Answer ALL SIX questions from Section A and THREE questions from Section B.

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

You may assume the following values:

Planck constant $h = 6.63 \times 10^{-34}\,\mathrm{J\,s}$; $\hbar = 1.05 \times 10^{-34}\,\mathrm{J\,s}$;

Electronic charge $e = 1.60 \times 10^{-19}\,\mathrm{C}$;

Mass of electron $m_e = 9.11 \times 10^{-31}\,\mathrm{kg}$;

Bohr magneton $\mu_B = \frac{e\hbar}{2m_e} = 9.27 \times 10^{-24}\,\mathrm{J\,T^{-1}}$.

SECTION A

[Part marks]

1. Sketch the setup of a Compton scattering experiment. Give a brief description of the results, including a formula (which you need *not* derive) for the change in wavelength of the scattered radiation. **[5]**

   What do the results tell us about the nature of electromagnetic radiation in quantum physics? (No mathematical derivations required.) **[2]**

2. State the Born interpretation of the wave-function $\Psi(x,t)$ in quantum mechanics in one dimension. **[2]**

   State *three* conditions that the wave-function of a particle must satisfy in order to be physically admissable. **[6]**

3. Explain what is meant by the concept of “tunnelling” in quantum mechanics. **[3]**

   Give one example of a physical process in which tunnelling is important, and explain why. **[3]**

4. How is the *expectation value* of an operator related to the results of many measurements on an ensemble of identically prepared quantum systems? **[2]**

Suppose $\psi(x)$ is a normalized solution to the time-independent Schrödinger equation of a particular one-dimensional system. Give *two* expressions for the expectation value of a Hermitian operator $\hat{O}$ in the state ψ. The first expresssion should involve $\psi(x)$ directly. The second should involve the eigenvalues o_n of $\hat{O}$, and the coefficients c_n defined by

$$\psi(x) = \sum_n c_n \phi_n(x),$$

where the $\phi_n(x)$ are the orthonormal eigenfunctions of $\hat{O}$. **[4]**

5. Give the defining equation for the *eigenfunction* and an *eigenvalue* of an operator $\hat{O}$, defining the symbols appearing in it. **[3]**

In spherical polar coordinates (r, θ, ϕ) the angular momentum operator is

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

An eigenfunction $f_m(\phi)$ of $\hat{L}_z$ has the form

$$f_m(\phi) = C \exp(\mathrm{i}m\phi),$$

where C and m are constants. What is the corresponding eigenvalue of $\hat{L}_z$? **[4]**

6. If we neglect spin, an electron in a hydrogen atom is described by three quantum numbers: n, l and m. Explain the physical significance of the quantum numbers l and m. **[2]**

For a given n, what are the possible values of l? **[2]**

For a given l, what are the possible values of m? **[2]**

SECTION B

7. The time-*dependent* Schrödinger equation obeyed by the wavefunction $\Psi(x,t)$ for a particle moving in one dimension through a potential $V(x,t)$ is

$$\mathrm{i}\hbar\frac{\partial\Psi}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x,t)\Psi(x,t).$$

Suppose the potential energy V is independent of time and depends on position only: $V = V(x)$. Separate the position and time variables by writing the wavefunction as $\Psi(x,t) = \psi(x)T(t)$. Hence show that the spatial function $\psi(x)$ obeys the time-*independent* Schrödinger equation, and show that

$$T(t) = \exp(-\mathrm{i}Et/\hbar)$$

where E is a constant. **[6]**

What is the physical interpretation of the constant E? **[2]**

A beam of particles (with mass m) moving in free space where $V(x) = 0$ is described by the following plane-wave state:

$$\psi(x) = \exp(\mathrm{i}kx).$$

Show that this is a solution to the time-independent Schrödinger equation, and find the energy in terms of k. **[2]**

What is the corresponding time-dependent solution $\Psi(x,t)$? **[3]**

Show that the probability per unit length of finding a particle is a constant (independent of both space and time). **[2]**

Evaluate the probability flux (mean number of particles passing a point per unit time) for the state $\psi(x)$. Give a physical interpretation of your answer in terms of the velocity of the particles. **[5]**

[The probability flux is

$$\Gamma(x) = \frac{-\mathrm{i}\hbar}{2m}\left[\Psi^*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x}\right]$$

at position x.]

