PAPER CODE NO.
MATH325

THE UNIVERSITY *of* LIVERPOOL

JANUARY 2006 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) Determine which, if any, of the following operators could represent an observable in quantum mechanics

$$\hat{A} = i\,x\,\frac{d}{dx}\,, \quad \hat{B} = \frac{d^2}{dx^2}\,,$$

stating clearly any assumptions you make.
[*Hint: you may use the property of a Hermitian operator* $\hat{O}$ *that*

$$\langle \hat{O}\psi|\phi\rangle = \langle \psi|\hat{O}\phi\rangle$$

where $\psi(x)$ *and* $\phi(x)$ *are any two normalisable wave functions*]

[6 marks]

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

$$\psi(x) = \begin{cases} C\cos\left(\dfrac{x}{a}\right) & : \quad |x| \le \frac{\pi}{2}a \\ 0 & : \quad \text{otherwise}\,, \end{cases}$$

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

Find the expectation values $\langle\hat{x}\rangle$, $\langle\hat{x}^2\rangle$, $\langle\hat{p}\rangle$ and $\langle\hat{p}^2\rangle$ with respect to the given wave function.

Use these results to find the uncertainties Δx and Δp for the position and momentum of the particle, and comment on your result.

[14 marks]

2. A quantum mechanical system has the Hamiltonian

$$\hat{H} = \begin{pmatrix} A & -iB & 0 \\ iB & A & iB \\ 0 & -iB & A \end{pmatrix}$$

(i) Find the possible values which a measurement of the energy of this system could give, and the corresponding normalised eigenstates.

(ii) The system is in the state

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \\ 0 \end{pmatrix}$$

when an energy measurement is carried out. Calculate the probability of each possible outcome.

(iii) The matrices

$$\hat{F} = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix} \qquad \text{and} \qquad \hat{G} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix}$$

represent two observables of this system. One of these quantities is conserved, having an expectation value that doesn't depend on time. Say which is conserved, giving a reason for your choice.

[**20 marks**]

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

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

where

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

(a) Solve Schrödinger's time-dependent equation for this system and show that at time t the state of the electron is given by

$$\psi(t) = \begin{pmatrix} a\, e^{-i\omega t} \\ b\, e^{i\omega t} \end{pmatrix} ,$$

where a and b are constants.

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

$$\hat{Q} = \begin{pmatrix} 9 & 2i \\ -2i & 6 \end{pmatrix} F$$

where F is a real constant. Compute the eigenvalues and normalised eigenvectors of $\hat{Q}$ and deduce the possible result of a measurement of $\hat{Q}$.

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

$$\psi(0) = \frac{1}{5}\begin{pmatrix} 4 \\ 3 \end{pmatrix} .$$

Write down $\psi(t)$, and use this to calculate the expectation value of $\hat{Q}$ as a function of time.

[20 marks]

4. 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

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

where V_0 is a constant. Suppose that $0 < E < V_0$.

(i) Write down an expression for the current density j_I for a beam of particles with wave-function $\psi(x) = Ae^{ikx}$. For the potential step above, evaluate the reflection coefficient R, defined as the ratio of the reflected current density to the incident current density.

(ii) Deduce the transmission coefficient T, and comment on the result.

(iii) Sketch the particles' probability density as a function of x.

[**20 marks**]

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5. The Hamiltonian of a particle of mass m undergoing simple harmonic motion along the x-axis is given by

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

where $\hat{p}$ is the momentum operator and ω is a positive constant.

(i) Show that, if we define

$$a = \frac{\alpha}{\sqrt{2}}(\frac{1}{m\omega}\hat{p} - i\hat{x}) \qquad \text{and} \qquad a^\dagger = \frac{\alpha}{\sqrt{2}}(\frac{1}{m\omega}\hat{p} + i\hat{x})$$

where $\alpha^2 = m\omega/\hbar$, then it follows from the commutator $[\hat{x}, \hat{p}] = i\hbar$ that $[a, a^\dagger] = 1$.

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

(iii) Given that the normalised eigenfunctions of the Hamiltonian are

$$\psi_n = \frac{1}{\sqrt{n!}}(a^\dagger)^n\psi_0 \qquad \text{where} \qquad a\psi_0 = 0\,,$$

show that

$$a\psi_n = \sqrt{n}\psi_{n-1} \qquad \text{and} \qquad a^\dagger\psi_n = \sqrt{n+1}\psi_{n+1}\,.$$

(iv) Write

$$(a + a^\dagger)^2\psi_n$$

in terms of ψ_{n-2}, ψ_n and ψ_{n+2}. Use this result to calculate

$$\langle\psi_n|\hat{p}^2|\psi_n\rangle \quad \text{and} \quad \langle\psi_n|\hat{p}^4|\psi_n\rangle\,.$$

[*You may find the following identity useful:*

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

for operators A, B and C.]

[20 marks]

6. (i) Define I_n as

$$I_n \equiv \int_{-\infty}^{\infty} x^n e^{-sx^2}\,dx$$

where $s > 0$. The value of I_0 is

$$I_0 = \int_{-\infty}^{\infty} e^{-sx^2}\,dx = \sqrt{\frac{\pi}{s}}$$

By differentiating this expression with respect to s find expressions for I_2, I_4 and I_6.

[6 marks]

(ii) The Hamiltonian for a particle of mass m moving in a one-dimensional harmonic oscillator potential is

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2\ .$$

(a) The normalised ground state wave function has the form

$$\psi_0(x) = Ae^{-bx^2}$$

where A and b are real positive constants. Find A, b and the ground state energy E_0.

(b) The Hamiltonian is perturbed by the addition of a term

$$ux^6$$

to the potential, where u is a small parameter. Use first order perturbation theory to find an approximation to the perturbed ground state energy in the form

$$E_0' = E_0 + Cu,$$

where C is a constant which you should find.

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

[14 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 $V(\mathbf{r}) = \sigma r$, where $r = |\mathbf{r}| = \sqrt{x^2 + y^2 + z^2}$. The quantum mechanical Hamiltonian for this system is

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

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**]