**2MA65 January 1996**

In this paper bold-face quantities like $\mathbf{r}$ represent three-dimensional vectors.

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

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

$$V = 0 \qquad 0 \le x \le a$$
$$V = \infty \qquad x < 0 \quad \text{and} \quad x > a.$$

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

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

At a certain time the particle is in a state described by the normalised wavefunction

$$\psi(x) = A\left(1 - \cos\frac{2\pi x}{a}\right) \qquad 0 \le x \le a$$
$$\psi(x) = 0 \qquad x < 0 \quad \text{and} \quad x > a.$$

(i) Determine the normalisation constant $A$.

(ii) Calculate the probability that a measurement of the energy will give the result $E_1$.

**2.** A particle of mass $m$ and energy $E < 0$ moves on the $x$-axis subject to a potential $V$ given by

$$V = 0 \qquad |x| > a$$
$$V = -V_0 \qquad |x| \le a$$

where $V_0$ is a positive constant. Suppose that $E > -V_0$. Define

$$K^2 = -\frac{2mE}{\hbar^2} \qquad \text{and} \qquad k^2 = \frac{2m(E + V_0)}{\hbar^2}.$$

(i) Write down the energy eigenfunction equation in the regions $|x| \le a$ and $|x| > a$, and hence write down the general form of an *even* solution to this equation in these two regions.

(ii) Show that for such an even solution, $k$ must satisfy

$$(ka)\tan(ka) = \sqrt{\alpha^2 a^2 - k^2 a^2},$$

where

$$\alpha^2 = \frac{2mV_0}{\hbar^2}.$$

(iii) Show graphically that the above condition on $k$ always has at least one solution.

**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

$$p = -i\hbar\frac{d}{dx}$$

and $\omega$ is a positive constant.

(i) Show that 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 $\alpha = \sqrt{\frac{m\omega}{\hbar}}$, then it follows from the basic commutator $[x, p] = i\hbar$ that $[a, a^\dagger] = 1$.

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

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

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

where $a\psi_0 = 0$. Show that

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

(iv) A particle is in the state with normalised wave-function

$$\psi = \frac{1}{\sqrt{2}}(\psi_n + \psi_{n+1}).$$

Compute the expectation value $< p >$ in this state.

[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 $\psi_{l,m}$ such that

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

where $2l$ is an integer and the possible values of $m$ are $-l, -l+1, \ldots l-1, l$. It can be shown that

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

and

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

where $L_+ = L_1 + iL_2$ and $L_- = L_1 - iL_2$, and $N_{l,m}$ and $M_{l,m}$ are 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) 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) A normalised angular momentum state $\psi$ is a linear combination

$$\psi = a\psi_{1,-1} + b\psi_{1,0} + c\psi_{1,1}$$

such that $L_1\psi = \hbar\psi$. By writing $L_1$ in terms of $L_+$ and $L_-$, deduce the values of $a$, $b$ and $c$.

**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

$$\sigma_\theta = \sigma_3 \cos\theta + \sigma_1 \sin\theta,$$

be the spin operator in the direction in the $xz$ plane making an angle $\theta$ with the $z$-axis.

(i) Show that the normalised eigenvectors of $\sigma_\theta$ are

$$\xi_1 = \begin{pmatrix} \cos\frac{1}{2}\theta \\ \\ \sin\frac{1}{2}\theta \end{pmatrix} \quad \text{and} \quad \xi_2 = \begin{pmatrix} \sin\frac{1}{2}\theta \\ \\ -\cos\frac{1}{2}\theta \end{pmatrix},$$

with eigenvalues $+1$ and $-1$ respectively. What are the possible results of a measurement of $S_\theta$?

(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 $\omega = \frac{eB}{2m}$. Write down the eigenvalues and eigenvectors of $H$ and hence 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 $\psi(0) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$. Show that the probability of getting the result $\frac{1}{2}\hbar$ in a measurement of $S_\theta$ at time $t$ is $\frac{1}{2}[1 + \sin\theta\cos\omega t]$.

[If the eigenstates of the Hamiltonian are $\phi_n$ with eigenvalues $E_n$, then the solution of the Schrödinger equation is

$$\psi(t) = \sum a_n e^{-\frac{iE_n t}{\hbar}} \phi_n$$

where $a_n$ are constants.]

**6.** The Hamiltonian for the simple harmonic oscillator is

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

where $\omega$ is a positive constant.

The normalised ground state and first excited state wave functions are given by

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

where $\alpha = \sqrt{\frac{m\omega}{\hbar}}$, and $A$ and $B$ are constants.

(i) If

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

show that $I_n = \frac{n-1}{2\alpha^2} I_{n-2}$. Hence write down $I_2$ and $I_4$, given that $I_0 = \frac{\sqrt{\pi}}{\alpha}$.

(ii) Calculate $A$ and $B$.

(iii) The Hamiltonian is perturbed by the addition of $\lambda V(x)$, where $V(x) = \frac{1}{2}mx^2$ and $\lambda$ is a small parameter. Calculate the energies of the ground state and first excited state to first order in $\lambda$.

(iv) By observing that the perturbed Hamiltonian is also of harmonic oscillator form, write down the exact energies of the ground state and first excited state for the perturbed Hamiltonian. Check that these exact results, when expanded to first order in $\lambda$, agree with the results of (iii).

**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

$$V(\mathbf{r}) = -V_0 \frac{e^{-\lambda r}}{r},$$

where $V_0$ and $\lambda$ are positive constants, and $r = |\mathbf{r}| = (x^2 + y^2 + z^2)^{\frac{1}{2}}$. Using a trial wave function of the form $\psi(\mathbf{r}) = Ae^{-\alpha r}$, $\alpha > 0$, where $A$ is chosen so that $\psi(\mathbf{r})$ is normalised, show that

$$E(\alpha) = \frac{\hbar^2 \alpha^2}{2m} - \frac{4\alpha^3 V_0}{(2\alpha + \lambda)^2}$$

is an upper bound to the ground state energy for all $\alpha > 0$. Given that the ground state energy in this potential is negative, show that the best upper bound is $\min(0, E(\alpha_0))$, where $\alpha_0$, if it exists, is a positive root of the cubic

$$\hbar^2 (2\alpha + \lambda)^3 = 4mV_0 \alpha (2\alpha + 3\lambda).$$

[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

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