8. A beam of particles, having mass m and energy E and moving in one dimension is incident from the left on a potential barrier in which the potential energy is:

$$V(x) = \begin{cases} 0 & \text{Region 1} \quad (x < 0); \\ V_2 & \text{Region 2} \quad (0 \leq x < a); \\ V_3 & \text{Region 3} \quad (x \geq a), \end{cases}$$

where V_2 and V_3 are constants and $0 \leq V_3 \leq V_2$. There is no incoming beam from the right.

Sketch the potential energy $V(x)$. **[2]**

What *two* conditions must apply to the wavefunction at each junction between different regions? **[2]**

The wavefunction in Region 1 consists of an incident wave from the left, plus a reflected wave:

$$\psi_1(x) = \exp(\mathrm{i}k_1 x) + r \exp(-\mathrm{i}k_1 x),$$

where $E = \hbar^2 k_1^2/2m$ and r is a complex constant to be determined. Assume that the energy E is such that $0 < E < V_2$. Write down expressions for

(a) the wavefunction in Region 2, in terms of the parameter $\kappa_2 = \sqrt{2m(V_2 - E)}/\hbar$, and

(b) the wavefunction in Region 3. Here, distinguish between the cases where

(i) $E < V_3$ and

(ii) $E > V_3$;

In case (i) define the parameter $\kappa_3 = \sqrt{2m(V_3 - E)}/\hbar$ and in case (ii) define $k_3 = \sqrt{2m(E - V_3)}/\hbar$.

In each case take care to include a sufficient number of arbitrary constants in your answer, and to explain which terms (if any) are ruled out by the boundary conditions at infinity. **[9]**

In the case (i) above (where $0 < E < V_3$), write down the four matching conditions satisfied by the wavefunction. **[4]**

In this case, the matching conditions may be solved to show that

$$r = \frac{\mathrm{i}k_1(\alpha + \beta) - \kappa_2(\alpha - \beta)}{\mathrm{i}k_1(\alpha + \beta) + \kappa_2(\alpha - \beta)},$$

where α and β are real quantities that depend on κ_2 and κ_3. (You are *not* required to obtain this result yourself.) What is the probability that the particles are reflected from the potential barrier? **[3]**

9. Define the *commutator* $[\hat{A}, \hat{B}]$ of two operators $\hat{A}$ and $\hat{B}$. **[2]**

Show that

(i) $[\hat{A} + \hat{B}, \hat{C}] = [\hat{A}, \hat{C}] + [\hat{B}, \hat{C}]$;

(ii) $[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}$.

[4]

Hence show that

(i) $[\hat{L}_x + \mathrm{i}\hat{L}_y, \hat{L}_z] = -\hbar(\hat{L}_x + \mathrm{i}\hat{L}_y)$;

(ii) $[\hat{L}^2, \hat{L}_z] = 0$,

where $(\hat{L}_x, \hat{L}_y, \hat{L}_z)$ are the components of the angular momentum vector and $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$. **[6]**

Two operators in quantum mechanics are *compatible* if they share the same eigenfunctions. Use the expansion postulate to show that if $\hat{A}$ and $\hat{B}$ are compatible operators, then $[\hat{A}, \hat{B}] = 0$. **[4]**

The total angular momentum, $\hat{L}^2$, the z-component of angular momentum, $\hat{L}_z$, and the Hamiltonian are all compatible operators (provided the spin of the electron is neglected). What is the consequence of this fact for the energy levels of the hydrogen atom? **[4]**

