King's College London

UNIVERSITY OF LONDON

B.Sc. EXAMINATION

CP/2201 Introduction to Quantum Mechanics

Summer 2004

Time allowed: THREE Hours

Candidates should answer no more than SIX parts of SECTION A, and no more than TWO questions from SECTION B. No credit will be given for answering further questions.

The approximate mark for each part of a question is indicated in square brackets.

You must not use your own calculator for this paper. Where necessary, a College calculator will have been supplied.

TURN OVER WHEN INSTRUCTED

Physical Constants

Permittivity of free space	ϵ_0	$=$	8.854×10^{-12}	$\mathrm{F\,m^{-1}}$
Permeability of free space	μ_0	$=$	$4\pi \times 10^{-7}$	$\mathrm{H\,m^{-1}}$
Speed of light in free space	c	$=$	2.998×10^{8}	$\mathrm{m\,s^{-1}}$
Gravitational constant	G	$=$	6.673×10^{-11}	$\mathrm{N\,m^2\,kg^{-2}}$
Elementary charge	e	$=$	1.602×10^{-19}	C
Electron rest mass	m_{e}	$=$	9.109×10^{-31}	kg
Unified atomic mass unit	m_{u}	$=$	1.661×10^{-27}	kg
Proton rest mass	m_{p}	$=$	1.673×10^{-27}	kg
Neutron rest mass	m_{n}	$=$	1.675×10^{-27}	kg
Planck constant	h	$=$	6.626×10^{-34}	$\mathrm{J\,s}$
Boltzmann constant	k_{B}	$=$	1.381×10^{-23}	$\mathrm{J\,K^{-1}}$
Stefan-Boltzmann constant	σ	$=$	5.670×10^{-8}	$\mathrm{W\,m^{-2}\,K^{-4}}$
Gas constant	R	$=$	8.314	$\mathrm{J\,mol^{-1}\,K^{-1}}$
Avogadro constant	N_{A}	$=$	6.022×10^{23}	$\mathrm{mol^{-1}}$
Molar volume of ideal gas at STP		$=$	2.241×10^{-2}	$\mathrm{m^3}$
One standard atmosphere	P_0	$=$	1.013×10^{5}	$\mathrm{N\,m^{-2}}$
Bohr magneton	μ_B	$=$	9.274×10^{-24}	$\mathrm{J\ T^{-1}}$

The Pauli spin matrices are

$$\mathbf{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \mathbf{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \mathbf{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

$$\int_{-\infty}^{\infty} \exp(-\alpha x^2) dx = \sqrt{\frac{\pi}{\alpha}}.$$

$$\sin^2\theta = \frac{1-\cos 2\theta}{2}$$

SECTION A – Answer SIX parts of this section

1.1) A particle is confined in a region of length L along the x axis. Wavefunctions for the particle are $\psi(x) = \exp(ikx)/\sqrt{L}$ where $k = 2n\pi/L$ and n is an integer. Show that any two states which have different values of n are orthogonal.

[7 marks]

1.2) A particle is confined in a region of length L along the x axis and has a normalised wavefunction of $\psi(x) = \exp(ikx)/\sqrt{L}$. What is the expectation value of the operator $-i\hbar d/dx$, and what physical quantity does this value represent?

1.3) An electron is trapped in a length $\Delta x = 0.5$ nm. Estimate the uncertainty in its momentum. At time $t = 0$ the barriers trapping the electron are removed. Over what range of x is the electron likely to be found at $t = 1$ ns?

[7 marks]

1.4) Electrons in the atoms of a gas are excited to a state that has a lifetime of 10 ns before they emit a photon by de-exciting to a lower energy state in the atom. Estimate the minimum spread in energy of the photons emitted by the gas. The mean energy of the photons is $h\nu = 2.5$ eV. What is the spread in energy as a fraction of $h\nu$?

[7 marks]

1.5) The normalised state of a harmonic oscillator is described by a wavefunction

$$\psi(x) = \sqrt{\frac{1}{6}}u_0(x) + \sqrt{\frac{1}{3}}u_1(x) + \sqrt{\frac{1}{2}}u_2(x),$$

where $u_n(x)$ is the nth normalised energy eigenfunction of the oscillator, corresponding to an eigenvalue $E_n = (n + \frac{1}{2})\hbar\omega$, $n = 0,\ 1,\ 2, \ldots$. What are the possible results of a measurement of the energy of this system, and what are their relative probabilities? Using these probabilities, show that the expectation value of the energy of the oscillator is $(11/6)\hbar\omega$.

[7 marks]

1.6) A rotational state of a molecule has an energy given by $E = l(l+1)\hbar^2/2I$, where l is an integer and I is the moment of inertia. Calculate the energy diference, in Joules, between the $l = 0$ and $l = 1$ states of $^{12}C^{16}O$, given that the bond length is 0.1121 nm.

[7 marks]

1.7) An electron orbits an atom with an orbital quantum number $l = 1$. A magnetic field of 5 Tesla is applied to the atom. Write down expressions for the components of the angular momentum along the field direction. What are the changes in the energy of the electron, in Joules, resulting from the interaction of the orbital angular momentum and the magnetic field?

