

UNIVERSITY COLLEGE LONDON

University of London

EXAMINATION FOR INTERNAL STUDENTS

For The Following Qualifications:–

B.Sc. *M.Sc.*

Physics 3C26: Quantum Mechanics

COURSE CODE : PHYS3C26

UNIT VALUE : 0.50

DATE : 05–MAY–06

TIME : 10.00

TIME ALLOWED : 2 Hours 30 Minutes

Answer ALL SIX questions from Section A and TWO 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.

The following results may be used:

In spherical polar co-ordinates, $dr = r^2 \sin \theta dr d\theta d\phi$, and

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2}.$$

If n is a positive integer,

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

The spin angular momentum operator \hat{S} is given by $\hat{S} = \frac{\hbar}{2} \hat{\sigma}$ where $\hat{\sigma} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$ and, in the basis formed by $|\alpha\rangle$ and $|\beta\rangle$, the Pauli spin matrices are

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

with

$$|\alpha\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |\beta\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

SECTION A

1. Explain what is meant by an **observable** in quantum mechanics. [2]

When does a measurement of the expectation value of an observable correspond to an eigenvalue of the observable? [1]

An observable \hat{Q} has just two orthonormal eigenstates ϕ_1 and ϕ_2 corresponding to eigenvalues -1 and $+1$ respectively. A system is described by a wave function ψ

$$\psi = c_1 \phi_1 + c_2 \phi_2,$$

which is normalised to unity.

What is the probability of a measurement of \hat{Q} giving the result $+1$? [1]

What is the expectation value of \hat{Q} before any measurement is made? [2]

2. The variance of an observable \hat{Q} in a state with wave function Ψ is defined by

$$(\Delta\hat{Q})^2 = \langle (\hat{Q} - \langle \hat{Q} \rangle)^2 \rangle .$$

Explain the meaning of the terms in this expression. [3]

Show that the variance can also be expressed as

$$(\Delta\hat{Q})^2 = \langle \hat{Q}^2 \rangle - \langle \hat{Q} \rangle^2$$
 [3]

3. Determine a real positive constant N such that the spherically symmetric three dimensional wave function

$$\psi(\mathbf{r}) = N e^{-r}$$

is normalised to unity. [6]

4. The conceptual problems of quantum mechanics may be grouped under the three headings of **determinism**, **locality** and **reduction** of the wave function. Very briefly outline the problems in each of these three areas. [8]

5. What is meant by a **stationary state** in quantum mechanics? [2]

The time rate of change of the expectation value of an observable \hat{A} , for a system with wave function Ψ , is given by

$$\frac{\partial \langle \hat{A} \rangle}{\partial t} = \frac{i}{\hbar} \int \Psi^* [\hat{H}, \hat{A}] \Psi d\tau + \langle \frac{\partial \hat{A}}{\partial t} \rangle .$$

Explain the meaning of the terms on the right hand side of this equation and the significance of this result. [4]

6. Using Dirac notation, express

- The fact that a complete set of states $|u_n\rangle$ are orthonormal [2]
- That any state $|x\rangle$ may be expanded in terms of the $|u_n\rangle$ [2]
- The coefficients of the expansion of $|x\rangle$ in terms of the $|u_n\rangle$ [2]
- That an operator \hat{A} is Hermitian [2]

SECTION B

7. (a) A Hermitian operator \hat{A} has a complete set of orthonormal eigenfunctions $|n\rangle$. Show that in the basis $|n\rangle$, the matrix representing \hat{A} is diagonal with elements $A_{nn'} = a_n \delta_{nn'}$ where a_n is the eigenvalue of \hat{A} corresponding to eigenvector $|n\rangle$. [3]

- (b) If $\hat{\mathbf{J}}$ is a quantum mechanical angular momentum operator, \hat{J}^2 and \hat{J}_z satisfy the commutation relation $[\hat{J}^2, \hat{J}_z] = 0$. What does this tell us about these two observables? [2]

If \hat{J}_+ and \hat{J}_- are defined by

$$\hat{J}_+ = \hat{J}_x + i\hat{J}_y \quad ; \quad \hat{J}_- = \hat{J}_x - i\hat{J}_y,$$

show that

$$[\hat{J}_z, \hat{J}_+] = \hbar \hat{J}_+ \quad [4]$$

- (c) Given that, in addition,

$$[\hat{J}_z, \hat{J}_-] = -\hbar \hat{J}_-$$

and if, also

$$\hat{J}_z |j, m\rangle = m\hbar |j, m\rangle$$

show that $\hat{J}_+ |j, m\rangle$ is an eigenfunction of \hat{J}_z corresponding to the eigenvalue $(m+1)\hbar$. [4]

- (d) A particle has total spin quantum number $s = 1$. If the spin operator is $\hat{\mathbf{S}}$, what are the eigenvalues of \hat{S}_z and \hat{S}^2 ? [2]

Write down the matrices of \hat{S}_z and \hat{S}^2 in the basis formed from the normalised eigenstates $|s, m\rangle$ of \hat{S}^2 and \hat{S}_z . [3]

- (e) Verify that they commute. [2]

- (f) Given that

$$\hat{S}_\pm |s, m\rangle = \hbar \sqrt{s(s+1) - m(m \pm 1)} |s, m \pm 1\rangle$$

find the matrix of \hat{S}_x in the same basis. [6]

- (g) Verify that the eigenvalues of \hat{S}_x are the same as those of \hat{S}_z . [4]

8. (a) The Hamiltonian operator \hat{H} for a one-dimensional harmonic oscillator of mass m and angular frequency ω is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2.$$

The operators \hat{a}_+ and \hat{a}_- are defined by

$$\hat{a}_{\pm} = \frac{1}{\sqrt{2m\hbar\omega}}(\hat{p} \pm im\omega\hat{x}),$$

where \hat{p} and \hat{x} are momentum and position operators satisfying $[\hat{x}, \hat{p}] = i\hbar$.

