Imperial College
London

BSc, MSci and MSc EXAMINATIONS (MATHEMATICS)

May – June 2015

This paper is also taken for the relevant examination for the Associateship of the Royal College of Science.

Mathematical Physics I: Quantum Mechanics

Date: Tuesday, 19 May 2015. Time: 2.00pm – 4.00pm. Time allowed: 2 hours.

This paper has FOUR questions.

Candidates should use ONE main answer book.

Supplementary books may only be used after the main book is full.

Statistical tables will not be provided.

- DO NOT OPEN THIS PAPER UNTIL THE INVIGILATOR TELLS YOU TO.
- Affix one of the labels provided to each answer book that you use, but DO NOT USE THE LABEL WITH YOUR NAME ON IT.
- Credit will be given for all questions attempted, but extra credit will be given for complete or nearly complete answers to each question as per the table below.

Raw mark	up to 12	13	14	15	16	17	18	19	20
Extra credit	0	$\frac{1}{2}$	1	$1\frac{1}{2}$	2	$2\frac{1}{2}$	3	$3\frac{1}{2}$	4

- Each question carries equal weight.
- Calculators may not be used.

1. Energy quantisation for the finite square well potential

Consider a particle of mass m under the influence of the potential

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

where V_0 is a real positive constant.

(a) Write down an ansatz for possible bound states using the known form of solutions of the time-independent Schrödinger equation in the different regions.

(b) Use the symmetry of the potential to simplify the ansatz from (a).

(c) Use the boundary conditions between the different regions to derive quantisation conditions for the energies of the bound states for odd and even states.

2. **The principles of quantum mechanics**

Consider a system on the Hilbert space $\mathbb{C}^3$ and a Hamiltonian $\hat{H}$ represented by the matrix

$$\hat{H} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & E & 0 \\ E & 0 & E \\ 0 & E & 0 \end{pmatrix},$$

with $E \in \mathbb{R}$. Let another observable $\hat{A}$ be described by the matrix

$$\hat{A} = \begin{pmatrix} a & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -a \end{pmatrix},$$

with $a \in \mathbb{R}$.

(a) Calculate the eigenvalues and a set of normalised eigenvectors of $\hat{H}$.

(b) Assume that at some specific time the system is in the state

$$|\psi\rangle = \frac{1}{\sqrt{11}} \begin{pmatrix} 3 \\ -\mathrm{i} \\ 1 \end{pmatrix}.$$

How likely is it that a measurement of the observable $\hat{A}$ yields which outcome? Calculate the expectation value of A.

(c) At time $t = 0$ the measurement of the observable A yields the result a. What is the probability that a subsequent measurement of A at time $t > 0$ yields the same result a?

3. **The variational method for the approximate calculation of eigenfunctions**

(a) Prove that the expectation value of a Hamiltonian is bounded from below by the lowest energy eigenvalue. For simplicity you only need to consider the case of discrete eigenvalues here.

(b) The statement in (a) can be used to provide an approximation for the lowest energy state by minimising the expectation value for a trial wave function depending on a set of parameters. Apply this idea to approximate the ground state energy and wave function for the Hamiltonian

$$\hat{H} = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}x^4,$$

using the normalised trial function

$$\phi(x) = \left(\frac{\lambda}{\pi}\right)^{\frac{1}{4}} \mathrm{e}^{-\lambda x^2/2},$$

where λ is a real positive constant. Here we use rescaled units such that $\hbar = 1 = m$. Compare the approximate ground state energy with the numerically exact value $E_0 = 0.530\ldots$.

Hint: The following integrals might be useful:

$$\int_{-\infty}^{\infty} \mathrm{e}^{-ax^2}\,dx = \sqrt{\frac{\pi}{a}}, \qquad \int_{-\infty}^{\infty} x^2\mathrm{e}^{-ax^2}\,dx = \frac{1}{2a}\sqrt{\frac{\pi}{a}}, \qquad \int_{-\infty}^{\infty} x^4\mathrm{e}^{-ax^2}\,dx = \frac{3}{4a^2}\sqrt{\frac{\pi}{a}},$$

for $\mathrm{Re}(a) > 0$. You might also need the approximate numerical value $3^{1/3} = 1.442\ldots$.

4. **Orbital angular momentum.**

Consider the quantum operators for three dimensional orbital angular momentum defined in terms of position and momentum operators as

$$\hat{L}_1 = \hat{q}_2\hat{p}_3 - \hat{q}_3\hat{p}_2$$
$$\hat{L}_2 = \hat{q}_3\hat{p}_1 - \hat{q}_1\hat{p}_3$$
$$\hat{L}_3 = \hat{q}_1\hat{p}_2 - \hat{q}_2\hat{p}_1,$$

where the position and momentum operators for the three spatial dimensions fulfil the canonical commutation relations

$$[\hat{q}_j, \hat{p}_k] = \mathrm{i}\hbar\delta_{jk}, \qquad [\hat{q}_j, \hat{q}_k] = 0 = [\hat{p}_j, \hat{p}_k]. \tag{1}$$

(a) Deduce the commutator of $\hat{L}_1$ and $\hat{L}_3$ from the fundamental commutators in equation (1).

(b) Can L_1 and L_3 be measured simultaneously?

(c) Consider the possible eigenvalues of $\hat{L}_3$.

(i) Introduce the new set of operators $\hat{x}$ and $\hat{y}$, and $\hat{p}_x$ and $\hat{p}_y$, defined as

$$\hat{x} = \frac{1}{\sqrt{2}}(\hat{q}_1 + \hat{p}_2), \qquad \hat{p}_x = \frac{1}{\sqrt{2}}(\hat{p}_1 - \hat{q}_2)$$
$$\hat{y} = \frac{1}{\sqrt{2}}(\hat{q}_1 - \hat{p}_2), \qquad \hat{p}_y = \frac{1}{\sqrt{2}}(\hat{p}_1 + \hat{q}_2),$$

deduce the commutation relations for the new operators and rewrite $\hat{L}_3$ in terms of $\hat{x}$, $\hat{y}$, $\hat{p}_x$, and $\hat{p}_y$.

(ii) Remembering that the eigenvalues of the harmonic oscillator $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2$ are given by $\hbar\omega(n + \frac{1}{2})$, where n are the non-negative integers, what can you deduce for the eigenvalues of $\hat{L}_3$?

(d) What are the eigenvalues of $\hat{L}_1$?