PAPER CODE NO.
MATH325

THE UNIVERSITY
of LIVERPOOL

JANUARY 2004 EXAMINATIONS

Bachelor of Arts : Year 3
Bachelor of Science : Year 2
Bachelor of Science : Year 3
Master of Mathematics : Year 3
Master of Mathematics : Year 4

QUANTUM MECHANICS

TIME ALLOWED : Two Hours and a Half

INSTRUCTIONS TO CANDIDATES

In this paper, bold-face quantities such as $\mathbf{r}$ represent three-dimensional vectors.

Full marks can be obtained for complete answers to FIVE questions. Only the best FIVE answers will be counted. Marks for parts of questions may be subject to small adjustments

1. (i) Consider the following operators acting on a two-state system.

$$\hat{A} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \; \hat{B} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \; \hat{C} = \begin{pmatrix} 3 & 0 \\ 0 & 2 \end{pmatrix}, \; \hat{D} = \begin{pmatrix} 0 & 3i \\ -3i & 0 \end{pmatrix}.$$

Three of them could represent an observable in quantum mechanics, and one could not. Say which is the operator that can not correspond to an observable, giving reasons for your choice.

Of the three valid operators, for which pair would it be possible to simultaneously know the value of both observables? Give the reason for your choice.

(ii) A particle moving in one dimension is described at some moment in time by the wave function

$$\psi(x) = Be^{-a|x|}$$

where B and a are real positive constants. Find the normalisation constant B in terms of a.

Find the expectation values $\langle\hat{x}\rangle, \langle\hat{x}^2\rangle, \langle\hat{p}\rangle$ and $\langle\hat{p}^2\rangle$ for the given wave function. Thus find the uncertainties Δx and Δp for the position and momentum of the particle, and comment on your result.

Note: you may use without proof the result

$$I_n(b) \equiv \int_0^\infty x^n e^{-bx}\,dx = \frac{n!}{b^{n+1}}$$

when $b > 0$.

[20 marks]

2. A particle of mass m moves on the x-axis in a potential $V(x)$ which has the values

$$\begin{array}{rl} V(x) = \infty & x < 0 \\ V(x) = 0 & 0 \leq x \leq L \\ V(x) = U & x > L \end{array}$$

where U is a positive constant.

What boundary conditions would the wave function of a bound state (i.e. a state with energy E such that $0 < E < U$) fulfill at $x = 0$ and at $x = \infty$? What conditions must the wave function satisfy at $x = L$?

Define the two quantities

$$q^2 = \frac{2mE}{\hbar^2} \quad \text{and} \quad K^2 = \frac{2m(U-E)}{\hbar^2}$$

and use them to write down the energy eigenfunction.

Show that bound states will exist at energies where

$$-q \cot qL = \sqrt{\frac{2mU}{\hbar^2} - q^2} \; .$$

What is the minimum value of U which will allow such a bound state to exist?

[20 marks]

3. The Hamiltonian of a particle undergoing simple harmonic motion in one dimension is given by

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

Define the operators

$$a = \frac{\alpha}{\sqrt{2}}\Big(\frac{\hat{p}}{\hbar\alpha^2} - i\hat{x}\Big) \quad \text{and} \quad a^\dagger = \frac{\alpha}{\sqrt{2}}\Big(\frac{\hat{p}}{\hbar\alpha^2} + i\hat{x}\Big)\,, \qquad \text{where} \quad \alpha^2 = \frac{m\omega}{\hbar} \ .$$

Let ϕ_0 be the normalised ground state wave function such that $a\phi_0 = 0$.

(a) Use the fact that $[\hat{x}, \hat{p}] = i\hbar$ to show that $[a, a^\dagger] = 1$.

(b) Show by induction that $[a, (a^\dagger)^n] = n(a^\dagger)^{n-1}$.

(c) The normalised eigenfunctions of the Hamiltonian are given by

$$\phi_n = \frac{1}{\sqrt{n!}}(a^\dagger)^n\phi_0.$$

Show that

$$a\phi_n = \sqrt{n}\phi_{n-1} \quad \text{and} \quad a^\dagger\phi_n = \sqrt{n+1}\phi_{n+1}.$$

(d) Write $(a^\dagger - a)^2\phi_n$ in terms of ϕ_{n-2}, ϕ_n and ϕ_{n+2}, and use the result to find $\langle\phi_n|\hat{x}^4\phi_n\rangle$.

[The identity

$$[A, BC] = B[A, C] + [A, B]C$$

for operators A, B and C may be useful.]

