MATH325 QUANTUM MECHANICS

JANUARY 2000

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 is confined to the region of the x-axis between $x = 0$ and $x = L$.

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

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

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

$$\psi(x) = A\left(6\sqrt{2}\sin\frac{\pi x}{L} + 3\sqrt{2}\sin\frac{2\pi x}{L} + 2\sqrt{2}\sin\frac{3\pi x}{L}\right) \qquad (0 \leq x \leq L),$$

$$\psi(x) = 0 \quad (x < 0, \quad x > L),$$

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) Compute the expectation value of the energy.

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

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

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

(i) Write down the current density for a beam of particles with wave-function $\psi(x) = Ae^{ikx}$. 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 can be written in the form

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

where the frequency ω is a positive constant, and where $[a, a^\dagger] = 1$. The position x and momentum p are given by

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

where $\alpha = \sqrt{\frac{m\omega}{\hbar}}$.

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

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

$$\psi_n = \frac{1}{\sqrt{n!}}(a^\dagger)^n \psi_0, \quad n \geq 0,$$

where $a\psi_0 = 0$. Show that

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

(iii) By writing $x\psi_n$, $p\psi_n$ in terms of ψ_{n-1}, ψ_{n+1}, compute the uncertainties Δx and Δp for the state ψ_n.

[You may find the following identity useful:

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

for operators A, B and C.]

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 $|l, m\rangle$ 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 $-l, -l+1, \ldots l-1, l$. Moreover,

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

and

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

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 by considering the norm of $L_-|l, m\rangle$, and noting that $(L_-)^\dagger = L_+$, show that

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

(ii) The angular momentum operator in the direction in the xz plane making an angle θ with the z-axis is given by $L_\theta = L_3 \cos\theta + L_1 \sin\theta$. By writing L_1 in terms of L_+ and L_-, compute $< L_\theta >$ and $< L_\theta^2 >$ for the state $|1, 1\rangle$.

(iii) By symmetry, the possible results of a measurement of L_θ for the state $|1, 1\rangle$ are clearly $\pm\hbar$ and 0. Use your results for $< L_\theta >$ and $< L_\theta^2 >$ to deduce the probabilities of obtaining each possible result.

[You may assume that $N_{l,m}$ is given by

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

5. The Pauli matrices are given by

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

and the spin operator S_i in the direction of the x_i-axis is given by $S_i = \frac{1}{2}\hbar\sigma_i$.

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 $\omega = \frac{eB}{2m}$.

(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) Compute the eigenvalues and normalised eigenvectors of σ_1. Hence deduce that the possible results of a measurement of S_1 are $\pm\frac{1}{2}\hbar$.

(iii) S_1 is measured at $t = 0$ and again at $t = T$. Let $p(k, l)$ be the probability that the result $\frac{1}{2}l\hbar$ is obtained at $t = T$, given that the result $\frac{1}{2}k\hbar$ was obtained at $t = 0$. Compute $p(1, 1)$ and $p(1, -1)$.

(iv) S_1 is measured at $t = 0$, again at $t = T$ and yet again at $t = 2T$. Given that the result of the measurement at $t = 0$ is $S_1 = \frac{1}{2}\hbar$, show that the probability P that the result $-\frac{1}{2}\hbar$ is obtained at $t = 2T$ is given by

$$P = \tfrac{1}{2}\sin^2(2\omega T).$$

[You may assume that $p(-1, -1) = p(1, 1)$.]

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) The normalised wave function for the first excited state with zero angular momentum is

$$\psi(\mathbf{r}) = Be^{-\frac{1}{2}\beta r}\left(1 - \tfrac{1}{2}\beta r\right),$$

where $B = \sqrt{\frac{\beta^3}{8\pi}}$. Determine β in terms of m, A and $\hbar$, and show that the energy E is given by

$$E = -\frac{mA^2}{8\hbar^2}.$$

(ii) The particle is now subjected to an additional potential λr, where λ is a small parameter. Show that the new energy of this state to first order in λ is given by $E + \delta E$ where

$$\delta E = 6\frac{\lambda\hbar^2}{mA}.$$

[Standard results from perturbation theory may be assumed without proof. Moreover, 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. A particle of mass m moves on the x-axis subject to a potential

$$V(x) = \lambda x^4,$$

where λ is a positive constant.

Consider a normalised wave function of the form

$$\psi(x) = Ae^{-\frac{1}{2}\beta^2 x^2}$$

where A, β are real, and A is positive.

(i) Compute the normalisation constant A.

(ii) Show that with this wave function, the expectation value of the Hamiltonian is given by

$$< H >= \frac{1}{4}\frac{\hbar^2\beta^2}{m} + \frac{3\lambda}{4\beta^4}.$$

(iii) Hence use the variational principle to show that an estimate for the ground state energy is given by

$$E_0 \approx \frac{3}{8}\left(\frac{6\hbar^4\lambda}{m^2}\right)^{\frac{1}{3}}.$$

Is the true ground state energy less than, or greater than, this value?

[You may assume that, if

$$I_n = \int_{-\infty}^{\infty} x^n e^{-\alpha^2 x^2}\, dx,$$

then $I_0 = \frac{\sqrt{\pi}}{\alpha}$, and $I_n = \frac{n-1}{2\alpha^2} I_{n-2}$ for $n > 1$.]