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.

SECTION A

[Part marks]

1. Compton investigated the scattering of X-rays passing through a thin metal film. What feature of his results was inconsistent with the classical theory of electromagnetic radiation? **[2]**

   Outline, without using mathematics, show the Compton Effect can be explained. **[4]**

2. Define the commutator of two operators $\hat{P}$ and $\hat{Q}$. **[2]**

   What does it mean if $\hat{P}$ and $\hat{Q}$ are *compatible* operators? What does this imply about their commutator? **[2]**

   Suppose that $\hat{P}$ and $\hat{Q}$ are not compatible. For a given system, $\hat{P}$ is first measured yielding the value p, then $\hat{Q}$ is measured yielding the value q. If $\hat{P}$ is then measured again, what can be said about the possible results of the measurement, and why? **[2]**

3. A particle of mass m moves in a one-dimensional square well potential

$$V(x) = \begin{cases} 0 & (-a \leq x \leq a) \\ V_0 & (\text{otherwise}) \end{cases}$$

   For the case of an infinitely deep well, $V_0 = \infty$, sketch the form of the wavefunction of the two lowest energy states. Does the energy difference between these states increase or decrease as the width of the well, $2a$, decreases? Give reasons for your answer. **[4]**

   How does the number of bound states change as the depth of the well decreases (i.e. V_0 decreases)? Sketch carefully the wavefunction of the lowest energy state for a well that is both shallow and broad (i.e. small V_0 and large a). **[4]**

4. What is meant by the concept of "tunnelling" in quantum mechanics? **[3]**

   Briefly explain why tunnelling plays an important role in both nuclear fusion and alpha decay. **[3]**

5. The wavefunction of an electron in the hydrogen atom may be written in the form:

$$\psi = \frac{\chi(r)}{r} Y(\theta, \phi),$$

which leads to a Schrödinger-like equation for the function $\chi(r)$, with an *effective* potential given by

$$V_{\text{eff}}(r) = \frac{-e^2}{4\pi\epsilon_0 r} + \frac{l(l+1)\hbar^2}{2m_e r^2},$$

where m_e is the electron mass and l is the orbital quantum number. What is the physical significance of the two terms in this effective potential? **[4]**

Given that the function $Y(\theta, \phi)$ is chosen such that

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

state the condition that χ must satisfy in order for the wavefunction ψ to be correctly normalized. **[2]**

6. Quantum mechanical operators are *Hermitian*. What mathematical property do the eigenvalues of a Hermitian operator possess? What do these eigenvalues correspond to? **[2]**

Explain what is meant if it is stated that the set of eigenfunctions $\{\phi_n\}$ of a Hermitian operator is *orthonormal*. **[2]**

In a one-dimensional system, an arbitrary function ψ may be expressed in terms of such a set of eigenfunctions, as

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

Give an expression for the expansion coefficient c_n. What is the interpretation of the value of $|c_n|^2$? **[4]**

SECTION B

7. The time-independent Schrödinger equation for a single particle moving in a one-dimensional potential is given by

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi.$$

In addition to being a solution to this equation, what other conditions must the wavefunction $\psi(x)$ satisfy? **[3]**

For all parts of the remainder of this question, use the above Schrödinger equation specifically with $V(x) = -U\delta(x)$, where $\delta(x)$ is the Dirac delta function and U is a positive constant.

For this special potential, the derivative of ψ has a discontinuity at the origin resulting in the boundary condition

$$\frac{d\psi}{dx}|_{x=0^+} - \frac{d\psi}{dx}|_{x=0^-} = -\frac{2m}{\hbar^2}U\psi(0),$$

where $x = 0^-$ and $x = 0^+$ are positions immediately to the left and right of the origin.

(a) Find the general solutions to this Schrödinger equation for $E < 0$ in the two regions $x < 0$ and $x > 0$. **[3]**

By using these solutions with the usual boundary condition on ψ and the boundary condition on $d\psi/dx$ given above, find the energy eigenvalue and the normalized eigenfunction of the single bound state for $E < 0$. **[5]**

(b) Find the general solutions to this Schrödinger equation for $E > 0$ in the two regions $x < 0$ and $x > 0$. **[3]**

Using these solutions and the same boundary conditions as in (a) above, show that the proportion T of particles that are transmitted for a beam of particles incident from $x < 0$ on the above potential is **[6]**

$$T = \frac{2E\hbar^2}{2E\hbar^2 + mU^2}.$$

8. Write down the time-independent Schrödinger equation for a single electron orbiting a nucleus of atomic number Z (assumed to be stationary). **[2]**

The ground state eigenfunction of this equation, ψ_{1s}, and the radially symmetric eigenfunction with next lowest energy, ψ_{2s}, are:

$$\psi_{1s} = 2\left(\frac{Z}{a_0}\right)^{3/2} \exp(-Zr/a_0), \quad \psi_{2s} = \frac{1}{\sqrt{2}}\left(\frac{Z}{a_0}\right)^{3/2}\left(1 - \frac{Zr}{2a_0}\right)\exp(-Zr/2a_0),$$

where $a_0 = 4\pi\epsilon_0\hbar^2/(m_e e^2)$ is the Bohr radius and the wavefunctions are normalized such that

$$\int_0^\infty r^2|\psi^2|dr = 1.$$

(a) Use the Schrödinger equation to show that the energy in state ψ_{1s} is **[4]**

$$E_{1s} = -\frac{1}{2}\frac{\hbar^2 Z^2}{m_e a_0^2}.$$

(b) Determine the most probable distance from the nucleus at which the electron is located in the state ψ_{1s}. **[5]**

(c) An atom of tritium (^{3}H) is in its ground state when the nucleus suddenly decays into a helium nucleus (^{3}He), by emission of a fast electron and an electon antineutrino, without perturbing the single extranuclear electron.

Write down the wavefunction of the ground state of tritium. Explain how this wavefunction may be written in terms of the energy eigenfunctions of the resulting He^+ ion. **[2]**

Calculate the probability of finding the resulting He^+ ion in the 2s eigenstate. **[5]**

What are the other energy eigenstates in which the He^+ ion could possibly be found, immediately following this nuclear decay? **[2]**

[*The radial component of the Laplacian operator is*

$$\nabla_r^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right).$$

You may assume the value of the following definite integral

$$\int_0^\infty r^n \exp(-r/a)dr = n!\, a^{n+1}.$$

]

9. It may be shown, from the time-dependent Schrödinger equation, that for an operator $\hat{O}$ that does not explicitly depend on time, the time-derivative of the expectation value is

$$\frac{\mathrm{d}\langle\hat{O}\rangle}{\mathrm{d}t} = \frac{1}{\mathrm{i}\hbar}\langle[\hat{O},\hat{H}]\rangle.$$

Consider the case where $\hat{O}$ is the momentum operator

$$\hat{p}_x = -\mathrm{i}\hbar\frac{\partial}{\partial x},$$

and where $\hat{H}$ is the one-dimensional Hamiltonian for a particle of mass m moving in a harmonic potential $V(x) = \frac{1}{2}kx^2$.

By considering the action of $[\hat{p}_x, \hat{H}]$ on a general state, find an expression for the rate of change of $\langle\hat{p}_x\rangle$. **[3]**

Comment on the relationship to the classical expression for the rate of change of momentum. **[2]**

To what quantity does the variable $\omega_0 = \sqrt{k/m}$ correspond in the classical system? In terms of ω_0, state the allowed energy eigenvalues according to quantum mechanics. **[2]**

Making the substitution $y = x\sqrt{m\omega_0/\hbar}$, the time-independent Schrödinger equation for this system is

$$-\frac{d^2\psi}{dy^2} + y^2\,\psi = \frac{2E}{\hbar\omega_0}\psi.$$

The ground state eigenfunction of this equation is $\psi_0 \propto \exp(-y^2/2)$, with eigenvalue $E_0 = \hbar\omega_0/2$.

