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 Davisson-Germer experiment and its implications for our understanding of wave-particle duality. [7]

2. Prove that if the complete set of functions ϕ_n are simultaneous eigenfunctions of two Hermitian operators $\hat{R}$ and $\hat{Q}$ then $[\hat{R}, \hat{Q}] = 0$. [7]

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

4. Explain the terms **eigenvalue**, **eigenfunction** and **operator** . [5]
   Give an example of an eigenvalue equation other than the Schrödinger equation. [2]

5. The operators corresponding to components of quantum angular momentum obey the relations $[\hat{L}_i, \hat{L}_j] = i\hbar\hat{L}_k$ (where i, j, k represent a cyclic permutation of x, y, z) and $[\hat{L}_z, \hat{L}^2] = 0$. Discuss the physical significance of these commutation relations and the implications for the eigenfunctions and eigenvalues. [7]

6. The wavefunction of a particular quantum particle in a simple harmonic potential is given as $u(x) = e^{-\alpha x^2/2}$. What is meant by the statement that $u(x)$ is not normalised? Explain one important consequence of the eigenfunction not being normalised. [3]
   Give $u(x)$ in normalised form given that,
   $$\int_{-\infty}^{\infty} e^{-\beta y^2} dy = \sqrt{\frac{\pi}{\beta}}.$$
   [4]

7. The wavefunction of an electron in hydrogen is given by: $R_{nl}(r)\ Y_{lm}(\theta, \phi)$. Explain the physical significance of the subscripts n, l, m and give their possible values. [4]
   What quantum numbers are implied by the notation $4f$ and how many states correspond to them? [3]

8. One can model the Zeeman effect 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? [3]

SECTION B

9. A quantum particle moves in a one-dimensional potential well, with a potential $V = 0$ for $0 < x < 2b$ and $V = \infty$ elsewhere.

(a) Show that the corresponding wavefunction satisfies the following equation inside the well,

$$\frac{d^2u(x)}{dx} + \; k^2u(x) = 0.$$

What is the value of k? [6]

(b) By considering appropriate boundary conditions derive the form of the <u>normalised</u> solutions $u_n(x)$ and the values of the eigenvalues E_n. [10]

(c) For what value(s) of x is one most likely to find the particle if it is in the first excited state? [4]

10. (a) The fine-structure splitting for an atom is given by:

$$E_{SO} = \frac{A(L,S)}{2}\; [J(J+1) - L(L+1) - S(S+1)],$$

where A is a constant for given L and S. Hence derive the Landé interval rule. [6]

(b) An atom has a set of terms $^3D^o$, ^3P and ^1S. What levels are involved? (List them in spectroscopic notation). [7]

(c) Sketch a plausible energy level diagram given that the energy $E(^3D^o) > E(^3P) > E(^1S)$. Between which terms are transitions forbidden and which are allowed? [7]

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

$$\text{Region } 1: \; x \leq 0 \;, \; V = 0$$
$$\text{Region } 2: \; x > 0 \;, \; V = V_0$$

A particle approaches the step with energy $E > V_0$ from region 1.
(a) Write down model solutions 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. [6]

(b) Hence show that $T = 2k/(k+q)$ and $R = (k-q)/(k+q)$. [10]

(c) Evaluate the probability flux current $j(x) = \frac{\hbar}{2im}(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x})$ and show that it is conserved across the two regions [4]

12. The operator $\hat{L}_z$ can be expressed in terms of polar angles

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial \phi}.$$

(a) Derive the normalized eigenfunctions of $\hat{L}_z$, hence proving that they take the form $\frac{1}{\sqrt{2\pi}} e^{im\phi}$ and obtain the corresponding eigenvalues. [10]

(b) An electron is described by the following angular wavefunction:

$$u(\theta, \phi) = \frac{1}{4}\sqrt{\frac{15}{\pi}} \sin^2 \theta \cos 2\phi.$$

Re-express u in terms of spherical harmonics given below. Hence give the probability that a measurement will yield the eigenvalue of $\hat{L}^2$ equal to $6\hbar^2$. [6]

(c) What is the probability that $u(\theta, \phi)$ will yield the eigenvalue of $\hat{L}_z$ (i) equal to $2\hbar$? (ii) equal to zero? [4]

You may use the following:
$Y_{20}(\theta, \phi) = \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1)$
$Y_{2\pm1}(\theta, \phi) = \pm\sqrt{\frac{15}{8\pi}} \sin\theta \cos\theta e^{\pm i\phi}$
$Y_{2\pm2}(\theta, \phi) = \sqrt{\frac{15}{32\pi}} \sin^2\theta e^{\pm 2i\phi}$

13. The radial Schrödinger equation, in atomic units, for an electron in a hydrogenic ion of nuclear charge Z is

$$\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + \frac{2Z}{r} + 2E\right) F(r) = 0,$$

where E is the total electron energy and ℓ is the orbital angular momentum quantum number.

(a) By making the substitution $\rho = Zr$, show that

$$\left(\frac{d^2}{d\rho^2} - \frac{\ell(\ell+1)}{\rho^2} + \frac{2}{\rho} + \frac{2E}{Z^2}\right) F(\rho) = 0.$$

[5]

(b) The series solution of this equation can be written

$$F(\rho) = \mathrm{e}^{-\frac{\ell}{\nu}} \rho^{\ell+1} \sum_{k=0}^{\infty} a_k \rho^k,$$

where the coefficients in the summation are related by the recurrence relation

$$k(2\ell + 1 + k)a_k = \frac{2}{\nu}(\ell + k - \nu)a_{k-1},$$

where $a_0 \neq 0$ and ν is defined by $E = \frac{-Z^2}{2\nu^2}$. Solutions of the radial Schrödinger equation exist which are bounded for all r provided that $\nu = n$, where n is a positive integer. If the solutions are normalised so that

$$\int_0^\infty F^2(r)\mathrm{d}r = 1,$$

show that for the 2s state,

$$F(r) = \left(\frac{Z}{2}\right)^{\frac{1}{2}} (Zr)(1 - \frac{Zr}{2})\mathrm{e}^{-Zr/2}.$$

[8]

(c) The *Darwin* term is a relativistic correction to the energies of the s states in hydrogenic systems whose magnitude is $D = \frac{1}{8} Z\alpha^2 \lim_{r\to 0} \left(\frac{F(r)}{r}\right)^2$, where $\alpha = 1/137$ is the fine-structure constant. Use the series solution to show that the Darwin correction for a general s state is $D = \frac{1}{8} Z^3 \alpha^2 a_0^2$, where a_0 is the leading coefficient in the above expansion. [4]

(d) Calculate the magnitude of the correction for the 2s state in hydrogen-like iron ($Z = 26$) as a fraction of the ionization energy of that state. [3]

The following result may be assumed: $\int_0^\infty r^m \mathrm{e}^{-\alpha r} dr = \frac{m!}{\alpha^{m+1}}$.

END OF PAPER