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B.Sc. (Honours) Experimental Physics

Paper III: Quantum Mechanics (EP405)


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Time allowed: TWO hours
Answer THREE questions.

Q.1 Show that, for a particle of mass $m$ moving in a field described by the potential energy function $V(\boldsymbol{r})$, we have

$$d\langle \boldsymbol{r}\rangle /dt = \langle \boldsymbol{p}\rangle /m$$

$$d\langle \boldsymbol{p}\rangle /dt = -\langle \nabla V\rangle$$

where all the terms have their usual meanings.

You may recall that $[\boldsymbol{p}^2, \boldsymbol{r}] = -2i\hbar \boldsymbol{p}$.

Consider the case of a particle in a one-dimensional infinite square well potential:

$V = 0$, $0 \le x \le 2a$; $V = \infty$ elsewhere. The normalised stationary state wavefunctions are

$$\Psi_n(x,t) = a^{-1/2} \sin(n\pi x/2a).\exp(-in\omega t), \qquad 0 \le x \le 2a,$$

$$\Psi_n(x,t) = 0 \qquad \text{elsewhere.}$$

where $n$ has integer values 1, 2, 3, ... , and the energy values are $E_n = n^2 \hbar \omega$, where $\omega$ is a constant.

Show that $\Psi(x,t) = 2^{-1/2} (\Psi_1 + \Psi_2)$ is also a normalised wavefunction.

Calculate $\langle x\rangle_n$, the expectation value of $x$ for the $n$th stationary state. Hence derive the values for $\langle p_x \rangle_n$ for these states.

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If the origin of coordinates is shifted to the centre of the well, the stationary state wavefunctions can be expressed in terms of the new $x$ coordinate by replacing $x$ by $(x-a)$ in the $\Psi_n(x,t)$ functions. In this form, the stationary state wavefunctions are found to be either even or odd under inversion. Explain clearly why this is the case.

Q.2 Define the quantum mechanical operators for the linear momentum, $\boldsymbol{p}$, and the orbital angular momentum, $\boldsymbol{l}$, of a particle in terms of the Cartesian co-ordinates of the particle. State the commutation relationships between the Cartesian components of $\boldsymbol{l}$.

Show that $[l_x, p_x] = 0$, $[l_x, p_y] = i\hbar p_z$, $[l_x, p_z] = -i\hbar p_y$, and hence show that $[l, p^2] = 0$.

The Hamiltonian for the simple hydrogen atom (neglecting spin) is

$$H = \frac{p^2}{2m} - \frac{1}{4\pi\varepsilon_0}\frac{e^2}{r}$$

Show that $[l, H] = 0$, from which it follows that $[l^2, H] = 0$, $[l_z, H] = 0$, and $[l_\pm, H] = 0$.

The eigenfunctions of $H$ can be chosen to be eigenfunctions of $l^2$ and of $l_z$. Why cannot they also be chosen to be eigenfunctions of $l_x$? These eigenfunctions can be written symbolically as $|n\, l\, m\rangle$, where the symbols $n$, $l$, $m$ have their usual meanings.

Explain why the energy of the state, i.e., the value of $E_{nlm} = \langle n\, l\, m \mid H \mid n\, l\, m\rangle$, is independent of the value of $m$, as long as $m$ has one of the integer values between $-l$ and $+l$.

Q.3 Write down and briefly discuss the Fermi Golden Rule formula for the probability of a transition from an initial state ($i$) to a final state ($f$) under a perturbation of the form $V.\exp(\pm i\omega t)$, where $V$ is independent of time.

Planck, in his analysis of the interaction of electromagnetic radiation with matter, employed the linear harmonic oscillator as a model of the interacting atom. In our quantum formulation, the linear harmonic oscillator is described by the Hamiltonian

$$H = \frac{p_x^2}{2m} + \tfrac{1}{2}m\omega^2 x^2 .$$

The eigenstates can be written as $|n\rangle$, and $H|n\rangle = (n+\tfrac{1}{2})\hbar\omega\,|n\rangle$.

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It is convenient to define the operators

$$a = \sqrt{\frac{m\omega}{2\hbar}}\,(x + i\frac{p_x}{m\omega}), \qquad a^+ = \sqrt{\frac{m\omega}{2\hbar}}\,(x - i\frac{p_x}{m\omega})$$

which have the property that

$$a|n\rangle = \sqrt{n}\,|n-1\,\rangle, \quad \text{and} \quad a^+|n\rangle = \sqrt{n+1}\,|n+1\,\rangle.$$

Analyse the interaction of a linear harmonic oscillator with electromagnetic radiation of frequency $\omega$, explaining how radiative transitions can be induced between the eigenstates of the linear harmonic oscillator according to the selection rule $\Delta n = \pm 1$, which was assumed by Planck in his analysis.

Discuss the selection rule from the viewpoint of the parity of the eigenstates.

Q.4 Explain what is meant by the matrix representation of an operator.

Show how diagonalising the Hamiltonian matrix is equivalent to solving for the eigenvalues of the Hamiltonian operator.

An electronic spin system in the absence of a magnetic field has energy $E_o$. This state is doubly degenerate; $|\xi\rangle$ and $|\eta\rangle$ are the two orthogonal eigenstates. In the presence of a magnetic field $\boldsymbol{B}$ the Hamiltonian matrix has the form

$$\begin{matrix} E_o & (e\hbar/2m)B \\ (e\hbar/2m)B & E_o \end{matrix}$$

Calculate the eigenstates and eigenvalues in the presence of the magnetic field.

Q.5 Answer *each* of the following.

(a) Explain, briefly and with illustrative examples, how, by allowing the outer electrons in the carbon atom to occupy hybrid orbitals, one can understand the spatial structure of some simple molecules involving carbon atoms.

(b) Show that the eigenfunctions of a Hermitian operator with different eigenvalues are orthogonal to each other.

(c) The operator for an infinitesimal rotation through $d\phi$ about the $z$-axis can be written as

$$\mathrm{P}_{d\phi} = 1 + i\,d\phi\, l_z/\hbar$$

If a system is described by a Hamiltonian operator $H$, which is invariant under such a rotation, show that the $z$-component of orbital angular momentum is conserved for this system.