[7 marks]

1.8) Show that the eigenvalues of the Pauli spin matrix S_z are $\pm\frac{1}{2}\hbar$, with corresponding normalised eigenvectors

$$\psi_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \text{and} \quad \psi_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

[7 marks]

SECTION B – Answer TWO questions

2) A particle of mass m is completely confined in a three-dimensional cubic 'box' of edge-length a.

a) Write down the time-independent Schrödinger equation for the particle, and solve it to show that the allowed energy levels of the particle are

$$E = \frac{\left(n_1^2 + n_2^2 + n_3^2\right) h^2}{8ma^2},$$

where $n_1,\ n_2,\ n_3 = 1, 2, 3, \ldots$

[11 marks]

b) Derive an expression for the normalised wavefunction of the state of lowest energy, and show that the probability density P of the particle at the centre of the box is $P = 8/a^3$.

[9 marks]

c) A 'quantum dot' is made from a cube of silicon of edge $a = 2.0$ nm embedded inside a piece of quartz. Using m_e for the mass of the electron, what is the energy E_0, in Joules, of the lowest energy state of an electron in the dot?

[3 marks]

d) What is the fractional variation in E_0 if the dot is not a cube, but is a cuboid with edge-lengths 2 nm, 2 nm and 1.8 nm?

[4 marks]

e) Describe briefly how one can measure differences in size of a series of quantum dots that are buried inside another material.

[3 marks]

3) A particle of mass m that moves in one dimension (the x dimension) in a potential $V(x) = \frac{1}{2}m\omega^2x^2$ will perform harmonic oscillations about $x = 0$ with an angular fequency ω.

a) Write down the time-independent Schrödinger equation for the particle.

[2 marks]

b) Given that the lowest energy state has an un-normalised eigenfunction

$$\psi_0(x) = N \exp\left(-\alpha x^2/2\right),$$

where $\alpha = m\omega/\hbar$, show that normalisation requires $N = (\alpha/\pi)^{1/4}$.

[4 marks]

c) Show that the energy of this state is $E_0 = \hbar\omega/2$.

[9 marks]

d) Using the wavefunction $\psi_0(x)$, show that the probability of finding the particle in a very small length Δx centred at $x = 0$ is

$$\sqrt{\frac{\alpha}{\pi}}\Delta x.$$

[3 marks]

e) An atom of hydrogen (^{1}H) inside a crystal of silicon is observed to vibrate with an angular frequency of $\omega = 4.15 \times 10^{14}$ rad / s.

What is the probability of finding the hydrogen atom within 0.001 nm of the point $x = 0$ in its lowest energy state?

What is the fractional change in this probability if the hydrogen atom is replaced by a deuterium atom (^{2}H)?

[12 marks]

4) A beam of particles, each of mass m and energy E, travels in a region of zero potential energy from $x = -\infty$ in the positive x direction. At $x = 0$ the beam hits a potential step of height $V_0 > E$ which continues for all positive x. The wavefunction of the incident particles is represented by $A_0 \exp(ikx)$ where

$$k^2 = \frac{2mE}{\hbar^2}.$$

We will also define

$$\alpha^2 = \frac{2m(V_0 - E)}{\hbar^2}.$$

a) Write down the Schrödinger equations for the regions $x < 0$ and $x > 0$, and find the corresponding wavefunction for a particle at $x > 0$.

[6 marks]

b) Derive an expression in terms of α and k for the reflection coefficient R at the potential step.

[12 marks]

c) Justify your answer in terms of the physical situation.

[2 marks]

d) A beam of electrons of kinetic energy 1.0 eV hits a step potential of height 1.5 eV at $x = 0$. What is the ratio of the probability function $|\psi(x)|^2$ predicted at $x = +0.1$ nm and at $x = +0.2$ nm?

[10 marks]

5) The normalised wavefunction for the ground state of the H atom is a function of only the radial distance r of the electron from the nucleus :

$$\psi(r) = \frac{2}{a_0^{3/2}} \exp\left(-\frac{r}{a_0}\right),$$

where a_o is the 'Bohr radius'.

a) Find the value of r at which the probability of finding the electron is maximum.

[10 marks]

When the operator ∇^2 operates on a function $\psi(r)$ that only depends on r and not θ or ϕ,

$$\nabla^2\psi(r) = \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)\psi(r).$$

b) Write down the time-independent Schrödinger equation for the hydrogen atom in its ground state.

Assuming that the mass of the electron is negligible in comparison to that of the proton, show that $\psi(r)$ is an eigenfunction of the Hamiltonian only if

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_{\mathrm{e}}e^2}.$$

[10 marks]

c) Show that the energy of this state corresponds to the $n = 1$ state in the general expression

$$E_n = -\frac{m_{\mathrm{e}}e^4}{32\pi^2\epsilon_o^2\hbar^2 n^2}.$$

[3 marks]

d) What is the energy of a photon emitted when the atom makes a transition from the $n = 2$ state to the $n = 1$ state?

[2 marks]

e) Write down an expression for the effective mass of the electron orbitting a proton. What is the approximate fractional change in the energy of the photon when the atom is deuterium (^{2}H) instead of hydrogen (^{1}H)?

[5 marks]