Show that

$$\hat{H} = (\hat{a}_+\hat{a}_- + \frac{1}{2})\hbar\omega. \quad [5]$$

and

$$[\hat{a}_-, \hat{a}_+] = 1. \quad [5]$$

- (b) Assuming without proof that

$$[\hat{H}, \hat{a}_{\pm}] = \pm\hat{a}_{\pm}\hbar\omega$$

and using the notation $\hat{H}|n\rangle = E_n|n\rangle$, show that

$$\hat{H}\hat{a}_+|n\rangle = (E_n + \hbar\omega)\hat{a}_+|n\rangle \quad [5]$$

- (c) What is the interpretation of this result? [2]

- (d) Given also that,

$$\hat{H}\hat{a}_-|n\rangle = (E_n - \hbar\omega)\hat{a}_-|n\rangle,$$

show that the lowest eigenvalue of \hat{H} is $E_0 = \frac{1}{2}\hbar\omega$, that

$$E_n = (n + \frac{1}{2})\hbar\omega \quad [5]$$

and that the eigenstate corresponding to E_n is

$$|n\rangle = C_n(\hat{a}_+)^n|0\rangle,$$

where C_n is a normalisation constant. [2]

- (e) Given that, in the x -representation, the eigenstate $|0\rangle$ is

$$\psi_0(x) = A_0 e^{-m\omega x^2/2\hbar},$$

show that

$$\psi_2(x) = A_2 \left(1 - \frac{2m\omega x^2}{\hbar}\right) e^{-m\omega x^2/2\hbar} \quad [6]$$

where A_0 and A_2 are normalisation constants.

9. (a) A charged spin-1/2 particle is fixed in an external uniform magnetic field $\mathbf{B} = B\hat{z}$ where \hat{z} is a unit vector in the z -direction. The Hamiltonian operator is

$$\hat{H} = \gamma B \hat{S}_z$$

where \hat{S}_z is the z -component of the spin operator $\hat{\mathbf{S}}$ and γ is a constant. Find the energy eigenvalues of this system. [4]

- (b) If $|\alpha\rangle$ and $|\beta\rangle$ are eigenvectors of \hat{S}_z corresponding to eigenvalues $\hbar/2$ and $-\hbar/2$ respectively, determine ω such that the wave function at time t is

$$\Psi(t) = c_1 e^{-i\omega t/2} |\alpha\rangle + c_2 e^{i\omega t/2} |\beta\rangle,$$

where c_1 and c_2 are constants. [5]

- (c) Suppose that at time $t = 0$ the system is in an eigenstate of \hat{S}_x ,

$$\Psi(0) = \frac{1}{\sqrt{2}} (|\alpha\rangle + |\beta\rangle)$$

corresponding to eigenvalue $\hbar/2$. Write down the wave function at subsequent times and hence determine the times at which it will be an eigenstate of \hat{S}_x ,

$$\Psi = \frac{1}{\sqrt{2}} (|\alpha\rangle - |\beta\rangle)$$

corresponding to eigenvalue $-\hbar/2$. [6]

- (d) The operator \hat{S}_n represents the component of the spin operator $\hat{\mathbf{S}}$ in the direction of a unit vector \hat{n} lying in the $x - y$ plane:

$$\hat{S}_n = \hat{\mathbf{S}} \cdot \hat{n} = \hat{S}_x \cos \phi + \hat{S}_y \sin \phi$$

where ϕ is the angle between \hat{n} and the x -axis. Show that \hat{S}_n may be expressed in matrix form as

$$\hat{S}_n = \frac{\hbar}{2} \begin{pmatrix} 0 & e^{-i\phi} \\ e^{i\phi} & 0 \end{pmatrix} \quad [4]$$

- (e) Show that the eigenvalues of \hat{S}_n are $\pm\hbar/2$. [4]
- (f) Determine the eigenfunction of \hat{S}_n corresponding to the eigenvalue $\hbar/2$ and show that, if the system is initially in an eigenstate of \hat{S}_x , it will subsequently be in an eigenstate of \hat{S}_n where \hat{n} rotates in the $x - y$ plane with angular velocity ω . Comment on this result. [7]

10. (a) The Hamiltonian operator \hat{H} describing a quantum mechanical system in spherical polar coordinates has a lowest energy eigenvalue E_0 . Show, for any normalisable function $F(\mathbf{r})$ that satisfies the boundary conditions appropriate to a bound state, that the expectation value $E(F)$ of \hat{H} satisfies

$$E(F) = \frac{\int F^*(\mathbf{r})\hat{H}F(\mathbf{r})d\mathbf{r}}{\int F^*(\mathbf{r})F(\mathbf{r})d\mathbf{r}} \geq E_0 \quad [8]$$

- (b) Explain how this expression can be used to find an approximation to the ground state energy which is an upper limit to its true value. [3]
- (c) The Hamiltonian operator for a hydrogenic ion of nuclear charge number Z and reduced mass μ is, in atomic units,

$$\hat{H} = -\frac{1}{2\mu}\nabla^2 - \frac{Z}{r}.$$

Use the normalised three-dimensional trial function

$$F(\mathbf{r}) = \sqrt{\frac{\mu^3 Z^3}{\pi}} e^{-\alpha r},$$

where α is a variational parameter, to derive an upper bound on the ground state energy of this system. [15]

- (d) Demonstrate that this upper bound is also an exact energy for this system. [4]