Verify that $\psi_2 \propto (2y^2-1)\exp(-y^2/2)$ is also a solution of the time-independent Schrödinger equation, and that the corresponding energy eigenvalue is $E_2 = 5E_0$. **[5]**

What are the corresponding solutions, $\Psi_0(y,t)$ and $\Psi_2(y,t)$ of the *time-dependent* Schrödinger equation? **[2]**

The particle is initially prepared in the state

$$\Psi(y,0) = Ay^2\exp(-y^2/2),$$

where A is a constant chosen in such a way that Ψ is correctly normalized. Express $\Psi(y,0)$ in terms of $\Psi_0(y,0)$ and $\Psi_2(y,0)$. Hence show that the probability density per unit length ρ of finding the particle at the origin $x=0$ varies with time as **[6]**

$$\rho = \frac{A^2}{2}\sqrt{m\omega_0/\hbar}\,[1-\cos(2\omega_0 t)]\,.$$

10. Starting from the classical definition of angular momentum $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, show that the quantum mechanical operator for the z-component of angular momentum may be written as

$$\hat{L}_z = -\mathrm{i}\hbar \left[x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} \right].$$

[3]

In spherical polar coordinates, the corresponding expression is

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

Consider the two states

$$\psi_0 = Az\exp(-r/a), \quad \psi_1 = Ay\exp(-r/a),$$

where a is a constant, $r = \sqrt{x^2 + y^2 + z^2}$ and A is a constant whose value is chosen to correctly normalize the wavefunctions.

Express ψ_0 and ψ_1 in spherical polar coordinates. **[2]**

Using either coordinate system, show that ψ_0 is an eigenfunction of $\hat{L}_z$ and find the corresponding eigenvalue. Show also that ψ_1 is not an eigenfunction of $\hat{L}_z$. **[3]**

Show that ψ_1 is an eigenfunction of the total squared angular momentum

$$\hat{L}^2 = -\hbar^2 \left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial^2\phi} \right]$$

and find the corresponding eigenvalues. What is the corresponding value of the orbital quantum number l? **[5]**

The completeness postulate implies that the angular part of ψ_1 can be expanded in terms of the spherical harmonics, such that

$$\psi_1(r,\theta,\phi) = \sum_{lm} a_{lm} Y_l^m(\theta,\phi) R(r).$$

By comparing your expression for $\psi_1(r,\theta,\phi)$ with the expressions given below for the spherical harmonics Y_l^m, find the expansion coefficients a_{lm} and determine the form of the function $R(r)$. **[3]**

Hence determine the possible results of measuring the z-component of the angular momentum in the state ψ_1, and the corresponding probabilities. **[4]**

[The first few spherical harmonics Y_l^m are:

$$Y_0^0 = \sqrt{\frac{1}{4\pi}} \quad Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta; \quad Y_1^1 = -\sqrt{\frac{3}{8\pi}}\sin\theta\exp(\mathrm{i}\phi); \quad Y_1^{-1} = \sqrt{\frac{3}{8\pi}}\sin\theta\exp(-\mathrm{i}\phi).$$

]

11. The solution to the time-dependent Schrödinger equation for the hydrogen atom may be written in the form

$$\psi_{nlm} = R_{nl}(r)\Theta_{lm}(\theta)\Phi_m(\phi).$$

Outline how the boundary conditions on the wavefunction restrict the possible values of the quantum numbers n, l and m. For a given value of n, state the allowed values of l and m. **[4]**

Which three physical quantities do n, l and m provide a measure of? **[3]**

A hydrogen atom is prepared in one of its energy eigenstates, with given n, l and m, and a magnetic field $\mathbf{B} = (0, 0, B_z)$ is then applied along the z-axis. Explain qualitatively why the energy changes by an amount

$$\Delta E = \mu_B B_z(m + gm_s)$$

where $\mu_B = e\hbar/2m_e$, $g \approx 2$ and m_s is the magnetic spin quantum number. **[4]**

Briefly describe the Stern-Gerlach experiment. What feature of its results indicated that the spin term must be included in the above expression. What are the possible values of m_s for an electron? **[4]**

If a hydrogen atom is prepared in a state with $n = 3$ and the measured change in energy is $\Delta E \approx 3\mu_B B_z$, deduce the values of l and m. Also determine the squared magnitude, J^2, of the total angular momentum of the electron. **[5]**

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SECTION A

[Part marks]

1. What relationship did de Broglie postulate between the momentum of a particle and the wavelength of the corresponding matter wave? **[2]**

   Explain briefly how a beam of electrons may be used to investigate the atomic structure of the surface of a metallic substance. Estimate the potential difference through which the electron beam should be accelerated for this purpose, showing your reasoning. **[6]**

   [*electron mass* $m_e = 9.11 \times 10^{-31}$ kg, *electron charge* $e = 1.60 \times 10^{-19}$ C
   Planck constant $h = 6.63 \times 10^{-34}$ Js]

2. State the Heisenberg uncertainty relation concerning the simultaneous measurement of the position and the momentum of a particle. **[2]**

   Explain briefly why attempting to measure the position of an electron by Compton scattering of a high energy photon leads to an uncertain knowledge of the electron's momentum, consistent with the Heisenberg uncertainty relation. **[4]**

3. 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

$$\frac{-\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V(x)\psi(x) = E\psi(x)\,,$$

   and give the physical interpretation of the constant E. **[6]**

   Find an expression for the time dependence $T(t)$. **[2]**

4. Let the functions $\{\phi_n\}$ be the eigenfunctions of some Hermitian operator $\hat{Q}$, with corresponding eigenvalues q_n. Explain what is meant if it is stated that this set of functions is *orthonormal*. **[2]**

   State why a general wavefunction ψ may be expressed as

   $$\psi = \sum_n c_n \phi_n \, .$$

   and give a condition that the coefficients c_n must satisfy if ψ is correctly normalized. **[2]**

   Give an expression for the expectation value of the operator $\hat{Q}$ in the state ψ, in terms of the eigenvalues q_n of $\hat{Q}$, and the coefficients c_n. **[2]**

5. The quantum state of an electron in the hydrogen atom may be described by four quantum numbers: n, l, m and m_s.

   What are the permitted values of n?

   For given n, what are the permitted values of l?

   For given l, what are the permitted values of m?

