UNIVERSITY OF SWAZILAND

Re-Sit 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) Briefly outline 3 experiments that drove scientists to view that energy can be transferred only in discrete amounts [12]

b) Show that the operators for position and momentum do not commute [4]

c) What are the advantages of working with normalized wavefunctions [4]

d) Given that an O_2 molecule is confined in one dimensional container of length 5cm.

   i. Calculate the separation between the two lowest energy levels [3]

   ii. At what value of n does the energy of the molecule reach 1/2kT at 300K [3]

   iii. What is the separation of this level (ii above) from the one immediately below it [3]

e) The normalized wavefunction for a particle confined to move on a circle is $\psi(\phi)=\left(\frac{1}{2\pi}\right)^{\frac{1}{2}}e^{im\phi}$ where $m=0,\pm1,\pm2,\ldots$, Determine $\langle\phi\rangle$. [5]

f) Determine whether the angular momentum operator, expressed in cylindrical coordinates, $\left(\hat{l}_z=\frac{\hbar\partial}{i\partial\phi}\right)$, has the eigenfunction of the form $\psi_{ml}(\phi)=\frac{e^{im\phi}}{(2\pi)^{1/2}}$ [3]

g) The total energy eigenvalues of the hydrogen atom are given by $E_n=-\frac{e^2}{8\pi\varepsilon_0 a_0 n^2}$, n = 1, 2, 3,... and the three quantum numbers associated with the total energy eigenvalues are related by n = 1, 2, 3,...; l = 0, 1, 2,... n − 1; and m_l = 0, ± 1,±2,±3,...,±l. Using the notation ψ_{nlm_l}, list all eigenfunction that have the following energy eigenvalues and hence give the degeneracy of these energy levels:

   i. $E=-\frac{e^2}{32\pi\varepsilon_0 a_0}$ [3]

ii. $E = -\frac{e^2}{72\pi\varepsilon_0 a_0}$ [3]

h) Calculate the mean value of the radius, <r>, at which you would find an electron if the H atom wavefunction is $\psi_{210}(r,\theta,\phi) = \frac{1}{4\sqrt{2\pi a_0^3}}\frac{r}{a_0}e^{-\frac{r}{2a_0}}\cos\theta$ [7]

SECTION B [50 MARKS]

QUESTION 1 (25 MARKS)

a) Explain how Einstein's introduction of quantization of energy accounted for the properties of heat capacity at low temperatures [4]

b) In an x-ray photoelectron experiment, a photon of wavelength 121 pm ejects an electron and it emerges with speed of 5.69 x 10^7 m/s. Calculate the binding energy of the electron. [3]

c) For the following operator and function, show that the function is an eigenfunction of the operator and determine the eigenvalue.

Operator	Eigenfunction	
$\frac{d^2}{dx^2} - 4$	$3\cos 2x$	[3]

d) What is the de Broglie wavelength of an electron accelerated to 100 eV [3]

e) A photon of radiation with a wavelength of 305 nm ejects an electron from a metal with a kinetic energy of 1.77 eV. Calculate the maximum wavelength of radiation capable of ejecting an electron from the metal. [4]

f) By evaluating the commutator, $[x, P_x]$, show whether the operators for position and momentum commute. [4]

g) Two (un-normalized) excited state wavefunctions of the hydrogen atom are

A) $\psi(r) = \left(2 - \frac{r}{a_0}\right) e^{-r/2a_0}$

B) $\psi(r,\theta,\phi) = r \sin\theta \cos\phi e^{-r/2a_0}$

Show that these two functions are mutually orthogonal. [4]

QUESTION 2 (25 MARKS)

a) 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 $2\hbar$ [3]

b) Consider the energy eigenvalues of a particle in a one dimensional box

$E_n = \frac{h^2 n^2}{8mL^2}$, n =1,2,3,...as a function of *n, m* and *L.*

i. By what factor do you need to change the box length **L** to decrease the zero point energy by a factor of 400 for a fixed value of *m*? [3]

ii. By what factor would you have to change ***n*** for fixed values of **L** and **m** to increase the energy by a factor of 400? [3]

iii. By what factor would you have to increase **L** to have the zero point energy of an electron be equal to the zero point energy of a proton? [4]

c) The function $\psi(x) = x\left(1 - \frac{x}{L}\right)$, is an acceptable function for a particle in a one dimensional box of length L and with infinitely high walls.

i. Normalize $\psi(x)$ [6]

ii. Calculate the expectation value <x> [6]

QUESTION 3 [25 MARKS]

a) The force constant of $^{1}H^{19}F$ molecule is 966N/m. [Isotopic masses are ^{1}H 1.0078 u and ^{19}F 18.9984 u].

i. Calculate the zero point vibrational energy of this molecule [5]

ii. If this amount of energy were to be converted to translational energy, how fast would the molecule be moving? [3]

iii. Calculate the frequency of light needed to excite the molecule from the ground state to the first excited state. [3]

b) A gas phase $^{1}H^{19}F$ molecule, with a bond length of 91.7 pm, rotates in a three dimensional space. Calculate the smallest quantum of energy that can be absorbed by this molecule in a rotational state. [4]

c) Consider a one dimensional harmonic oscillator

i. Write down the expression for the energy and define all terms [4]

ii. Assuming that the vibrations of a $^{14}N_2$ molecule are equivalent to those of a harmonic oscillator with force constant k = 2293.8N/m, what is the zero point energy of vibration of this molecule. [Take the mass of ^{14}N to be 14.0041 u]. [4]

iii. Calculate the wavelength of a photon needed to excite a transition between neighboring levels in the nitrogen molecule. [2]

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

Atomic mass → Symbol → Atomic No.

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								

*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.