Imperial College London

BSc/MSci EXAMINATION June 2012

This paper is also taken for the relevant Examination for the Associateship

QUANTUM MECHANICS

For 2nd-Year Physics Students

Friday, 8th June 2012: 10:00 to 12:00

Answer THREE questions.

All questions carry equal marks.

Marks shown on this paper are indicative of those the Examiners anticipate assigning.

General Instructions

Complete the front cover of each of the THREE answer books provided.

If an electronic calculator is used, write its serial number at the top of the front cover of each answer book.

USE ONE ANSWER BOOK FOR EACH QUESTION.

Enter the number of each question attempted in the box on the front cover of its corresponding answer book.

Hand in THREE answer books even if they have not all been used.

You are reminded that Examiners attach great importance to legibility, accuracy and clarity of expression.

1. (i) The fundamental predictions of quantum mechanics are the probabilities of obtaining any particular result from a measurement of a dynamical variable. Show that the probabilities are not affected by multiplying the wavefunction ψ by any phase factor $e^{i\alpha}$, where α is a real number which is not a function of x.

[4 marks]

(ii) Write down the time independent Schrödinger equation for a particle of mass m moving in one dimension in a potential $V(x)$. Consider the potential described by

$$\begin{aligned} V(x) &= 0 : \quad 0 \le x \le a, \\ V(x) &= \infty : \quad x < 0 \text{ or } x > a. \end{aligned}$$

Solve the Schrödinger equation for this potential and show that the energy eigenstates $u_n(x)$ have energy eigenvalues given by

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2},$$

where n is a positive integer. [6 marks]

(iii) Consider a particle in the ground state, so at $t = 0$ its wavefunction is

$$\psi(x, t = 0) = u_1(x).$$

Write down the time dependence of this wavefunction and explain why this is called a "stationary state". [3 marks]

(iv) Consider a particle with a wavefunction at $t = 0$ given by

$$\psi(x, t = 0) = \frac{1}{\sqrt{2}}\left[u_1(x) + u_2(x)\right].$$

Calculate an expression for the first later time at which the wavefunction is physically equivalent to the wavefunction at $t = 0$. [5 marks]

(v) If the potential in the region $0 \le x \le a$ was $V = K$ for some non-zero constant K, rather than $V = 0$, explain how the answers to parts (iii) and (iv) would change. Is such a potential shift observable? [2 marks]

[Total 20 marks]

2. The ground state energy eigenfunction of a one dimensional harmonic oscillator centred on $x = 0$ is given by

$$u_0 = Ae^{-\alpha x^2/2},$$

where α is a constant, and A is a normalisation constant which can be taken to be real and positive.

(i) The first excited state energy eigenfunction is given by

$$u_1 = Bxe^{-\alpha x^2/2},$$

where B is a normalisation constant. Show that these two eigenfunctions are orthogonal. [2 marks]

(ii) Normalise u_0. [3 marks]

(iii) Calculate the following quantities for the state u_0:

(a) The expectation value of the position of the particle. Briefly give a physical justification for your answer. [2 marks]

(b) The expectation value of the momentum of the particle. Briefly give a physical justification for your answer. [2 marks]

(c) The root mean squared (rms) uncertainty in the position of the particle. [4 marks]

(d) The rms uncertainty in the momentum of the particle. Hint: the momentum operator is Hermitian. [4 marks]

(iv) Show that the ground state of the system is a “minimum uncertainty state”. [3 marks]

[Total 20 marks]

Standard integrals:

$$\int_{-\infty}^{\infty} e^{-y^2}\, dy = \sqrt{\pi}, \qquad \int_{-\infty}^{\infty} y^2 e^{-y^2}\, dy = \sqrt{\pi}/2.$$

3. A particle of mass m is confined by a one dimensional harmonic oscillator potential corresponding to a classical angular frequency ω.

(i) Write down the quantum mechanical Hamiltonian in terms of $\hat{x}$ and $\hat{p}$, the operators corresponding to position and momentum and show that it can be written in the form

$$\hat{H} = \hbar\omega(\alpha^2\hat{x}^2 + \beta^2\hat{p}^2),$$

where $\alpha^2 = m\omega/2\hbar$ and $\beta^2 = 1/2m\omega\hbar$. [3 marks]

(ii) By defining new operators

$$\begin{aligned} \hat{a} &= \alpha\hat{x} + i\beta\hat{p}, \\ \hat{a}^\dagger &= \alpha\hat{x} - i\beta\hat{p}, \end{aligned}$$

and given that $[\hat{x}, \hat{p}] = i\hbar$, calculate expressions for $\hat{a}\hat{a}^\dagger$ and $\hat{a}^\dagger\hat{a}$ and hence show that

$$[\hat{a}, \hat{a}^\dagger] = 1.$$

[6 marks]

(iii) By expressing $\hat{H}$ in terms of the combination $\hat{a}^\dagger\hat{a}$, show that the commutator of $\hat{H}$ and $\hat{a}$ is

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

Hence, show that the action of the operator $\hat{a}$ on u_n is to convert it to another eigenstate ($\hat{a}u_n$) of energy lower than that of u_n by an amount $\hbar\omega$. [6 marks]

