2MA65 January 1998

In this paper bold-face quantities like **r** represent three-dimensional vectors.

Full marks can be obtained for complete answers to FIVE questions. Only the best FIVE answers will be counted.

1. A particle of mass m moves on the x-axis in a potential V such that

$$V = 0 \qquad (0 \leq x \leq L)$$
$$V = \infty \qquad (x < 0 \quad \text{and} \quad x > L).$$

Find the normalised eigenfunctions of the Hamiltonian, and show that the energy eigenvalues are E_n where

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

At a certain instant the particle has the following wave function:

$$\psi(x) = A(\sin\frac{\pi x}{L} + \sin\frac{2\pi x}{L}) \qquad (0 \leq x \leq L)$$
$$\psi(x) = 0 \qquad (x < 0 \quad \text{and} \quad x > L)$$

where A is a real, positive normalisation constant.

(i) By writing $\psi(x)$ in terms of the normalised eigenfunctions, compute A.

(ii) Show that

$$\int_0^L x \cos\frac{n\pi x}{L} dx = -\frac{2L^2}{n^2\pi^2} \qquad (n \text{ odd})$$
$$= 0 \qquad (n \text{ even})$$

and hence show that the expectation value $<x>$ of x in the state ψ is given by

$$<x> = \frac{L}{2}\left(1 - \frac{32}{9\pi^2}\right).$$

[The following identity may be useful:

$$2 \sin A \sin B = \cos(A - B) - \cos(A + B).]$$

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

$$V(x) = -V_0 \qquad 0 \leq x \leq L$$
$$V(x) = 0 \qquad x < 0, \quad x > L$$

where V_0 is a positive constant.

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

$$T = \frac{16k^2k_1^2}{|(k+k_1)^2e^{-ik_1L} - (k-k_1)^2e^{ik_1L}|^2},$$

where $k^2 = \frac{2mE}{\hbar^2}$ and $k_1^2 = \frac{2m(E+V_0)}{\hbar^2}$.

(ii) Comment on what happens if $k_1L = n\pi$.

3. The Hamiltonian for a particle of mass m moving on the x-axis in a harmonic oscillator potential is

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

where $[x, p] = i\hbar$ and ω is a positive constant.

(i) If we define

$$a = \frac{1}{\sqrt{2}}\left(\frac{1}{\hbar\alpha} p - i\alpha x\right) \qquad \text{and} \qquad a^\dagger = \frac{1}{\sqrt{2}}\left(\frac{1}{\hbar\alpha} p + i\alpha x\right),$$

where $\alpha = \left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}}$, show that

$$[a, a^\dagger] = 1.$$

(ii) You may assume that H may be rewritten in the form

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

Hence show that, given an energy eigenstate ψ of H such that $H\psi = E\psi$, then

$$H(a^\dagger\psi) = (E + \hbar\omega)a^\dagger\psi, \qquad H(a\psi) = (E - \hbar\omega)a\psi.$$

Assuming that the energy eigenvalues are all greater than or equal to zero, deduce that there must be a state ψ_0 such that $a\psi_0 = 0$, and that the energy eigenvalues of H are of the form $(n + \frac{1}{2})\hbar\omega$, where n is a positive integer or zero.

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

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

where $\psi_0 = Ae^{-\frac{1}{2}\alpha^2 x^2}$, with $A = \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}}$. Using the explicit form for $a^\dagger$ given above, with the representation

$$p = -i\hbar\frac{\partial}{\partial x},$$

show that

$$\psi_1 = i\left(\frac{4m^3\omega^3}{\hbar^3\pi}\right)^{\frac{1}{4}} x e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2},$$

$$\psi_2 = \left(\frac{m\omega}{4\hbar\pi}\right)^{\frac{1}{4}}\left(1 - 2\frac{m\omega}{\hbar}x^2\right) e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2}$$

and check explicitly that ψ_2 is orthogonal to ψ_0.

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

4. The angular momentum operators satisfy the commutation relations

$$[L_1, L_2] = i\hbar L_3 \qquad \text{and cyclic permutations,}$$

which imply

$$[\mathbf{L}^2, L_1] = [\mathbf{L}^2, L_2] = [\mathbf{L}^2, L_3] = 0$$

(where $\mathbf{L}^2 = L_1^2 + L_2^2 + L_3^2$).

