PAPER CODE NO.
MATH325

THE UNIVERSITY
of LIVERPOOL

JANUARY 2001 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. The normalised eigenfunctions of the Hamiltonian of a particle of mass m confined to the region of the x-axis between $x = 0$ and $x = L$ are

$$\phi_n(x) = \begin{cases} A \sin \frac{n\pi x}{L} & : \quad 0 \le x \le L \\ 0 & : \quad x < 0 \quad \text{or} \quad x > L \end{cases}$$

where A is a real, positive normalisation constant and the corresponding energy eigenvalues are

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

Find the value of A.

The particle is initially in the *ground state* of this potential well of width L. Suddenly the well expands to twice its original size, the right wall moving from $x = L$ to $x = 2L$, leaving the wavefunction momentarily undisturbed. A measurement of the energy is now made.

(a) Write down the wavefunction ψ of the particle in the modified potential (indicating its value for *all* x).

(b) By expressing ψ in terms of eigenfunctions of the modified system, find the probabilities for each possible result of the energy measurement. What is the most likely result?

(c) By using the result that

$$\sum_{n=1,3,5\ldots} \frac{1}{(n^2 - 4)^2} = \frac{\pi^2}{64},$$

verify that the probabilities evaluated in (b) do indeed add to 1.

(d) If the result of the energy measurement was in fact E'_1, where

$$E'_n = \frac{\hbar^2 \pi^2 n^2}{8mL^2} \qquad (n = 1, 2, 3 \ldots),$$

what is the probability that a subsequent energy measurement will give E'_2?

[*For part (b), you may find it helpful to use the result:* $2 \sin A \sin B = \cos(A - B) - \cos(A + B)$].

[20 marks]

2. A beam of particles of mass m and energy E is incident in the positive x direction on a potential well whose potential V is given by

$$V(x) = \begin{cases} 0 & : \quad x < 0 \qquad \text{(region I)} \\ -V_0 & : \quad 0 \le x \le a \quad \text{(region II)} \\ 0 & : \quad x > a \qquad \text{(region III)} \end{cases}$$

where $E > 0$ and $V_0 > 0$.

(a) Show that the particle wave function in the x regions defined above can be written

$$\begin{aligned} \psi_{\mathrm{I}} &= Ae^{iKx} + Be^{-iKx} \\ \psi_{\mathrm{II}} &= Ce^{iqx} + De^{-iqx} \\ \psi_{\mathrm{III}} &= Fe^{iKx} \end{aligned} \tag{1}$$

where you should find expressions for K and q.

(b) State the conditions on the particle wave function ψ and its derivative ψ' which must be satisfied at the boundaries between regions I, II and III and use these to show that

$$\frac{A}{F} = \frac{(K+q)^2 e^{i(K-q)a} - (K-q)^2 e^{i(K+q)a}}{4Kq} .$$

(c) The incident particle current density for the above scattering problem is defined by

$$j_I = \frac{\hbar K}{m} |A|^2 .$$

Give the corresponding expressions for the reflected and transmitted particle current densities j_R and j_T. Hence define the reflection and transmission coefficients R and T.

(d) Use the result of part (b) to evaluate the transmission coefficient T in the case when $qa = n\pi$ (where n is some integer). Without explicitly evaluating it, state what the value of R will be, giving reasons.

[20 marks]

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

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

and ϕ_0 is the normalised ground state wave function such that $a\phi_0 = 0$ where

$$a = \frac{\alpha}{\sqrt{2}}\left(\frac{1}{m\omega}\hat{p} - i\hat{x}\right), \qquad \alpha^2 = \frac{m\omega}{\hbar}.$$

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

(b) Show that one may write the Hamiltonian in the form

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

and hence find the eigenvalue corresponding to the ground-state wave function ϕ_0.

(c) Show that $\phi_1 = Aa^\dagger\phi_0$ is also an eigenfunction of $\hat{H}$ and find the associated eigenvalue. [Here, A is a normalisation constant.]

(d) Given that the properly normalised ground state wave function is

$$\phi_0 = \sqrt{\frac{\alpha}{\sqrt{\pi}}}e^{-\frac{1}{2}\alpha^2x^2},$$

obtain the properly normalised eigenfunction $\phi_1(x)$.

[**13 marks**]

(ii) Establish, giving reasons, which of the following operators could represent quantum mechanical observables:

$$\hat{A} = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{B} = \begin{pmatrix} 0 & i \\ -i & 2 \end{pmatrix}, \quad \hat{C} = x\frac{d}{dx}, \quad \hat{D} = i(x\frac{d}{dx} + \tfrac{1}{2})$$

where the space of wave functions $\psi(x)$ acted upon by $\hat{C}$ and $\hat{D}$ is such that $a \le x \le b$ and $\psi(a) = \psi(b) = 0$.