[20 marks]

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4. The Hamiltonian for a stationary electron of mass m and charge e in a constant magnetic field B along the z-axis is given by

$$\hat{H} = \hbar\omega\sigma_3$$

where

$$\omega = \frac{eB}{2m} \quad \text{and} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} .$$

(a) By solving Schrödinger's equation, show that at time t the state of the electron is given by

$$\psi(t) = \begin{pmatrix} ae^{-i\omega t} \\ \\ be^{i\omega t} \end{pmatrix},$$

where a, b are constants.

(b) An observable $\hat{Q}$ is represented by

$$\hat{Q} = \begin{pmatrix} 1 & 2i \\ -2i & 1 \end{pmatrix} .$$

Compute the eigenvalues and normalised eigenvectors of $\hat{Q}$ and deduce the possible results of a measurement of $\hat{Q}$.

(c) At $t = 0$, the electron is in the normalised state

$$\psi(0) = \frac{1}{\sqrt{5}} \begin{pmatrix} 2 \\ 1 \end{pmatrix} .$$

By writing $\psi(t)$ as a linear combination of the eigenvectors of $\hat{Q}$, find the probabilities of each possible result of a measurement of $\hat{Q}$ at time t.

If this measurement gives a result greater than 0, what is the state of the system immediately after the measurement?

[20 marks]

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5. A beam of identical particles of mass m and energy $E > 0$ is travelling along the x-axis from $x < 0$ and is incident on a potential step

$$\begin{aligned} V(x) &= V_0 \qquad x \geq 0 \\ V(x) &= 0 \qquad x < 0 \end{aligned}$$

where V_0 is a constant. Suppose that $E > V_0$.

(i) Write down an expression for the probability flux (current density) j_I for a beam of particles with wave-function $\psi(x) = Ae^{ikx}$. For the potential step above, show that the transmission coefficient T, defined as the ratio of the transmitted flux to the incident flux, is

$$T = \frac{4kq}{(k+q)^2}$$

where $\hbar^2 k^2 = 2mE$ and $\hbar^2 q^2 = 2m(E - V_0)$.

(ii) Calculate the probability density $|\psi(x)|^2$ as a function of x, and sketch the result when $0 < V_0 < E$.

[**20 marks**]

6. A particle of mass m moves on the x-axis in a potential $V(x)$ such that

$$\begin{aligned} V(x) &= \infty \qquad x < 0 \text{ or } x > 2L \\ V(x) &= 0 \qquad 0 \leq x \leq 2L\ . \end{aligned}$$

(i) Find the normalised eigenfunctions of the Hamiltonian, and show that the energy levels are given by

$$E_n = \frac{\hbar^2 n^2 \pi^2}{8mL^2} \qquad (n = 1, 2, 3, \cdots).$$

(ii) The potential in the region $0 \leq x \leq 2L$ is perturbed so that the new potential is

$$\begin{aligned} V(x) &= \infty \qquad x < 0 \text{ or } x > 2L \\ V(x) &= \lambda x \qquad 0 \leq x \leq 2L\ . \end{aligned}$$

where λ is a small parameter. Use first order perturbation theory to obtain an approximation to the perturbed ground state energy.

[*Standard results from perturbation theory may be assumed without proof.*]
[**20 marks**]

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7. An arbitrary, normalised wave function ψ is expanded in terms of orthogonal, normalised eigenfunctions ϕ_n of the Hamiltonian $\hat{H}$:

$$\psi = \sum_n c_n \phi_n \qquad \hat{H}\phi_n = E_n \phi_n$$

and the eigenfunctions are ordered so that $E_0 \leq E_1 \leq E_2 \cdots$.

(i) Show that

$$E_0 \leq \langle \psi | \hat{H} \psi \rangle$$

and use this result to explain the variational method for estimating an upper bound on the ground state energy of a system with Hamiltonian $\hat{H}$.

(ii) A particle of mass m is moving in three dimensions in a spherical potential $V(\mathbf{r}) = \lambda r^4$, where $r = |\mathbf{r}| = \sqrt{x^2 + y^2 + z^2}$. The quantum mechanical Hamiltonian for this system is

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + \lambda r^4 \,,$$

and the radial part of the Laplacian operator is

$$\nabla^2_{\text{rad}} = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}.$$

Find the expectation value of the Hamiltonian for the normalised trial function

$$\psi(\mathbf{r}) = \sqrt{\frac{\alpha^3}{\pi}} e^{-\alpha r}.$$

By varying α find an estimate of the ground state energy of this system.

Note: you may use without proof the result

$$I_n(b) \equiv \int_0^\infty x^n e^{-bx} dx = \frac{n!}{b^{n+1}}$$

when $b > 0$.

[20 marks]