   How many different quantum states are there in total for a given value of n? **[4]**

   On which of the four quantum numbers does the energy of the electron principally depend, and what is the functional form of that dependence? **[2]**

6. An excited state of a helium atom contains one electron in the 1s state and a second electron in the 2p state.

   What are the possible values of the quantum number L representing the combined orbital angular momentum of the pair of electrons? **[2]**

   What are the possible values of the quantum number S representing the combined spin angular momentum of the pair of electrons? **[2]**

   For each permitted combination of L and S, state the possible values of the quantum number J representing the total angular momentum of the pair of electrons. **[2]**

SECTION B

7. A beam of particles of energy E and mass m is incident from the left on a potential step of height V_0 such that

$$V(x) = \begin{cases} 0 & (x \le 0) \\ V_0 & (x > 0)\,. \end{cases}$$

For the case $E > V_0$, explain why the spatial part of the wavefunction may by written as

$$\psi(x) = \begin{cases} e^{ikx} + Be^{-ikx} & (x \le 0) \\ Ce^{ik'x} & (x > 0)\,, \end{cases}$$

where B and C are constants, if there is one particle per unit length in the incident beam. **[4]**

Determine the value of k as a function of E and m, and show that **[4]**

$$k^2 - k'^2 = \frac{2mV_0}{\hbar^2}\,.$$

What two matching conditions must the wavefunction $\psi(x)$ satisfy at $x = 0$? By applying these conditions, show that

$$C = \frac{2k}{k + k'}\,.$$

[4]

What is the full time-dependent solution $\Psi(x,t)$, and what is its interpretation in terms of travelling waves? **[4]**

Evaluate the probability flux (mean number of particles passing a point per unit time) in the region $x > 0$. Give a physical interpretation of your answer in terms of the velocity of the particles in this region. **[4]**

[*The probability flux is*

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

at position x.]

8. A particle of mass m moves in a finite one-dimensional square well, located between $x = -a$ and $x = +a$, such that the potential is

$$V(x) = \begin{cases} 0 & (|x| \le a); \\ V_0 & (|x| > a), \end{cases}$$

with $V_0 = \pi^2\hbar^2/16ma^2$.

Within the well, the ground state wavefunction has the form

$$\psi(x) = A\cos(kx), \quad (|x| \le a)\,,$$

with $k = \pi/4a$, where A is a constant.

Write down the time-independent Schrödinger equation inside the well, $|x| \le a$, and hence determine the energy E of the ground state in terms of V_0. **[2]**

What is the time-independent Schrödinger equation in the regions outside the well, $|x| > a$? **[2]**

Give the general solution to this equation and explain why the ground state wavefunction in the regions outside the well may be written as

$$\psi(x) = \begin{cases} Ce^{\kappa x} & (x < -a); \\ De^{-\kappa x} & (x > a), \end{cases}$$

where C and D are constants. **[3]**

Find an expression for κ in terms of V_0 and hence in terms of a. **[2]**

By considering one of the conditions that the solutions for ψ in the different regions must satisfy at the edges of the well $x = \pm a$, find how C and D are related to A. **[2]**

What condition must the wavefunction satisfy in order for it to be correctly normalized? **[2]**

By applying this condition, show that

$$|A|^2 = \frac{1}{(1 + 4/\pi)\,a}\,.$$

[5]

If the particle is in the ground state and a measurement is made of its position, with what probability will it be located outside the well (i.e. outside the region $|x| \le a$)? **[2]**

9. The quantum mechanical operator for the z-component of angular momentum may be written in spherical polar coordinates as

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

and the operator for the total squared angular momentum is

$$\hat{L}^2 = -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right] .$$

Define the commutator $[\hat{L}^2, \hat{L}_z]$ and show that $[\hat{L}^2, \hat{L}_z] = 0$. What is the implication of this result for measurement of the total angular momentum and of its z-component? **[4]**

Show that the function $\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} \exp(\mathrm{i}m\phi)$ is an eigenfunction of $\hat{L}_z$, and find the corresponding eigenvalue. **[2]**

Why must m be an integer in order for this to be a physically acceptable eigenfunction? **[2]**

Show that the functions Φ_m are orthogonal for different values of m, and are normalized so that

$$\int_0^{2\pi} [\Phi_m(\phi)]^* \Phi_{m'}(\phi) \mathrm{d}\phi = \delta_{m,m'},$$

where $\delta_{m,m'} = 0$ if $m \neq m'$, and 1 if $m = m'$. **[3]**

A particle has the wave-function

$$\psi(\theta, \phi) = \frac{1}{2} Y_1^{-1} + \frac{1}{\sqrt{2}} Y_1^0 + \frac{1}{2} Y_1^1 ,$$

where Y_l^m are the spherical harmonics given below.

Show that $\psi(\theta, \phi)$ is an eigenfunction of $\hat{L}^2$ and determine the corresponding eigenvalue. **[3]**

State what the possible results of a measurement of L_z in this state would be, and what would be the corresponding probabilities of obtaining each one (given that $\psi(\theta, \phi)$ is correctly normalized). **[4]**

If a measurement of L^2 were made immediately after a measurement of L_z, what possible results could be obtained and what would be the probabilities of each? **[2]**

[*The first few spherical harmonics Y_l^m are:*

$$Y_0^0 = \sqrt{\frac{1}{4\pi}} \quad Y_1^0 = \sqrt{\frac{3}{4\pi}} \cos\theta; \quad Y_1^1 = -\sqrt{\frac{3}{8\pi}} \sin\theta \exp(\mathrm{i}\phi); \quad Y_1^{-1} = \sqrt{\frac{3}{8\pi}} \sin\theta \exp(-\mathrm{i}\phi).$$

]

10. A particle of mass m moves in the one-dimensional harmonic potential $V(x) = \frac{1}{2}kx^2$.

State the classical angular frequency ω_0 of oscillations as a function of k and m. **[2]**

State the quantum-mechanical energy eigenvalues as a function of ω_0. **[2]**

The ground state wavefunction $\psi_0(x)$ and the first excited state $\psi_1(x)$ are

$$\psi_0(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}\,, \qquad \psi_1(x) = \left(\frac{4\alpha^3}{\pi}\right)^{1/4} x\, e^{-\alpha x^2/2}\,,$$

where $\alpha = m\omega_0/\hbar$. Sketch these two functions. **[2]**

Suppose that an infinite potential barrier is placed at $x = 0$, confining the particle in the region $x > 0$ such that the potential becomes

$$V(x) = \begin{cases} \infty\,, & (x \le 0) \\ \frac{1}{2}kx^2\,, & (x > 0)\,. \end{cases}$$

By considering what conditions any acceptable wavefunction must satisfy at $x = 0$, explain why the ground-state wavefunction ϕ_0 now has the form **[2]**

$$\phi_0(x) = \begin{cases} 0\,, & (x \le 0) \\ A\, x\, e^{-\alpha x^2/2}\,, & (x > 0)\,. \end{cases}$$

Sketch this wavefunction and find the value of the normalization constant A. **[2]**

What is the new ground state energy, and what other values of the energy are permitted? **[2]**

Determine the expectation value of the potential energy when the particle is in the ground state ϕ_0. **[4]**

The particle is in state ϕ_0 and its energy is measured. The barrier is then removed, and the energy is measured again. What is the probability that the two measurements yield the same value? **[4]**

[*You may use the identity*

$$\int_0^\infty x^{2n} e^{-\alpha x^2}\, dx = \frac{(2n-1)(2n-3)...1}{2^{n+1}\alpha^n}\sqrt{\frac{\pi}{\alpha}}\,,$$

valid for $n \ge 1$.]