[**7 marks**]

4. Given that 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), show that
$$[\mathbf{L}^2, L_1] = [\mathbf{L}^2, L_2] = [\mathbf{L}^2, L_3] = 0\,,$$
where $\mathbf{L}^2 = L_1^2 + L_2^2 + L_3^2$.

From the above commutation relations it is possible to deduce the following results (*which you may assume*). There exist normalised eigenfunctions $|l, m\rangle$ such that
$$L_3|l, m\rangle = \hbar m|l, m\rangle, \qquad \mathbf{L}^2|l, m\rangle = \hbar^2 l(l+1)|l, m\rangle,$$
where $2l$ is a positive integer and the possible values of m are $-l, -l+1, \dots l-1, l$. Moreover,
$$L_+|l, m\rangle = M_{l,m}|l, m+1\rangle \quad \text{and} \quad L_-|l, m\rangle = N_{l,m}|l, m-1\rangle,$$
where $L_+ = L_1 + iL_2$ and $L_- = L_1 - iL_2$, and $M_{l,m}$ and $N_{l,m}$ are real, positive constants.

(a) Show that
$$L_-L_+ = \mathbf{L}^2 - L_3^2 - \hbar L_3$$
and, by considering the norm of $L_+|l, m\rangle$, show that
$$M_{l,m} = \hbar\sqrt{l(l+1) - m(m+1)}\,.$$

(b) A particle is in the normalised angular momentum state
$$|\psi\rangle = A(|1, -1\rangle + |1, 1\rangle - 2|1, 0\rangle)$$
where A is a real normalisation constant which you should find. By expressing L_1 in terms of L_+ and L_-, find the expectation values $\langle L_1\rangle$ and $\langle L_1^2\rangle$ for this state. Hence find the standard deviation ΔL_1 for this state. $((\Delta A)^2 \equiv \langle (A - \langle A\rangle)^2\rangle$.)
[*You may assume that*
$$N_{l,m} = \hbar\sqrt{l(l+1) - m(m-1)} \quad \textit{and} \quad L_+L_- = \mathbf{L}^2 - L_3^2 + \hbar L_3\,.]$$

[20 marks]

5. 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 $\hat{O}$ is represented by

$$\hat{O} = \gamma \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$$

where γ is a real constant. Compute the eigenvalues and normalised eigenvectors of $\hat{O}$ and deduce the possible results of a measurement of $\hat{O}$.

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

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

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

What is the effect on the system of such a measurement?

[20 marks]

6. (i) Use integration by parts to show that for $n \geq 2$

$$I_{n-2} = \frac{2\beta^2}{n-1} I_n \,, \qquad \text{where} \quad I_n \equiv \int_0^\infty r^n e^{-\beta^2 r^2}\, dr \,.$$

Given that

$$I_0 = \frac{\sqrt{\pi}}{2\beta} \,,$$

find I_2. Evaluate I_1 and deduce the value of I_3.

[**6 marks**]

(ii) The Hamiltonian for a particle of mass m moving in three dimensions under the influence of a three-dimensional harmonic oscillator potential is

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

where $r = |\mathbf{r}| = \sqrt{x^2 + y^2 + z^2}$ and the radial part of the Laplacian operator is

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

(a) Given that the normalised ground state wave function is

$$\psi_0(\mathbf{r}) = A e^{-\frac{1}{2}\beta^2 r^2}$$

where A is real, determine β and the ground state energy E_0.

(b) Calculate the normalisation constant A.

(c) The potential is perturbed by the addition of a term λH_1 where

$$H_1(r) = r^3 \left(\frac{m\omega}{\hbar}\right)^{\frac{3}{2}} \quad \text{and } \lambda \text{ is small.}$$

Show that, to first order in λ, the perturbed ground state energy can be written in the form

$$\tfrac{3}{2}\hbar\omega + \lambda K$$

where K is a numerical 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 $E_0 \leq E_1 \leq E_2 \ldots$.

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 $\hat{H}$.

A particle of mass m moves on the x-axis subject to a potential $V(x) = \eta |x|$, where η is a positive constant.

(a) Normalise the trial wave function

$$\psi(x) = A e^{-\frac{1}{2}\beta^2 x^2},$$

(i.e. find A) and show that

$$\langle \psi | \hat{H} \psi \rangle = \frac{\hbar^2 \beta^2}{4m} + \frac{\eta}{\sqrt{\pi}\beta}.$$

(b) Hence use the variational method to show that the ground state energy is at most

$$E_0^{\max} = \tfrac{3}{2}\Big(\frac{\hbar^2 \eta^2}{2m\pi}\Big)^{\frac{1}{3}}.$$

How might you improve on this estimate of the ground state energy and how would you know if you had succeeded?

You may use the results:

$$\int_{-\infty}^{\infty} e^{-\beta^2 x^2}\, dx = \frac{\sqrt{\pi}}{\beta}, \qquad \int_{-\infty}^{\infty} x^2 e^{-\beta^2 x^2}\, dx = \frac{\sqrt{\pi}}{2\beta^3}.$$

[20 marks]