(iv) What must be the result of operating with $\hat{a}$ on the ground state u_0? Use this to determine the ground state energy eigenvalue E_0. [2 marks]

(v) Use the equation of part (iv) for $\hat{a}u_0$ to determine the (unnormalised) functional form of $u_0(x)$. [3 marks]

[Total 20 marks]

4. A spinless particle of mass m is bound in a central potential $V(r)$. Energy eigenfunctions have the form

$$u_{nlm_l} = R_{n\,l}(r) Y_{l\,m_l}(\theta, \phi).$$

The radial dependence is given by solutions to the equation

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2mr^2} + V(r)\right] G_{n\,l}(r) = EG_{n\,l}(r),$$

where $G_{n\,l}(r) = rR_{n\,l}(r)$, E is the energy and l is the total angular momentum squared quantum number.

A spherically symmetric infinite well has a potential

$$\begin{aligned} V(r) &= 0 \qquad \text{for} \qquad r \leq a, \\ &= \infty \qquad \text{for} \qquad r > a. \end{aligned}$$

(i) $R_{n\,l}(r)$ must be finite at $r = 0$ and zero for $r > a$. Use this to write down the boundary conditions for $G_{n\,l}(r)$ at $r = 0$ and $r = a$. [2 marks]

(ii) By direct substitution (or otherwise) show that in the absence of angular momentum, the solutions of $G_{n\,0}$ have the form

$$G_{n\,0} = A \sin kr,$$

where A is a normalisation constant. Find the allowed values of k and hence determine the lowest energy which has zero angular momentum. [6 marks]

(iii) By direct substitution (or otherwise) show that for $l = 1$, the solutions of $G_{n\,1}$ have the form

$$G_{n\,1} = B\left(\frac{\sin k'r}{r} - k' \cos k'r\right),$$

where B is a normalisation constant. [7 marks]

(iv) By considering the $r \to 0$ limit, show that $G_{n\,1}$ satisfies the boundary condition at $r = 0$. Use the boundary condition at $r = a$ to show that k' must satisfy

$$\tan k'a = k'a.$$

[3 marks]

(v) By sketching the functions in part (iv) or otherwise, deduce whether the lowest energy solution for $l = 1$ is lower than, the same as, or greater than the lowest energy solution for $l = 0$. Explain your reasoning. [2 marks]

[Total 20 marks]

5. (i) A quantum rigid rotor with a moment of inertia I, constrained to rotate in the xy plane, has a Hamiltonian operator

$$\hat{H} = -\frac{\hbar^2}{2I}\frac{\partial^2}{\partial\phi^2}$$

where ϕ is the xy plane polar angle to the x axis. Physically justify this expression, given that the angular momentum operator for rotations in the xy plane is $L = -i\hbar\,\partial/\partial\phi$ [3 marks]

(ii) Considering just the ϕ dependence, show by substitution that the energy eigenstates can be written in the form

$$u(\phi) = Ne^{im\phi}.$$

Find a suitable value for the normalisation constant N and give an expression for the energy eigenvalues, paying attention to the requirement for the wavefunction to be physical. [6 marks]

(iii) State the level of degeneracy of these energy eigenstates. Explain how L can be used to label the states uniquely. [4 marks]

(iv) Consider a rotor with a normalised wavefunction

$$\psi(\phi) = \frac{1}{\sqrt{3\pi}}\left(1 + \cos\phi\right).$$

Find the possible results of an energy measurement and evaluate the probability of getting each possible value. [7 marks]

[Total 20 marks]

6. (i) Describe the use of Hermitian operators in quantum mechanics and explain why it is important that they are Hermitian. [4 marks]

(ii) In quantum mechanics, particles have an intrinsic quantity called spin; for example electrons are "spin 1/2" particles and photons are "spin 1" particles. When handling spin variables, the spin operators are represented using matrices. Define what is meant by an Hermitian matrix. Hence, for a general Hermitian matrix, written figuratively as

$$\begin{pmatrix} a & b & c & \dots \\ d & e & \dots & \dots \\ f & \vdots & \ddots & \\ \vdots & \vdots & & \ddots \end{pmatrix},$$

write down a condition for the diagonal elements, e.g. a or e, and derive a relation between the opposite off-diagonal elements, e.g. b and d, or c and f. [3 marks]

(iii) Consider the three matrices

$$A = \hbar \begin{pmatrix} 0 & i & 0 \\ -i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad B = \hbar \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \qquad C = \hbar \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & i \\ 0 & -i & 0 \end{pmatrix}.$$

(a) Find the eigenvalues of A. [3 marks]

(b) Find the commutator $[A, B]$. [2 marks]

(c) Calculate A^2 and by analogy write down B^2 and C^2. Hence calculate the matrix $A^2 + B^2 + C^2$. [2 marks]

(d) Explain why A, B and C have the correct properties to act as appropriate matrices to represent operators for spin components. [3 marks]

(e) State the total spin value that these matrices would correspond to. Give TWO justifications for your answer. [3 marks]

[Total 20 marks]