2MA65 January 1997

In this paper bold-face quantities like ${\bf r}$ 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

$$V=0$$
 $0 \le x \le L$ $V=\infty$ $x < 0$ and $x > L$.

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

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

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

$$\psi(x) = A\left(\sqrt{2}\sin\frac{\pi x}{L} + 2\sqrt{2}\sin\frac{2\pi x}{L} + 2\sqrt{2}\sin\frac{3\pi x}{L}\right) \quad (0 \le x \le L),$$

where A is a real, positive normalisation constant.

- (i) Write an expression for $\psi(x)$ in terms of $\phi_n(x)$, the normalised eigenfunctions of the Hamiltonian. Calculate the normalisation constant A.
- (ii) What are the possible results of a measurement of energy and with what probability would they occur?
 - (iii) Show that the expectation value of the energy is given by

$$< H > = \frac{53}{18} \frac{\hbar^2 \pi^2}{mL^2}.$$

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 step

$$V(x) = V_0 \qquad x \ge 0$$
$$V(x) = 0 \qquad x < 0$$

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

- (i) Write down the current density for a beam of particles with wavefunction $\psi(x) = Ae^{ikx}$. For the potential step above, calculate the reflection and transmission coefficients R and T, defined as the ratios of the reflected and transmitted current densities to the incident current density.
 - (ii) Compute the sum R + T, and comment on the result.
- (iii) Consider the case $V_0 = -V_1$, with V_1 positive. What happens to R and T in the limit $V_1 >> E$? Is this surprising from the classical point of view?

3. 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 the frequency ω is a positive constant.

- (i) Show that the expectation value of H for any normalisable state of non-zero norm is positive or zero.
 - (ii) Given that the normalised ground state wave function is

$$\psi_0 = Ae^{-\frac{1}{2}\alpha^2 x^2},$$

where $A^2 = \frac{\alpha}{\sqrt{\pi}}$, determine the constant α and the ground state energy.

(iii) A particle is in the ground state ψ_0 of a harmonic oscillator potential with frequency ω . What is the expectation value of H in this state? The frequency is suddenly changed to ω' . By writing the new Hamiltonian H' in terms of the original Hamiltonian H, show that the expectation value of H' in the state ψ_0 is given by

$$< H'> = \frac{\hbar(\omega^2 + \omega'^2)}{4\omega}.$$

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

4. The angular momentum operators L_1 , L_2 and L_3 satisfy the commutation relations

$$[L_1, L_2] = i\hbar L_3$$
 and cyclic permutations,

which imply

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

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

Suppose that |l, m> are the normalised eigenstates such that

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

(i) Defining $L_+ = L_1 + iL_2$ and $L_- = L_1 - iL_2$, show that $[L_3, L_+] = \hbar L_+$, $[L_3, L_-] = -\hbar L_-$.

Hence, using also the commutation relations for L^2 above, deduce that

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

and

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

where $N_{l,m}$ and $M_{l,m}$ are constants.

(ii) A particle is in the angular momentum eigenstate |1,1>. By writing L_1 in terms of L_+ and L_- , compute the uncertainty ΔL_1 of L_1 in this state, defined by $(\Delta L_1)^2 = \langle L_1^2 \rangle - (\langle L_1 \rangle)^2$.

[You may assume that in (i), $N_{l,m}$ and $M_{l,m}$ are given by

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

5. The Pauli matrices are given by

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \text{and} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Let $S_{\theta} = \frac{1}{2}\hbar\sigma_{\theta}$, where

$$\sigma_{\theta} = \sigma_1 \cos \theta + \sigma_2 \sin \theta,$$

be the spin operator in the direction in the xy plane making an angle θ with the x-axis.

- (i) Show that $\sigma_{\theta} = \begin{pmatrix} 0 & e^{-i\theta} \\ e^{i\theta} & 0 \end{pmatrix}$. Compute the eigenvalues and the normalised eigenvectors of σ_{θ} . What are the possible results of a measurement of S_{θ} ?
- (ii) The Hamiltonian for a stationary electron of mass m and charge e in a magnetic field B along the z-axis is given by $H=\hbar\omega\sigma_3$, where $\omega=\frac{eB}{2m}$. 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.

(iii) Suppose that at time t=0 the wave-function has the normalised form $\psi(0)=\frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix}$. Show that the expectation value of S_{θ} at time t is given by

$$\langle S_{\theta} \rangle = \frac{1}{2} \hbar \sin(\theta - 2\omega t).$$

- **6.** A particle of mass m moves in three dimensions under the influence of a Coulomb potential $V = -\frac{A}{r}$, where $r = |\mathbf{r}| = (x^2 + y^2 + z^2)^{\frac{1}{2}}$ and A is a positive constant.
 - (i) Given that the normalised ground state wave function is

$$\psi(\mathbf{r}) = Be^{-\frac{r}{a_0}}$$

where B and a_0 are constants, determine a_0 , the ground state energy E_0 , and B in terms of m, A and \hbar .

(ii) The particle is now subjected to an additional potential $\lambda r^2 \sin \theta$, where λ is a small parameter, and $\{r, \theta, \phi\}$ are spherical polar co-ordinates. Calculate the new ground state energy to first order in λ .

[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

$$\int_0^\infty r^n e^{-\beta r} dr = \frac{n!}{\beta^{n+1}} \qquad (\beta > 0).]$$

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 on the x-axis subject to a potential $V(x) = \lambda |x|$, where λ is a positive constant. Using a normalised trial wave function $\psi(x) = Ae^{-\frac{1}{2}\beta^2x^2}$, where $A^2 = \frac{\beta}{\sqrt{\pi}}$, show that

$$< H > = \frac{1}{4} \frac{\hbar^2 \beta^2}{m} + \frac{\lambda}{\sqrt{\pi \beta}}.$$

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

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

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