \times 10^{-11}$ N m^{2} Kg^{-2}

Conversion factors

1 cal	=	4.184 joules (J)	1 erg	=	1×10^{-7} J
1 eV	=	$1.602\,2 \times 10^{-19}$ J	1 eV/molecule	=	96 485 kJ mol^{-1}

Prefixes

f	p	n	μ	m	c	d	k	M	G
femto	pico	nano	micro	milli	centi	deci	kilo	mega	giga
10^{-15}	10^{-12}	10^{-9}	10^{-6}	10^{-3}	10^{-2}	10^{-1}	10^{3}	10^{6}	10^{9}

PERIODIC TABLE OF ELEMENTS

GROUPS

PERIODS	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
	IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIIIB			IB	IIB	IIIA	IVA	VA	VIA	VIIA	VIIIA
1	1.008 H 1																	4.003 He 2
2	6.941 Li 3	9.012 Be 4											10.811 B 5	12.011 C 6	14.007 N 7	15.999 O 8	18.998 F 9	20.180 Ne 10
3	22.990 Na 11	24.305 Mg 12	TRANSITION ELEMENTS										26.982 Al 13	28.086 Si 14	30.974 P 15	32.06 S 16	35.453 Cl 17	39.948 Ar 18
4	39.098 K 19	40.078 Ca 20	44.956 Sc 21	47.88 Ti 22	50.942 V 23	51.996 Cr 24	54.938 Mn 25	55.847 Fe 26	58.933 Co 27	58.69 Ni 28	63.546 Cu 29	65.39 Zn 30	69.723 Ga 31	72.61 Ge 32	74.922 As 33	78.96 Se 34	79.904 Br 35	83.80 Kr 36
5	85.468 Rb 37	87.62 Sr 38	88.906 Y 39	91.224 Zr 40	92.906 Nb 41	95.94 Mo 42	98.907 Tc 43	101.07 Ru 44	102.91 Rh 45	106.42 Pd 46	107.87 Ag 47	112.41 Cd 48	114.82 In 49	118.71 Sn 50	121.75 Sb 51	127.60 Te 52	126.90 I 53	131.29 Xe 54
6	132.91 Cs 55	137.33 Ba 56	138.91 *La 57	178.49 Hf 72	180.95 Ta 73	183.85 W 74	186.21 Re 75	190.2 Os 76	192.22 Ir 77	195.08 Pt 78	196.97 Au 79	200.59 Hg 80	204.38 Tl 81	207.2 Pb 82	208.98 Bi 83	(209) Po 84	(210) At 85	(222) Rn 86
7	223 Fr 87	226.03 Ra 88	(227) **Ac 89	(261) Rf 104	(262) Ha 105	(263) Unh 106	(262) Uns 107	(265) Uno 108	(266) Une 109	(267) Uun 110								

Atomic mass → 10.811
Symbol → B
Atomic No. → 5

*Lanthanide Series	140.12 Ce 58	140.91 Pr 59	144.24 Nd 60	(145) Pm 61	150.36 Sm 62	151.96 Eu 63	157.25 Gd 64	158.93 Tb 65	162.50 Dy 66	164.93 Ho 67	167.26 Er 68	168.93 Tm 69	173.04 Yb 70	174.97 Lu 71
**Actinide Series	232.04 Th 90	231.04 Pa 91	238.03 U 92	237.05 Np 93	(244) Pu 94	(243) Am 95	(247) Cm 96	(247) Bk 97	(251) Cf 98	(252) Es 99	(257) Fm 100	(258) Md 101	(259) No 102	(260) Lr 103

( ) indicates the mass number of the isotope with the longest half-life.