11. Write down the three-dimensional time-independent Schrödinger equation for the electron in a hydrogen atom, using atomic units ($\hbar = m_e = e^2/(4\pi\epsilon_0) = 1$), under the assumption of a fixed and point-like nucleus. **[2]**

Write the wavefunction as $\psi(r,\theta,\phi) = R(r)Y_l^m(\theta,\phi)$ (where Y_l^m is a spherical harmonic). Hence show that if the radial wavefunction R is written as

$$R(r) = \frac{\chi(r)}{r}\,,$$

then $\chi(r)$ satisfies the equation

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

(An expression for the operator ∇^2 in spherical polar coordinates is given at the end of the question.) **[6]**

Which two terms in the above differential equation may be neglected close to the nucleus ($r \to 0$), and why? **[2]**

Hence show that close to the nucleus the radial part of the wavefunction varies as

$$R(r) \sim r^l\,.$$

[2]

The radial part of the hydrogen 2p wave-function (in atomic units) is

$$R_{2p}(r) = \frac{1}{\sqrt{3}}\,re^{-r/2}\,.$$

Sketch the function $\chi_{2p}(r) = rR_{2p}(r)$. **[2]**

Determine the most likely distance of an electron from the nucleus (in atomic units) when it is in the 2p state of the hydrogen atom. **[2]**

Show that $\chi_{2p}(r)$ is a solution to the above differential equation for $\chi(r)$ with $l = 1$, and calculate the corresponding energy E (in atomic units). **[4]**

[*The Laplacian operator in spherical polar coordinates can be written as*

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2\frac{\partial}{\partial r}\right] - \frac{\hat{L}^2}{r^2},$$

where $\hat{L}^2$ is the operator representing the square of the total angular momentum and atomic units have been used.]

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

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SECTION A

[Part marks]

1. In the Compton experiment, a beam of X-rays with known wavelength is scattered from a solid target. What main features of the results contradict the expectation of classical physics, which treats the X-rays as a wave of electromagnetic radiation? **[2]**

   Explain briefly how the results can be explained by considering the incident radiation to be a beam of photons with particle-like properties, giving the explicit relations between the particle-like and wave-like properties. Describe also the effect of the scattering on the electrons in the target. [*No mathematical derivations are required*]. **[4]**

2. A particle of mass m in free space in one-dimension has the wavefunction

$$\Psi(x,t) = e^{-i(kx+Et/\hbar)} \, .$$

   Give an expression for the momentum p of the particle. **[2]**

   Give an expression for the energy E of the particle in terms of k and m. **[2]**

   The general expression for particle flux $\Gamma(x)$, i.e. number of particles per unit time passing the point x, is

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

   What is the particle flux for the above wavefunction? **[2]**

3. In terms of the Hamiltonian operator $\hat{H}(\mathbf{r},t)$, write down the *time-dependent* Schrödinger equation for the wavefunction $\Psi(\mathbf{r},t)$. **[2]**

   For a Hamiltonian that does not explicitly depend on time, i.e. $\hat{H} = \hat{H}(\mathbf{r})$, a particle is initially in the state

$$\Psi(\mathbf{r}, t=0) = \sum_n a_n \psi_n(\mathbf{r}) \, ,$$

   where the functions $\psi_n(\mathbf{r})$ are solutions of the *time-independent* Schrödinger equation

$$\hat{H}(\mathbf{r})\psi_n(\mathbf{r}) = E_n\psi_n(\mathbf{r}) \, .$$

   Give a physical interpretation of the quantities E_n and write down the wavefunction $\Psi(\mathbf{r},t)$ at a later time t. **[4]**

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 wavefunction of a particular one-dimensional system. Give an expression for the expectation value of a Hermitian operator $\hat{Q}$ in the state ψ. **[2]**

   According to the expansion postulate, $\psi(x)$ may be expressed in terms of the set of eigenfunctions $\{\phi_n\}$ of $\hat{Q}$, as

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

   Give an expression for the coefficient c_n. **[2]**

   With the system in state ψ, express the expectation value of $\hat{Q}$ in terms of the set of coefficients $\{c_n\}$ and the set of eigenvalues $\{q_n\}$ of $\hat{Q}$. **[2]**

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

   The angular momentum operators in the x, y and z directions, ($\hat{L}_x$, $\hat{L}_y$ and $\hat{L}_z$), obey the commutation relation

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

   What is the physical implication of the fact that the commutator is non-zero? **[2]**

   The *spherical harmonic* $Y_l^m(\theta, \phi)$ is an eigenfunction of L_z, and also an eigenfunction of the operator $\hat{L}^2$ which represents the squared magnitude of the angular momentum. State the corresponding eigenvalue for each of these operators. **[2]**

6. In a Stern-Gerlach-type experiment, a beam of hydrogen atoms in the ground state is passed through an inhomogeneous magnetic field. What feature of the result reveals that the electron has an intrinsic spin? What value of the spin quantum number s does the result imply, and why? **[4]**

   What is the value of the orbital angular momentum quantum number l for an electron in the 3d state of hydrogen? **[2]**

   What are the possible values of the total angular momentum quantum number j that could be produced by combining the orbital and spin angular momenta of an electron in the 3d state? **[2]**

SECTION B

7. A particle of mass m resides in a 3-dimensional box of dimensions $2a$, $2b$, $2c$, such that it experiences the potential

$$V(x,y,z) = \begin{cases} 0\,, & (-a \le x \le a,\ -b \le y \le b,\ -c \le z \le c)\,; \\ \infty\,, & \text{otherwise}\,. \end{cases}$$

Write down the time-independent Schrödinger equation for the particle within the box in the form of a partial differential equation. **[3]**

What boundary conditions must the wavefunction $\psi(x,y,z)$ satisfy at each wall of the box? **[3]**

By writing $\psi(x,y,z) = X(x)Y(y)Z(z)$, show that the time-independent Schrödinger equation may be separated into three ordinary differential equations. **[4]**

Hence show that the energy E of the particle is quantised, such that

$$E = \frac{\pi^2\hbar^2}{8m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right),$$

and specify the permitted values of n_x, n_y, and n_z. **[4]**

According to the Pauli exclusion principle, no two electrons may be in the same quantum state (including spin states). Suppose that eight electrons are in a box with equal sides, $a = b = c$. Determine the lowest energy of the system and the degeneracy of this energy level, assuming that the electrons do not interact with each other. **[3]**

What is the lowest energy of the system if the box contains seven non-interacting electrons, and what is the degeneracy of the energy level in this case? **[3]**

8. Without writing any equations, briefly describe the phenomenon of quantum tunnelling. **[2]**

An electron travelling in the $+x$ direction with energy E is incident, at $x = 0$, on a square potential barrier of width a and height V_0, with $V_0 > E$. Thus the potential is

$$V(x) = \begin{cases} 0, & (x \leq 0)\,; \\ V_0\,, & (0 < x < a)\,; \\ 0, & (x \geq a)\,. \end{cases}$$

The spatial part of the wavefunction $\psi(x)$ of the electron may be written

$$\psi(x) = \begin{cases} e^{ikx} + re^{-ikx}\,, & (x \leq 0)\,; \\ Ae^{\kappa x} + Be^{-\kappa x}\,, & (0 < x < a)\,; \\ te^{ikx}\,, & (x \geq a)\,. \end{cases}$$

Explain the functional form of the wavefunction in each of the three regions of space. **[3]**

By considering the time-independent Schrödinger equation, give expressions for the constants k and κ. **[4]**

If the barrier is sufficiently high and wide that the tunnelling is weak, then the amplitude of one of the waves within the barrier is much smaller than the other, i.e. $|A| \ll |B|$. Solve the time-independent Schrödinger equation with the appropriate boundary conditions, making the approximation that the component with amplitude A may be neglected at the *left-hand* boundary. Hence show that the transmitted wave has amplitude

$$t = \frac{4ik\kappa e^{-\kappa a} e^{-ika}}{(k + i\kappa)^2}\,.$$

[6]

Show that, with the above approximation, the probability of transmission is

$$T = \frac{16E(V_0 - E)}{V_0^2} e^{-2\kappa a}\,.$$

[2]

