

**Answer SIX questions from section A and THREE questions from section B.**

The numbers in square brackets in the right-hand margin indicate the provisional allocation of maximum marks per sub-section of a question.

SECTION A

[Part marks]

1. Briefly describe the 1991 experiment of Carnal and Mlynek and its implications for our understanding of wave-particle duality. [7]

2. State the **time-dependent** Schrödinger equation for a particle moving in a one-dimensional potential  $V(x, t)$ . [2]

If the potential is not explicitly time-dependent, show that the wavefunction, at fixed energy  $E$ , takes the general form  $u(x) \exp(-iEt/\hbar)$ . [5]

3. Describe the tunnelling phenomenon of quantum mechanics. [3]  
Briefly discuss a physical process in which it is important. [4]

4. A particle in an infinite symmetrical well ( $V = 0$  if  $|x| < a$  and  $V = \infty$  elsewhere) has wavefunction  $u(x) = A \sin \frac{\pi x}{a}$ . Calculate the expectation value of  $\hat{P}_x$ . [5]

Sketch the probability of finding the particle at any point in the well. [2]

5. The operators corresponding to components of quantum angular momentum obey the relations  $[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z$ . What is the physical significance of this result? [2]

The ladder operators are defined by  $\hat{L}_{\pm} = \hat{L}_x \pm i\hat{L}_y$ . Evaluate  $[\hat{L}_+, \hat{L}_-]$ . [5]

6. An atom has the normalised angular wavefunction:

$$u(\theta, \phi) = \frac{1}{\sqrt{3}}Y_{11}(\theta, \phi) + \frac{1}{\sqrt{6}}Y_{21}(\theta, \phi) + \frac{1}{\sqrt{2}}Y_{10}(\theta, \phi),$$

where the  $Y$  are spherical harmonics. Give the probability that its orbital angular momentum squared ( $L^2$ ) would be measured to be equal to  $2\hbar^2$ . [3]

Given the above wavefunction, work out the expectation value of  $\hat{L}_z$ . [4]

7. A level of a given multi-electron atom is denoted by  ${}^3D_1$ . Explain the meaning of this symbol in full. [3]

An excited state of helium has a configuration  $2p3d$ . Give all the corresponding terms in spectroscopic notation. [4]

8. The Zeeman effect can be modelled by adding a small extra term to the Hamiltonian (in atomic units):

$$\hat{V} = \frac{B}{2}(\hat{L}_z + 2\hat{S}_z).$$

Explain the physical origin of the terms on the right hand side. [4]

A particular atom has been assigned quantum numbers  $S = 0$ ,  $L = 2$ . How many Zeeman levels would one expect to observe? Give their quantum numbers. [3]

## SECTION B

9. Explain what is meant by the Heisenberg Uncertainty Principle for positions and momenta of a quantum particle. Discuss our current understanding of the Uncertainty Principle by considering in detail *two* of the following: [4]

(a) The Bohr microscope thought experiment

(b) The commutation relations  $[\hat{P}_x, \hat{x}]$  and  $[\hat{P}_y, \hat{x}]$  explaining their relevance to the Uncertainty Principle.

(c) The probability distribution of position and momentum coordinates of a *gaussian* wavepacket where the probability amplitudes in  $k$  is given by

$A(k) = \exp\{-\alpha(k - k_0)\}^2$ , where  $P = \hbar k$  is the momentum and  $k_0$  is a constant. [16]

10. A one-dimensional potential step is defined by:

Region 1 :  $x \leq 0$  ,  $V = 0$

Region 2 :  $x > 0$  ,  $V = V_0$

A particle approaches the step with energy  $E < V_0$  from region 1.

