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

2. Write down the differential operator which represents the kinetic energy of a particle moving in one dimension. [2]
   If the wave function of a particle moving in one dimension is $\Psi(x,t)$, write down an expression for the expectation value of the kinetic energy of the particle. [2]
   What does the expectation value represent in terms of physical measurements of the particle? [3]

3. Define the **commutator** of two operators $\hat{A}$ and $\hat{B}$. [2]
   Show that the commutation relation for the operators, $\hat{x}$ and $\hat{p_x}$ representing position and momentum in one dimension is $[\hat{x}, \hat{p_x}] = i\hbar$ [5]

4. The wave function of a particle moving in one dimension is $\Psi(x,t)$. What is meant by the statement that this wave function is normalised? [3]
   If the particle is localised between $x = 0$ and $x = +a$ and its wave function is $\Psi(x,t) = cx(a-x)\mathrm{e}^{-i\omega t}$, determine the normalisation constant, $c$. [4]

5. State the uncertainty principle for a particle moving in one dimension with momentum variable $p_x$ and position variable $x$. [2]
   Define the uncertainties in momentum and position in terms of the corresponding operators and explain the meaning of these definitions. [5]

6. A particle moves in a one-dimensional finite square potential well with boundaries located at $x = -a$ and $x = +a$. Contrast qualitatively the predictions of classical and quantum mechanics for this system including a sketch of the position probability distribution for the lowest quantum energy state in both cases. [7]

7. Neglecting spin, the bound states of the hydrogen atom are described by the quantum numbers $n, \ell, m_\ell$. Explain their significance and give their possible values. [4]
   What values of these quantum numbers are implied by the spectroscopic notation $4d$ and how many quantum states are included within it? [3]

8. (a) Define, in mathematical terms, an Hermitian operator. [1]
Show that its eigenvalues are always real numbers and that the eigenfunctions of different discrete eigenvalues are orthogonal. [3]
[3]

## SECTION B

9. (a) In Cartesian coordinates the components of the angular momentum vector operator $\hat{\mathbf{L}}$ are related by $[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z$, $[\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x$, $[\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y$. Show that

$$[\hat{L}^2, \hat{L}_z] = 0.$$ [6]

(b) What are the eigenvalues of the operator $\hat{L}^2$ and how are the eigenvalues of $\hat{L}_z$ related to them? [3]

(c) The operators $\hat{L}_z$ and $\hat{L}^2$ can be expressed in terms of the spherical polar angles $(\theta, \phi)$ as

$$\begin{aligned} \hat{L}_z &= -i\hbar\frac{\partial}{\partial\phi}, \\ \hat{L}^2 &= -\hbar^2\left[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right]. \end{aligned}$$

Given the unnormalised spherical harmonic function

$$Y(\theta, \phi) = N e^{i\phi}\sin\theta,$$

where $N$ is a constant, show that $Y(\theta, \phi)$ is an eigenfunction of $\hat{L}_z$ and $\hat{L}^2$ and determine the corresponding eigenvalues. [6]

(d) If the function $Y(\theta, \phi)$ is normalised according to

$$\int_0^{2\pi}\int_0^{\pi} |Y(\theta, \phi)|^2 \sin\theta \, d\theta \, d\phi = 1,$$

determine the constant $N$, [5]

10. The one-dimensional time-independent Schrödinger equation for a particle of mass $m$ moving in a potential $V(x)$ is given by

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right) u(x) = E u(x),$$

where $E$ is the total energy. A potential barrier is defined by

| | | | |
|---|---|---|---|
| Region 1 | $x \leq 0$ | and | $V = 0$ |
| Region 2 | $0 \leq x \leq a$ | and | $V = V_0$ |
| Region 3 | $x \geq a$ | and | $V = \infty$ |

where $V_0$ is positive.

(a) Consider the case where the total energy $E > V_0$. Demonstrate that in Region 1 the Schrödinger equation has the solution

$$u(x) = \mathrm{e}^{ikx} + A\mathrm{e}^{-ikx},$$

where $k^2 = \dfrac{2mE}{\hbar^2}$, and that in Region 2 it has the solution

$$u(x) = B\mathrm{e}^{iqx} + C\mathrm{e}^{-iqx},$$

where $q^2 = \dfrac{2m(E - V_0)}{\hbar^2}$. [4]

(b) State the continuity conditions that must be satisfied by the wave function at $x = 0$ and $x = a$. [3]

(c) From the continuity condition at $x = a$, show that the constants $B$ and $C$ are related by

$$C = -B\mathrm{e}^{2iqa}.$$ [2]

(d) Using this result and the continuity conditions at $x = 0$, show that the transmission coefficient $T = \dfrac{q|B|^2}{k}$, from Region 1 to Region 2 is given by

$$T = \frac{2kq}{(q^2 + k^2) + (q^2 - k^2)\cos 2qa}.$$ [8]

(e) Consider the case where the energy of the incident particles and the barrier width are such that $qa = \dfrac{\pi}{2}$. Determine the wave function $u$ in Regions 1 and 2 and sketch the position probability distribution, $|u|^2$ in all regions. [3]

11. 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

$$\frac{d^2 y}{dr^2} = \frac{2}{\nu}\left(\frac{d}{dr} - \frac{\nu}{r}\right) y.$$ [5]

(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,

$$p(p+1)a_p = \frac{2}{\nu}(p-\nu)a_{p-1}.$$ [7]

(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

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

(d) Given that the normalisation constant of the 2s state is $a_0 = \frac{1}{\sqrt{2}}$ and that the expectation value of $r^n$ is given, in atomic units, by

$$< r^n > = \int_0^{\infty} r^n F^2(r) \mathrm{d}r,$$

determine the expectation value of the Coulomb potential energy for this state. [4]

The following result may be assumed

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

12. Discuss the wave and particle nature of both matter and electromagnetic radiation. Make detailed reference to evidence from the photoelectric effect and the experiment of Davisson and Germer. [20]

13. (a) If $\hat{A}$ is an operator corresponding to a quantum observable and $\left\langle \hat{A} \right\rangle$ the corresponding expectation value, show that

$$\frac{\mathrm{d}\left\langle \hat{A} \right\rangle}{\mathrm{d}t} = \frac{1}{i\hbar}\left\langle \left[\hat{A}, \hat{H}\right] \right\rangle + \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle,$$

where $\hat{H}$ is the time-independent Hamiltonian for the quantum system. [8]

A Hamiltonian for motion in one-dimension is

$$\hat{H} = \frac{\hat{p}_x^2}{2m} - k\hat{x},$$

where $k$ is a constant. Show that the commutators for the operators for position and momentum $\hat{x}$ and $\hat{p}_x$, respectively, are

$$\left[\hat{x}, \hat{H}\right] = \frac{i\hbar \hat{p}_x}{m}\ ; \qquad \left[\hat{p}_x, \hat{H}\right] = ik\hbar.$$ [6]

Hence show that if at time $t = 0$, $\langle \hat{x} \rangle = 0$ and $\langle \hat{p}_x \rangle = 0$, then

$$\langle \hat{p}_x\,(t) \rangle = kt \qquad \text{and} \qquad \langle \hat{x}\,(t) \rangle = \frac{kt^2}{2m}.$$ [6]



**END OF PAPER**