In a scanning tunnelling microscope, an electron with energy 4 eV is incident on a barrier of width 1 nm and height 8 eV. Estimate the tunnelling probability. **[3]**

[*electron mass* $m_e = 9.11 \times 10^{-31}$ kg, *electron charge* $e = 1.60 \times 10^{-19}$ C
Planck constant $h = 6.63 \times 10^{-34}$ Js]

9. Write down the equation that defines an *eigenfunction* and an *eigenvalue* of a Hermitian operator $\hat{O}$, explaining carefully which quantity in your equation is which. **[2]**

An observable corresponding to operator $\hat{A}$ has eigenvalues $+1$ and -1 with eigenfunctions α_+ and α_-. Another observable corresponding to operator $\hat{B}$ also has eigenvalues $+1$ and -1, but its eigenfunctions are

$$\beta_+ = (\alpha_+ + \alpha_-)/\sqrt{2}\,,$$

$$\beta_- = (\alpha_+ - \alpha_-)/\sqrt{2}\,.$$

Find the results $\hat{B}\alpha_+$ and $\hat{B}\alpha_-$. Are $\hat{A}$ and $\hat{B}$ compatible operators? Give a reason for your answer. **[4]**

By considering the states produced when $\hat{C} = \hat{A} - \hat{B}$ acts on an un-normalized wavefunction of the form $\psi = \alpha_+ + c\ \alpha_-$, where c is an arbitrary constant, show that $\hat{C}$ corresponds to an observable. What will be the result when $\hat{C}$ is measured in a state of this form? **[4]**

Does the operator $\hat{A}\hat{B}$ correspond to an observable? Explain. **[4]**

$\hat{A}$ is measured with the result $+1$. $\hat{B}$ is measured immediately thereafter. What are the possible results, and what are their probabilities? **[3]**

Hence find the probability that the same result, $+1$, is obtained if $\hat{A}$ is measured a second time, immediately following the measurement of $\hat{B}$. **[3]**

10. Write down the Hamiltonian $\hat{H}$ for a particle of mass m moving in the one-dimensional potential $V(x)$. **[2]**

For an operator $\hat{O}$ that does not explicitly depend on time, the time-derivative of the expectation value is

$$\frac{\mathrm{d}\langle\hat{O}\rangle}{\mathrm{d}t} = \frac{1}{\mathrm{i}\hbar}\langle[\hat{O},\hat{H}]\rangle.$$

Define what is meant by a *stationary state* of a system, and show that for a stationary state $\langle\hat{O}\rangle$ has a constant value. **[2]**

Write down the expression for the quantum mechanical operator corresponding to the particle's linear momentum, $\hat{p}_x$. **[2]**

By considering the action of $[\hat{p}_x, \hat{H}]$ on a general wavefunction, show that

$$\frac{d\langle\hat{p}_x\rangle}{dt} = -\langle\frac{dV}{dx}\rangle\,.$$

[6]

Comment on the relationship to the classical expression for the rate of change of momentum. **[2]**

It can also be shown that

$$\frac{d\langle\hat{x}\rangle}{dt} = \frac{\langle\hat{p}_x\rangle}{m}\,,$$

where m is the mass of the particle. Using this and the preceding result, for a particle in the simple harmonic potential $V(x) = \frac{1}{2}m\omega_0^2x^2$, show that

$$\frac{d^2\langle\hat{x}\rangle}{dt^2} = -\omega_0^2\langle\hat{x}\rangle\,.$$

[4]

Hence find the general solution for the time-evolution of $\langle\hat{x}\rangle$ for a particle in a simple-harmonic potential. **[2]**

11. An electron in the 1s state of the hydrogen atom has the radial wavefunction

$$R(r) = 2a_0^{-3/2} e^{-r/a_0} \, ,$$

where $a_0 = 4\pi\epsilon_0\hbar^2/m_e e^2$ is the Bohr radius.

What is the probability that the distance of the electron from the nucleus is between r and $r + dr$? **[2]**

Show that the probability of finding the electron within a distance d of the nucleus varies as $(d/a_0)^3$ when $d \ll a_0$. **[2]**

At what distance from the nucleus is the electron most likely to be found? **[2]**

The general formula for the spatial part of the wavefunction of the hydrogen atom is

$$\psi_{nlm} = R_{nl}(r) Y_l^m(\theta, \phi) \, .$$

How do the energy and angular momentum of the electron depend on the quantum numbers n, l, and m? State the permitted values of these quantum numbers. **[6]**

The 2p wavefunction has the form

$$\psi_{210} \propto r e^{-r/2a_0} \cos\theta \, .$$

Normalize this wavefunction. **[4]**

Verify that ψ_{210} is an eigenfunction of the operator for total angular momentum

$$\hat{L}^2 = -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \sin^2\theta \frac{\partial^2}{\partial\phi^2} \right] ,$$

and explicitly evaluate the corresponding eigenvalue. Is this the value you expect for the 2p state? **[4]**

[*You may use the identity*

$$\int_0^\infty x^n e^{-\alpha x} dx = \frac{n!}{\alpha^{n+1}} \, .$$

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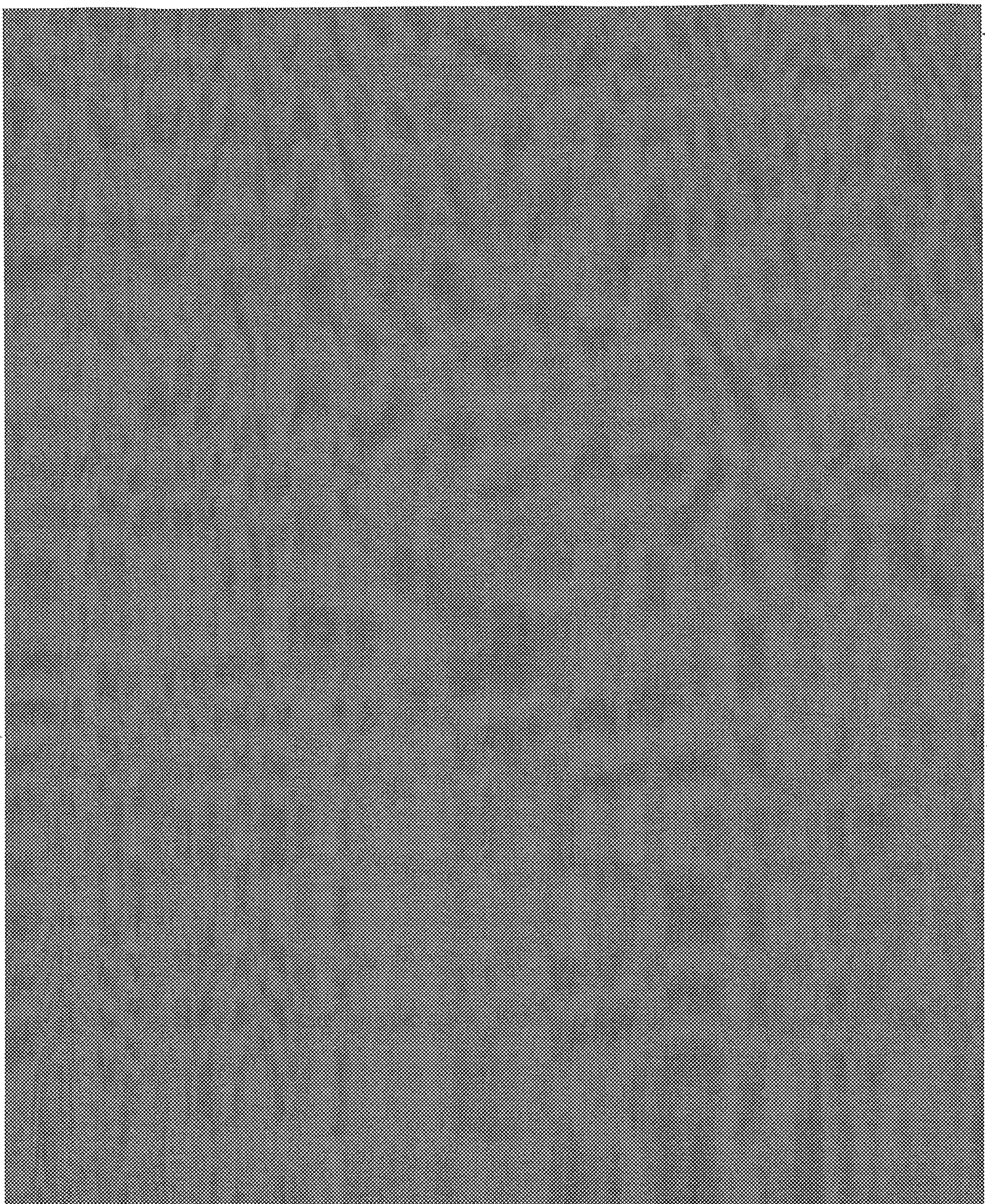
UNIVERSITY COLLEGE LONDON

