PAPER CODE NO.
MATH325

THE UNIVERSITY
of LIVERPOOL

JANUARY 2007 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

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1. (i) Define I_n as

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

where $s > 0$. By symmetry, I_n is zero for odd n. 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) A particle free to move along the entire x axis is described at some moment in time by the wave function

$$\psi(x) = C(a + ix) \exp\left(-\frac{x^2}{2a^2}\right)$$

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 results.

[14 marks]

2. A quantum mechanical system has the Hamiltonian

$$\hat{H} = \begin{pmatrix} A & B & 0 \\ B & A & 0 \\ 0 & 0 & 2A \end{pmatrix}$$

where A and B are real numbers.

(i) Find the eigenvalues and normalised eigenvectors of the Hamiltonian. What is the physical significance of the eigenvalues?

(ii) Initially, at $t = 0$, the system is in the state

$$\psi_0 = \frac{1}{2} \begin{pmatrix} 1 \\ 1 - i \\ i \end{pmatrix} .$$

Calculate $\psi(t)$, the wave function at time t.

(iii) An energy measurement is carried out on this system at time t. Calculate the probability of each possible outcome and the expectation value of the energy.

[**20 marks**]

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

$$
\begin{aligned}
V(x) &= \infty & \quad & x < 0 \\
V(x) &= -U_0 & & 0 \leq x \leq L \\
V(x) &= 0 & & x > L
\end{aligned}
$$

where U_0 is a positive constant.

What boundary conditions does the wave function of a bound state (i.e. a state with energy $-U_0 < E < 0$) fulfill at $x = 0$ and at $x = \infty$? What conditions must the wave function satisfy at $x = L$?

Define the two quantities

$$q^2 = \frac{2m(E + U_0)}{\hbar^2} \quad \text{and} \quad K^2 = -\frac{2mE}{\hbar^2}$$

and use them to write down the energy eigenfunction.

Solve the Schrödinger equation and show that bound states will exist at energies where

$$-q \cot qL = +\sqrt{\frac{2mU_0}{\hbar^2} - q^2}\ .$$

What is the minimum value of U_0 for which a bound state exists?

Sketch the probability distribution of the ground state.

[**20 marks**]

4. The the angular momentum operators L_i $(i = 1, 2, 3)$ satisfy the commutation relations $[L_1, L_2] = i\hbar L_3$ (and cyclic permutations). All three L_i operators commute with $\mathbf{L}^2 \equiv L_1^2 + L_2^2 + L_3^2$.

   In this question you can assume the following properties of the angular momentum operators and their eigenstates. There are normalised states $|l, m\rangle$ which are simultaneously eigenstates of $\mathbf{L}^2$ and L_3, satisfying

$$\begin{aligned} L_3|l,m\rangle &= \hbar m|l,m\rangle \\ \mathbf{L}^2|l,m\rangle &= \hbar^2 l(l+1)|l,m\rangle \end{aligned} \tag{1}$$

   where $2l$ is a positive integer and $m \in \{-l, -l+1, \cdots, l-1, l\}$. Moreover there are raising and lowering operators $L_+ = L_1 + iL_2$ and $L_- = L_1 - iL_2$ which act on the eigenstates according to

$$L_+|l,m\rangle = M_{l,m}|l,m+1\rangle \quad \text{and} \quad L_-|l,m\rangle = N_{l,m}|l,m-1\rangle, \tag{2}$$

   with

$$M_{l,m} = \hbar\sqrt{l(l+1) - m(m+1)} \quad \text{and} \quad N_{l,m} = \hbar\sqrt{l(l+1) - m(m-1)}\,.$$

   (i) Use the commutation relations to show that

$$L_-L_+ = \mathbf{L}^2 - L_3^2 - \hbar L_3 \tag{3}$$

   (ii) A particle is in a state such that $l = 1$. Write down the allowed values of m (corresponding to the eigenvalues of L_3) and use equations (1) and (2) to write down 3×3 matrices representing L_3, L_+ and L_-.

   (iii) Use your matrix representations for L_+, L_- to find matrix representations for L_1 and L_2.

   (iv) Calculate the matrix $\mathbf{L}^2 = L_1^2 + L_2^2 + L_3^2$.

   (v) Check whether you matrices satisfy equation (3).

[**20 marks**]

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5. The Hamiltonian of a particle of mass m in the potential of a 1-dimensional harmonic oscillator 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) Show that the Hamiltonian can be written

$$\hat{H} = \hbar\omega\left(a^\dagger a + \tfrac{1}{2}\right) .$$

(iv) Show that the normalised state $|\psi_0\rangle$ defined by

$$a|\psi_0\rangle = 0\,,\ \langle\psi_0|\psi_0\rangle = 1\ ,$$

is an eigenstate of the Hamiltonian, and find its energy.

(v) Show that

$$|\psi_n\rangle \equiv \frac{1}{\sqrt{n!}}(a^\dagger)^n|\psi_0\rangle$$

is a normalised eigenstate of $\hat{H}$, and find its energy.
[*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) By using the connection between trigonometrical functions and the complex exponential function, or otherwise, derive identities for $\sin A \sin B$ and $\sin A \cos B$, where A and B are numbers.

[4 marks]

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

$$V(x) = \begin{cases} 0 & : \quad 0 \le x \le L \\ \infty & : \quad x < 0 \quad \text{and} \quad x > L\,, \end{cases}$$

The Hamiltonian for this system is

$$\hat{H}_0 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

which has the normalised eigenfunctions

$$\phi_n(x) = \begin{cases} \sqrt{\frac{2}{L}}\,\sin\left(\frac{n\pi x}{L}\right) & : \quad 0 \le x \le L \\ 0 & : \quad x < 0 \quad \text{and} \quad x > L\,, \end{cases}$$

(a) Find the energy of the eigenstate $\phi_n(x)$.

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

$$-U \sin\left(\frac{\pi x}{L}\right)$$

to the potential in the region $0 \le x \le L$, where U is a small parameter.
Use first order perturbation theory to find an approximation to the energy levels of the perturbed system in the form

$$E_n' \approx E_n + C_n U,$$

where the C_n are constants which you should calculate.

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

[16 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 $V(\mathbf{r}) = \frac{1}{2}m\omega^2 r^2$, where $r = |\mathbf{r}| = \sqrt{x^2 + y^2 + z^2}$. The quantum mechanical Hamiltonian for this system is

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega^2 r^2$$

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 value of A needed to normalise the trial wave-function

$$\psi(r) = \begin{cases} A(b^2 - r^2) & : \quad r \leq b \\ 0 & : \quad \text{otherwise}, \end{cases}$$

and find the expectation value of the Hamiltonian as a function of b. By varying b find an estimate of the ground state energy of this system. How close is your estimate to the true value of E_0?

[**20 marks**]