From the commutation relations it is possible to deduce the following results (which you may assume): There exist normalised eigenfunctions $|l,m>$ such that

$$L_3|l,m> = \hbar m|l,m>, \qquad \mathbf{L}^2|l,m> = \hbar^2 l(l+1)|l,m>,$$

where $2l$ is a positive integer and the possible values of m are $-l, -l+1, \ldots l-1, l$. Moreover,

$$L_+|l,m> = N_{l,m}|l,m+1>$$

and

$$L_-|l,m> = M_{l,m}|l,m-1>,$$

where $L_+ = L_1 + iL_2$ and $L_- = L_1 - iL_2$, and $N_{l,m}$ and $M_{l,m}$ are real, positive constants.

(i) Show that

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

and

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

(ii) By considering the norms of $L_+|l,m>$ and $L_-|l,m>$, and noting that $(L_+)^\dagger = L_-$, show that

$$N_{l,m} = \hbar\{l(l+1) - m^2 - m\}^{\frac{1}{2}}, \qquad M_{l,m} = \hbar\{l(l+1) - m^2 + m\}^{\frac{1}{2}}.$$

(iii) The angular momentum operator in the direction in the xy plane making an angle θ with the x-axis is given by $L_\theta = L_1 \cos\theta + L_2 \sin\theta$. Show that this may be written in the form $L_\theta = \frac{1}{2}(L_+e^{-i\theta} + L_-e^{i\theta})$.

(iv) A particle is in the normalised state

$$A(|2,1> - |2,0>).$$

Calculate the normalisation constant A, and the expectation value of L_θ in this state.

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 $H = \hbar\omega\sigma_3$, where $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ and $\omega = \frac{eB}{2m}$.

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

$$\psi(t) = \begin{pmatrix} c_1 e^{-i\omega t} \\ \\ c_2 e^{i\omega t} \end{pmatrix},$$

where c_1, c_2 are constants.

(ii) A certain observable is represented by $A = \alpha \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$, where α is a real constant. Compute the eigenvalues and normalised eigenvectors of A. What are the possible results of a measurement of A?

(iii) Suppose that at $t = 0$ the state has the normalised form $\psi(0) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}$. By writing $\psi(t)$ as a linear combination of the eigenvectors of A, find the probabilities of each possible result for a measurement of A at time t. What is the effect on the system of such a measurement?

6. The Hamiltonian for a particle of mass m moving on the x-axis in a harmonic oscillator potential is

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2$$

where ω is a positive constant.

The normalised ground state and first excited state are given by

$$\psi_0 = Ae^{-\frac{1}{2}\alpha^2 x^2} \quad \text{and} \quad \psi_1 = Bxe^{-\frac{1}{2}\alpha^2 x^2},$$

where $\alpha = \left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}}$, and

$$|A|^2 = \frac{\alpha}{\sqrt{\pi}}, \qquad |B|^2 = \frac{2\alpha^3}{\sqrt{\pi}}.$$

Show by explicit calculation that ψ_0 and ψ_1 are both eigenfunctions of the above Hamiltonian, and write down the corresponding energy eigenvalues.

The Hamiltonian is perturbed by the addition of a potential $\lambda V(x)$, where $V(x) = |x|$ and λ is a small parameter. Show that to first order in λ, the energy of the first excited state is now

$$\frac{3}{2}\hbar\omega + 2\lambda\left(\frac{\hbar}{\pi m\omega}\right)^{\frac{1}{2}}.$$

[You may assume, without proof, general results from perturbation theory.]

7. State briefly how the variational method is used to estimate the ground state energy of a quantum mechanical system.

A particle of mass m moves in three dimensions subject to a potential

$$V(\mathbf{r}) = -\frac{\lambda}{r^{\frac{1}{2}}},$$

where λ is a positive constant, and $r = |\mathbf{r}| = (x^2+y^2+z^2)^{\frac{1}{2}}$. Using a trial wave function of the form $\psi(\mathbf{r}) = Ae^{-\beta r}$, $\beta > 0$, where A is chosen so that $\psi(\mathbf{r})$ is normalised, show that

$$<H> = \frac{\hbar^2\beta^2}{2m} - \frac{3\lambda}{4}\left(\frac{\beta\pi}{2}\right)^{\frac{1}{2}}.$$

Hence use the variational principle to show that an approximation to the ground state energy is given by

$$E_0 \approx -\frac{9}{32}\left(\frac{3m\pi^2\lambda^4}{4\hbar^2}\right)^{\frac{1}{3}}.$$

[You may assume that the radial part of the Laplacian in spherical polars is

$$\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}$$

and also that $\int_0^\infty r^n e^{-br}dr = \frac{n!}{b^{n+1}}$ for n a positive integer and $b > 0$ and $\int_0^\infty r^{\frac{3}{2}} e^{-br}dr = \frac{3\sqrt{\pi}}{4b^{\frac{5}{2}}}$ for $b > 0$.]