(a) Write down model solutions  $u(x)$  to the Schrödinger equation in terms of reflected amplitudes  $R$  and transmitted amplitudes  $T$  as well as two wavenumbers  $k$  and  $q$  relevant to region 1 and 2 respectively, explaining your answers and defining the wavenumbers. [8]

(b) By matching wavefunctions and derivatives, obtain the transmitted and reflected amplitudes in terms of  $k$  and  $q$ . [8]

(c) If  $|q| = 1/2$  evaluate the ratio  $|u(0)|^2 : |u(1)|^2$  explaining the physical significance of this quantity. [4]

11. A particle moves in a one-dimensional potential well, with a potential  $V = V_0$  for  $|x| > a$  and  $V = 0$  elsewhere. If  $E < V_0$ , the solution for the Time Independent Schrödinger equation (TISE) takes a different form in each of three spatial regions:  
 Region 1 :  $u_1(x) = C \exp(-Px)$   
 Region 2 :  $u_2(x) = D \exp(+Px)$   
 Region 3 :  $u_3(x) = A \cos Kx + B \sin Kx$ .  
 (a) Give the TISE for each of the three regions and identify the range of  $x$  corresponding to each of the three regions, justifying the form of the solutions. [10]

(b) Prove that, if  $B = 0$ , then:

$$\frac{P}{K} = \tan Ka$$
 [6]

(c) In this case, what is the maximum number of quantum states with energy  $E < (5^2 \hbar^2 \pi^2) / (8ma^2)$  ? [4]

12. In the context of dipole radiative transitions of hydrogen, explain briefly the form of the interaction between the atom and the electromagnetic radiation [4]

State the general **selection rules** on the angular momentum quantum numbers  $lm$ , for electric dipole transitions in the hydrogen atom and show, on an energy level diagram, the possible transitions among  $nl$  states with principal quantum number  $1 < n < 5$ . [8]

It can be shown rigorously that, within the dipole approximation, the probability  $P$  for a transition between two levels of hydrogen characterised by quantum numbers  $nlm$  and  $n'l'm'$  obeys the relation:

$$P \propto \left| \int Y_{lm}^*(\theta, \phi) V(\theta, \phi) Y_{l'm'}(\theta, \phi) \sin \theta d\phi d\theta \right|^2$$

where  $V$  represents the interaction with the radiation and the  $Y_{lm}$  are spherical harmonics.

(a) If we choose the photon polarization such that we can take  $V(\theta, \phi) = \epsilon \cos \theta$  show that there is a specific selection rule for the  $m$  quantum number,  $\Delta m = 0$ . [4]

(b) Derive the corresponding selection rules for the case  $V = \epsilon \cos \theta \sin \phi$ . [4]

You can use the fact that the general form of a spherical harmonic is  $Y_{lm}(\theta, \phi) = N P_{lm}(\theta) \exp\{im\phi\}$ , where  $N$  is a normalization constant and the  $P_{lm}$  are functions of  $\theta$ .

13. The radial Schrödinger equation, in atomic units, for an electron in a hydrogen atom for which the orbital angular momentum quantum number,  $\ell = 0$ , is

$$\left( \frac{d^2}{dr^2} + \frac{2}{r} + 2E \right) F(r) = 0,$$

where  $E$  is the total energy.

- (a) Put  $F(r) = \exp(-r/\nu)y(r)$ , where  $E = -1/(2\nu^2)$ , and show that

$$\frac{d^2y}{dr^2} = \frac{2}{\nu} \left( \frac{d}{dr} - \frac{\nu}{r} \right) y. \quad [4]$$

- (b) Assuming that  $y(r)$  can be expanded as the series

$$y(r) = \sum_{p=0}^{\infty} a_p r^{p+1},$$

where  $a_0 \neq 0$ , show that the coefficients  $a_p$  in the series satisfy the recurrence relation,

$$p(p+1)a_p = \frac{2}{\nu}(p-\nu)a_{p-1}. \quad [8]$$

- (c) Solutions of the radial Schrödinger equation exist which are bounded for all  $r$  provided that  $\nu = n$ , where  $n$  is a positive integer. Show that the unnormalized radial function for the  $n = 2$  state is

$$F_{2s}(r) = a_0 r \left( 1 - \frac{r}{2} \right) e^{-\frac{r}{2}}. \quad [4]$$

- (d) Show that the normalisation constant of the 2s state is  $a_0 = \frac{1}{\sqrt{2}}$  and hence determine the expectation value of  $r^2$  for this state. [4]

The following result may be assumed

$$\int_0^{\infty} r^m e^{-\alpha r} dr = \frac{m!}{\alpha^{m+1}}.$$