EXAMINATION FOR INTERNAL STUDENTS

MODULE CODE	:	**PHAS2222**
ASSESSMENT PATTERN	:	**PHAS2222A**
MODULE NAME	:	**Quantum Physics**
DATE	:	**14-May-12**
TIME	:	**14:30**
TIME ALLOWED	:	**2 Hours 30 Minutes**

2011/12-PHAS2222A-001-EXAM-205



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.

SECTION A

[Part marks]

1. de Broglie proposed that particles can behave as waves. What relationship did he postulate between a particle's momentum and a wave-like property? [2]

   Give a brief account of *two* different experiments that confirm that particles can behave as waves. [4]

2. Define the *eigenvalues* and *eigenfunctions* of a linear operator. [2]

   A *Hermitian* operator $\hat{Q}$ satisfies the relation

$$\int_{-\infty}^{\infty} f^* \hat{Q} g dx = \left(\int_{-\infty}^{\infty} g^* \hat{Q} f dx \right)^*$$

   where f and g are functions that vanish at $x = \pm\infty$. By setting both f and g equal to an eigenfunction of $\hat{Q}$, show that the eigenvalues of a Hermitian operator are real. [2]

   According to the postulates of quantum mechanics, what are the possible results of a measurement of the physical quantity corresponding to a particular operator, and what state is the system left in after the measurement? [2]

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

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

   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

$$\frac{-\hbar^2}{2m} \frac{\mathrm{d}^2 \psi}{\mathrm{d}x^2} + V(x)\psi(x) = E\psi(x)\,,$$

   and give the physical interpretation of the constant E. [6]

   Find an expression for the time dependence $T(t)$. [2]

4. Explain what is meant if it is stated that the set of eigenfunctions $\{\phi_n\}$ of a Hermitian operator is *orthonormal.* [2]

In a one-dimensional system, an arbitrary function ψ may be expressed in terms of such a set of eigenfunctions, as

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

State an expression for the expansion coefficient c_n. [2]

By considering the normalisation of $\psi(x)$, show that

$$\sum_n |c_n|^2 = 1 ,$$

and state the interpretation of the value of $|c_n|^2$. [4]

5. Define the *commutator* of two operators $\hat{P}$ and $\hat{Q}$. [2]

What can be said about the eigenfunctions of *compatible* operators? What does this imply about their commutator? [2]

The angular momentum operators in the x, y and z directions, ($\hat{L}_x$, $\hat{L}_y$ and $\hat{L}_z$), obey the commutation relation

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

What is the physical implication of the fact that the commutator is non-zero? [2]

6. What are the possible values of the spin quantum numbers s and m_s for an electron? [2]

What are the possible values of the total angular momentum quantum number j that could be produced by combining the orbital and spin angular momenta of an electron in the 2p state? What is the range of total magnetic quantum numbers m_j associated with each possibility? [2]

Whether the electron is described using the quantum numbers l, m, s and m_s, or using the quantum numbers j and m_j, the total number of distinct states should be the same. Show that this is the case for the example discussed above. [2]

SECTION B

7. A beam of particles of energy E and mass m is incident from the left on a potential step of height V_0. At a distance a beyond the step there is an impenetrable barrier, such that the potential varies as

$$V(x) = \begin{cases} 0 & (x \leq 0) \\ V_0 & (0 < x \leq a) \\ \infty & (x > a)\,. \end{cases}$$

For the special case $E = V_0$, explain why the spatial part of the wavefunction may by written as

$$\psi(x) = \begin{cases} e^{ikx} + Be^{-ikx}\,, & (x \leq 0)\,; \\ Cx + D\,, & (0 < x < a)\,; \\ 0\,, & (x \geq a)\,. \end{cases}$$

where B, C and D are constants, if there is one particle per unit length in the incident beam. [4]

Determine the value of k as a function of V_0 and m. [2]

What matching conditions must the wavefunction $\psi(x)$ satisfy at $x = 0$ and at $x = a$? [3]

Use the equations derived from the matching conditions to show that

$$C = \frac{2ik}{(1 - aik)}\,.$$

[3]

Hence show that the mean number of particles located in the region $(0 < x \leq a)$ at any given time is

$$\frac{4k^2a^3}{3(1 + a^2k^2)}\,.$$

[4]

Show that the total particle flux Γ in the region $(x < 0)$ is zero. [4]

[*The particle flux in one dimension is*

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

8. A particle of mass m moves in one dimension in an infinite square well extending from $x = -a$ to $x = +a$. Inside the well the potential is zero. Write down the time-independent Schrödinger equation for the particle when it is inside the well, and find the most general solution in this region. [4]

What are the boundary conditions on the wave function at $x = \pm a$? By applying these boundary conditions, find the energies and wavefunctions for the square well's *even* stationary states, i.e. those having $\psi(x) = \psi(-x)$. [5]

For the case of the ground state (the solution with lowest energy, E_1) determine the normalisation constant of the wavefunction so that

$$\int_{-\infty}^{\infty} |\psi|^2 \, \mathrm{d}x = 1.$$

[3]

At a certain instant a particle in the well has the normalized wave function

$$\phi(x) = \sqrt{\frac{8}{5a}} \cos^3\left(\frac{\pi x}{2a}\right)$$

Determine the probability that a measurement of the particle's energy, at that instant, will yield the value E_1. [4]

By expressing the cosine function in terms of exponential functions, or otherwise, determine what other value(s) of the energy could be measured. [4]

[*You may use without proof the result*

$$\int_{-\pi/2}^{\pi/2} \cos^n \theta \, \mathrm{d}\theta = \frac{(n-1)(n-3)\ldots 1}{n(n-2)\ldots 2}\pi, \qquad \text{for even } n \quad]$$

9. A particle of mass m moving in one dimension has potential energy $V(x) = \frac{1}{2}m\omega_0^2 x^2$. Explain the significance of the quantity ω_0 in classical mechanics. [2]

Write down the time-independent Schrödinger equation for this system. State the energy eigenvalues of this system according to quantum mechanics. [4]