[The commutation relations of the angular momentum components are:

$$[\hat{L}_x, \hat{L}_y] = \mathrm{i}\hbar\hat{L}_z; \quad [\hat{L}_y, \hat{L}_z] = \mathrm{i}\hbar\hat{L}_x; \quad [\hat{L}_z, \hat{L}_x] = \mathrm{i}\hbar\hat{L}_y.$$

]

10. (a) Neglecting spin, the Hamiltonian decribing the interaction of an electron with a magnetic field $\mathbf{B} = (0, 0, B_z)$ can be written

$$\frac{e}{2m_e}\hat{L}_z B_z,$$

where m_e is the electron mass and e is the electronic charge.

An electron in a hydrogen atom satisfies the time-independent Schrödinger equation with energy E_0 in zero magnetic field, and its state possesses the usual quantum numbers n, l and m. Show that the electron's state remains a solution of the time-independent Schrödinger equation when a magnetic field is applied, and find the corresponding energy. **[5]**

Hence show that states with a given n and l should always produce an odd number of energy levels through interaction with a magnetic field, if spin is neglected. Show that these states are predicted to be evenly spaced in energy, and find the spacing between them. **[3]**

Neglecting spin, how many levels are produced when a hydrogen atom whose electron is in a 3d state interacts with a magnetic field of strength 0.1 T? Calculate the spacing of these levels. **[2]**

(b) Briefly describe the Stern-Gerlach experiment, and explain why its results are inconsistent with the above predictions. **[4]**

Explain how the results may be explained in terms of the concept of electron spin. **[2]**

What values of the total spin quantum number j can arise when an electron (having spin $s = 1/2$) resides in the 3d state of hydrogen? Give the corresponding spectroscopic term symbols. **[4]**

11. The time-independent Schrödinger equation for the hydrogen atom, in atomic units, is

$$-\frac{1}{2}\nabla^2\psi - \frac{1}{r}\psi = E\psi.$$

If the solution is written as

$$\psi(r, \theta, \phi) = R(r)Y_{lm}(\theta, \phi),$$

where $Y_{lm}(\theta, \phi)$ is a spherical harmonic, show that the radial function $R(r)$ obeys the equation

$$-\frac{1}{2r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left[r^2\frac{\mathrm{d}R}{\mathrm{d}r}\right] + \left[\frac{l(l+1)}{2r^2} - \frac{1}{r}\right]R = ER,$$

[5]

By writing $R(r) = \chi(r)/r$, show that χ obeys the differential equation

$$-\frac{1}{2}\frac{\mathrm{d}^2\chi}{\mathrm{d}r^2} + \left[\frac{l(l+1)}{2r^2} - \frac{1}{r}\right]\chi = E\chi.$$

[4]

This equation is similar to a one-dimensional Schrödinger equation for a particle moving in an effective potential

$$V_{\mathrm{eff}}(r) = \frac{l(l+1)}{2r^2} - \frac{1}{r}.$$

Find an expression for the force corresponding to V_{eff}, and explain the physical origins of the two different terms appearing in it. **[4]**

Sketch the effective potential for the cases (a) $l = 0$ and (b) $l > 0$. **[4]**

Find the value of r where the function $V_{\mathrm{eff}}(r)$ is a minimum (assuming $l > 0$). Hence explain how you would expect the mean distance from the nucleus in the lowest state of a given l to vary with l, assuming that the corresponding probability density occurs mainly in the region near the minimum in V_{eff}. **[3]**

[The Laplacian operator may be written in spherical polar coordinates (using atomic units) as

$$\nabla^2 = \frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left[r^2\frac{\mathrm{d}}{\mathrm{d}r}\right] - \frac{\hat{L}^2}{r^2}.$$

The spherical harmonic Y_{lm} is an eigenfunction of $\hat{L}^2$ with eigenvalue (in atomic units) $l(l+1)$.]