Verify that

$$\psi_0 = c_0 \exp(-m\omega_0 x^2/2\hbar) \quad \text{and} \quad \psi_1 = c_1 x \exp(-m\omega_0 x^2/2\hbar),$$

are both solutions of the time-independent Schrödinger equation, and find the corresponding energy eigenvalues. [4]

What are the corresponding solutions of the *time-dependent* Schrödinger equation? [2]

The particle is initially prepared in the state

$$\Psi(x,0) = \frac{A}{c_0}\psi_0 + \frac{A}{c_1}\psi_1\,,$$

where A is a real constant chosen in such a way that Ψ is correctly normalized. Show that after a time t has elapsed, the probability density per unit length of finding the particle near position x is

$$A^2[1 + x^2 + 2x\cos(\omega_0 t)]\exp(-m\omega_0 x^2/\hbar).$$

[5]

Sketch this probability density at (a) $t = 0$, (b) $t = \pi/\omega_0$; (c) $t = 2\pi/\omega_0$. [3]

10. Write down the three-dimensional time-independent Schrödinger equation for the electron in a hydrogen atom, using atomic units ($\hbar = m_e = e^2/(4\pi\epsilon_0) = 1$), under the assumption of a fixed and point-like nucleus, using spherical polar coordinates. [2]

Write the wavefunction as $\psi(r, \theta, \phi) = R(r)Y_l^m(\theta, \phi)$ (where Y_l^m is a spherical harmonic). Hence show that if the radial wavefunction R is written as

$$R(r) = \frac{\chi(r)}{r},$$

then $\chi(r)$ satisfies the equation

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

(An expression for the operator ∇^2 in spherical polar coordinates is given at the end of the question.) [6]

This equation has the form of a one-dimensional time-independent Schrödinger equation for a particle in an effective potential

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

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

The radial part of the hydrogen 1s wavefunction (in atomic units) is

$$R_{1s}(r) = 2e^{-r}\,.$$

Show that $\chi_{1s}(r) = rR_{1s}(r)$ is a solution to the above differential equation for $\chi(r)$ with $l = 0$, and calculate the corresponding energy E (in atomic units). [4]

Given that the probability that the electron may be found in a spherical shell between distances r and $r + \delta r$ from the nucleus can be written as $r^2|R|^2\delta r$, determine the expectation value of the potential energy of the electron in the 1s state, due to the interaction with the nucleus. [4]

[*The Laplacian operator in spherical polar coordinates can be written as*

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2\frac{\partial}{\partial r}\right] - \frac{\hat{L}^2}{r^2},$$

where $\hat{L}^2$ is the operator representing the square of the total angular momentum and atomic units have been used.]

11. Starting from the classical definition of angular momentum $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, show that the quantum mechanical operator for the z-component of angular momentum may be written as

$$\hat{L}_z = -\mathrm{i}\hbar \left[x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} \right].$$

[3]

In spherical polar coordinates, the corresponding expression is

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

Consider the two states

$$\psi_0 = Az \exp(-r/a), \quad \psi_1 = Ay \exp(-r/a),$$

where a is a constant, $r = \sqrt{x^2 + y^2 + z^2}$ and A is a constant whose value is chosen to correctly normalize the wavefunctions.

Express ψ_0 and ψ_1 in spherical polar coordinates. [2]

Using either coordinate system, show that ψ_0 is an eigenfunction of $\hat{L}_z$ and find the corresponding eigenvalue. Show also that ψ_1 is not an eigenfunction of $\hat{L}_z$. [3]

Show that ψ_1 is an eigenfunction of the total squared angular momentum

$$\hat{L}^2 = -\hbar^2 \left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \right]$$

and find the corresponding eigenvalue. What is the corresponding value of the orbital quantum number l? [5]

The angular part of ψ_1 can be expanded in terms of the spherical harmonics, such that

$$\psi_1(r, \theta, \phi) = \sum_{lm} a_{lm} Y_l^m(\theta, \phi) R(r).$$

By comparing your expression for $\psi_1(r, \theta, \phi)$ with the expressions given below for the spherical harmonics Y_l^m, find the expansion coefficients a_{lm} and determine the form of the function $R(r)$. [3]

Hence determine the possible results of measuring the z-component of the angular momentum in the state ψ_1. Comment on the relative likelihood of observing the different results. [4]

[*The first few spherical harmonics* Y_l^m *are:*

$$Y_0^0 = \sqrt{\frac{1}{4\pi}} \quad Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta; \quad Y_1^1 = -\sqrt{\frac{3}{8\pi}}\sin\theta\exp(\mathrm{i}\phi); \quad Y_1^{-1} = \sqrt{\frac{3}{8\pi}}\sin\theta\exp(-\mathrm{i}\phi).$$

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UNIVERSITY COLLEGE LONDON

EXAMINATION FOR INTERNAL STUDENTS

MODULE CODE	:	**PHAS2222**
ASSESSMENT PATTERN	:	**PHAS2222A**
MODULE NAME	:	**Quantum Physics**
DATE	:	**07-May-13**
TIME	:	**14:30**
TIME ALLOWED	:	**2 Hours 30 Minutes**

2012/13-PHAS2222A-001-EXAM-196

TURN OVER

Answer ALL 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 question section.

Section A

1. Describe the tunnelling phenomenon in quantum mechanics. Briefly discuss a physical process in which it is important. **[6 marks]**

2. Describe briefly the two-slit experiment and its implications for wave-particle duality. In particular, given the expression for the fringe spacing $\Delta y \simeq \frac{\lambda D}{d}$, draw a sketch indicating the physical significance of the parameters Δy, λ, D and d. **[5 marks]**
For an experiment conducted with electrons with momentum of magnitude p_e, give an expression for Δy in terms of p_e. **[1 marks]**

3. State 3 conditions that the solutions of the Schrödinger equation must satisfy in order to be physically acceptable. **[6 marks]**
Give one example of an eigenvalue equation in quantum mechanics other than the Schrödinger equation. **[2 marks]**

4. Consider two wave-functions $\psi(x)$ and $e^{i\theta}\psi(x)$ where θ is an arbitrary (real) phase. Show that they give the same predictions with respect to measurement of any observable. Discuss both repeated measurements of the position of the particle as well as of some other observable. **[4 marks]**
Explain briefly why it is important that $\psi(x)$ is normalised. Also, if it is not, how you would normalise it? **[4 marks]**

5. State the time-independent Schrödinger equation for the Quantum Harmonic Oscillator (QHO). **[2 marks]**
Sketch the form of its quantum ground state. Give two ways in which the QHO differs from its classical equivalent. **[4 marks]**

6. For a hydrogen atom in its $n = 3$ state, what are the allowed values of the quantum numbers corresponding to the angular momenta L and z-component L_z, and in what combinations can they occur? State clearly the general range of allowed quantum numbers in each case. **[6 marks]**

Section B

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

$$V(x) = \begin{cases} 0 & \text{if } x \leq 0; \\ V_0 & \text{if } 0 \leq x \leq a \\ V_1 & \text{if } x > a. \end{cases}$$

Here V_0 and V_1 are constant potentials and $0 < V_1 < V_0$.

Assume that $E > V_0$ and that the wavefunction in the region $x \leq 0$ takes the form:

$$\psi(x) = \exp(ikx) + R\exp(-ikx).$$

(a) Discuss the physical significance of a solution of this form, giving the wavenumber k in terms of E. **[4 marks]**

(b) Give the form of the solutions in both regions for which $x > 0$ introducing corresponding wavenumbers k_0 and k_1. Take care to introduce the correct number of arbitrary constants and to define k_0 and k_1 in terms of V_0 and V_1. If any terms are excluded by physical boundary conditions, explain why. **[8 marks]**

(c) Give the set of matching equations which would enable you to obtain all arbitrary constants, stating clearly what you are matching, for the above case where $E > V_0$. **[4 marks]**

(d) Consider now the case where $V_0 = V_1$ and where we find that:

$$R = \frac{k - k_0}{k + k_0}.$$

Obtain an expression for the transmitted current. You may use ideas of conservation of current and may find useful the operator below: **[4 marks]**

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

8. A particle of energy E moves in a one-dimensional potential well, with potential $V(x) = 0$ when $|x| < a$ and $V(x) = V_0$ elsewhere, where V_0 is a positive constant and $E < V_0$.

(a) Give the general form of the solutions to the time-independent Schrödinger equation inside the well, in terms of wavenumbers k and with appropriate constants. **[2 marks]**

(b Give corresponding solutions outside the well in terms of functions $\exp(\pm\kappa x)$ explaining carefully physical constraints which determine the form of the solution. You should illustrate your answer with a sketch. **[3 marks]**

(c) State four matching conditions which enable you to determine the eigenstates of this system.
Give the form of the corresponding four equations for the case where the wavefunctions are constrained to be even with respect to reflection about $x = 0$ and thus show $\kappa = k \tan ka$. **[8 marks]**

(d) Give a general expression for the total probability of finding a particle outside the well. **[3 marks]**

(e) Consider a particle in the ground state of the well, for which the eigenfunction for $|x| \leq a$ is $\psi(x) = A \cos kx$ and for $x > a$ we have $\psi(x) = C \exp -\kappa x$. Show that if P_{IN} is the probability of finding the particle in the well, while P_{OUT} is the total probability of finding the particle outside the well, then:

$$\frac{P_{OUT}}{P_{IN}} = \frac{C^2 k e^{-2\kappa a}}{A^2 \kappa (ka + \frac{1}{2} \sin 2ka)} \quad (1)$$

[2 marks]

Give an expression for $\frac{P_{OUT}}{P_{IN}}$ which is independent of C and A. **[2 marks]**

9. (a) The wavefunction Ψ of a quantum particle is given in terms of a sum over orthonormal eigenfunctions, ie $\Psi = \sum_n C_n \phi_n$, for which $C_n = \int \Psi \phi_n^* d\tau$ and $\hat{A}\phi_n = \lambda_n \phi_n$ where $\hat{A}$ is a Hermitian operator. Discuss the relevance of the above for the quantum theory of measurement, considering in particular the probability of measuring an arbitrary eigenvalue λ_n as well as the averages obtained after many measurements on identical particles. **[8 marks]**

(b) An atom of tritium ($Z = 1$) is in a $2p$ state with $m = +1$ when its nucleus suddenly decays into a nucleus of helium ($Z = 2$) without perturbing the extranuclear electron. What will be the probability that we will measure the electron to be in a $2p$ state of the resulting He^+ ion? Explain carefully your reasoning. **[8 marks]**

(c) Calculate the expectation value of r immediately after the decay, but before the measurement. **[4 marks]**

You may assume for an atom of nuclear charge Z, $R_{2p}(r) = \frac{Z^{5/2}}{\sqrt{24}} r e^{-Zr/2}$ and use the result $\int_0^\infty r^n e^{-\alpha r} dr = \frac{n!}{\alpha^{n+1}}$.

10. In spherical polar coordinates, the operator $\hat{L}_z$ can be written as

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

(a) Show that the function $\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}}e^{(im\phi)}$ is an eigenfunction of $\hat{L}_z$ and find the corresponding eigenvalues. **[4 marks]**

(b) Why must m be an integer in order for this to be a physically acceptable eigenfunction? **[2 marks]**

(c) Consider the Hamiltonian of an electron in a central potential $V(r)$ with eigenfunctions $\Psi_{n,l,m}(r,\theta,\phi)$ and eigenvalues E_n

$$\hat{H}_0 = -\frac{\hbar^2}{2mr^2}\left\{\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right\} + V(r).$$

Note that the angular coordinate-dependent part of the Hamiltonian corresponds to the total angular momentum operator $\hat{L}^2$. Explain why the functions $\Phi_m(\phi)$ are also eigenfunctions of $\hat{H}_0$. **[3 marks]**

(d) Imagine that we now turn on a magnetic field B_z, so that the total Hamiltonian (neglecting spin) is now

$$\hat{H} = \hat{H}_0 + \frac{\mu_0}{\hbar}B_z\hat{L}_z$$

Consider a hydrogen atom in a $3d$ state. Justifying your answer, what are the new eigenfunctions of $\hat{H}$, in terms of the old ones? How many new eigenvalues are there? **[4 marks]**

(e) The expectation value of the time derivative of an arbitrary quantum operator $\hat{O}$ is given by the expression:

$$d\langle\hat{O}\rangle/dt \equiv \langle d\hat{O}/dt\rangle = \langle\partial\hat{O}/\partial t\rangle + i/\hbar\langle[\hat{H},\hat{O}]\rangle$$

Obtain an expression for $\langle d\hat{L}_x/dt + d\hat{L}_y/dt\rangle$, given the form of $\hat{H}$ given in part (d) of the question. You may use the fact that $[\hat{L}_i,\hat{L}_j] = i\hbar\hat{L}_k$ where i,j,k are cyclic permutations of cartesian coordinates x,y,z such as, for example, $[\hat{L}_x,\hat{L}_y] = i\hbar\hat{L}_z$.

[7 marks]

11. A particular solution $\Psi_n(x,t)$ of the time-dependent Schrödinger equation (TDSE), $i\hbar\partial\Psi/\partial t = \hat{H}\Psi$, can be constructed by taking

$$\Psi_n(x,t) = \psi_n(x)\exp\left(-iE_n t/\hbar\right)$$

where the ψ_n are solutions of the time-independent Schrödinger equation (TISE).

(a) Hence show that a linear combination of two such solutions $c_1\Psi_1(x,t) + c_2\Psi_2(x,t)$ is also a solution of the TDSE but is not a solution of the TISE. **[6 marks]**

(b) Consider a Hamiltonian $\hat{H}$ with eigenvectors ϕ_1 and ϕ_{-1} and corresponding energy eigenvalues $E_1 = \hbar\omega$ and $E_{-1} = -\hbar\omega$. If at time $t = 0$, the state of the system is $\Psi(t=0) = c_1\phi_1(t=0) + c_{-1}\phi_{-1}(t=0)$, give the state of the system at an arbitrary later time t. This system demonstrates recurrences, where $\Psi(t) = \Psi(0)$. At what times will this occur? **[4 marks]**

(c) Write down the expectation value of the energy $\langle E\rangle$ at an arbitrary later time t for the case $c_1 = c_{-1}$. **[3 marks]**

(d) Consider now the two (also orthonormal) quantum states:
$v_\pm(t) = (\phi_1(t) \pm \phi_{-1}(t))/\sqrt{2}$. Find $\phi_1(t)$ and $\phi_{-1}(t)$ in terms of the $v_\pm(t)$. **[3 marks]**

(e) If at time $t = 0$, the state of the system is found to be $\psi(0) = v_-$, find the probability as a function of time, that $\psi(t)$ will be found in the state v_+. **[4 marks]**

 END OF PAPER