Second Year Theory Option

QUANTUM MECHANICS

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Problem Set 1

A. Dirac notation

A1. A system has a complete orthonormal set of basis states $\mid 0\rangle, \mid 1\rangle, \mid 2\rangle, \mid 3\rangle, \ldots \equiv \{\mid n\rangle\}$.

(i) Explain why

$$\sum_n \mid n\rangle\langle n \mid = 1.$$

(ii) The linear operator A is represented in this basis by the matrix with elements $A_{mn} = \langle m \mid A \mid n\rangle$; a second linear operator B is represented by the matrix with elements $B_{pq} = \langle p \mid B \mid q\rangle$ (m, n, p, q run over the entire basis set). Show that the matrix representing the product AB is the product, in that order, of the matrices representing A and B.

A2. (i) A is a Hermitian linear operator; what is the relation between $\langle m \mid A \mid n\rangle$ and $\langle n \mid A \mid m\rangle$?

(ii) A is a Hermitian linear operator with a complete set of eigenstates $\mid 0\rangle, \mid 1\rangle, \mid 2\rangle, \ldots$ belonging to the eigenvalues $a_0, a_1, a_2, \ldots$. Prove
(a) that the a_n's are real;
(b) that the states $\mid m\rangle$ and $\mid n\rangle$ are orthogonal if $m \neq n$.

A3. (i) Verify the identities

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

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

$[A, [B, C]] + [C, [A, B]] + [B, [C, A]] = 0$

for arbitrary operators A, B, C. Using $[x, p] = i\hbar$, show that $[x, p^2] = 2i\hbar p$.

(ii) The Hamiltonian H of a system is given by

$$H = \frac{p^2}{2m} + V(x).$$

Show that $[x, [H, x]] = \hbar^2/m$.

By taking the $\langle 0 \mid \ldots\ldots \mid 0\rangle$ matrix element of this equation (where $\mid 0\rangle$ is the ground state with energy E_0) show that

$$\sum_n \mid \langle n \mid x \mid 0\rangle \mid^2 (E_n - E_0) = \hbar^2/2m,$$

where $\mid n\rangle$ is the n^{th} excited state, of energy E_n. [This is called a sum rule for the matrix elements $\langle n \mid x \mid 0\rangle$].

A4. (i) Show, using

$$\langle x \mid p\rangle = \frac{1}{(2\pi\hbar)^{\frac{1}{2}}} e^{ipx/\hbar},$$

that

$$\langle p \mid \hat{x} \mid a\rangle = i\hbar \frac{\partial}{\partial p}\phi_a(p)$$

where

$$\phi_a(p) = \frac{1}{(2\pi\hbar)^{\frac{1}{2}}} \int_{-\infty}^{\infty} e^{-ipx/\hbar}\psi_a(x)dx$$

and $\psi_a(x) = \langle x \mid a\rangle$.

(ii) Write down the Hamiltonian for the one-dimensional harmonic oscillator in the p-representation and *hence*, given that the ground state wave function in the x-representation is

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

obtain the momentum probability distribution of the oscillator ground state.
What other method might you use to find this distribution?

B. Finite state systems

B1. A certain two-state system can be described by two orthonormal base states $\mid 1\rangle$ and $\mid 2\rangle$. The Hamiltonian H is such that

$$H \mid 1\rangle = \alpha \mid 1\rangle + \beta \mid 2\rangle \ , \ H \mid 2\rangle = \beta \mid 1\rangle + \alpha \mid 2\rangle$$

where α and β are real.

(i) What column vectors represent the basis states in the $\mid 1\rangle, \mid 2\rangle$ basis? What matrix represents H in this basis?

(ii) What are the energy eigenvalues? What are the normalized energy eigenstates in terms of $\mid 1\rangle$ and $\mid 2\rangle$? What column vectors represent the energy eigenstates in the $\mid 1\rangle, \mid 2\rangle$ basis?

(iii) If the energy eigenvalues are called E_+ and E_-, and the corresponding energy eigenstates are called $\mid +\rangle$ and $\mid -\rangle$, find the matrix $\mathbf{R}$ that transforms from the $\mid 1\rangle, \mid 2\rangle$ basis to the $\mid +\rangle, \mid -\rangle$ basis. Show that $\mathbf{R}$ is orthogonal, and verify explicitly that if $\mathbf{H}$ is the matrix representing H in the $\mid 1\rangle, \mid 2\rangle$ basis, then $\mathbf{R}^{-1}\mathbf{H}\mathbf{R}$ is a diagonal matrix with diagonal elements E_+ and E_-.

(iv) At time $t = 0$, the system is in the state $\mid 1\rangle$. What is the state vector of the system at a later time t? What is the probability of finding the system in state $\mid 2\rangle$ at time t? If the first time at which the state vecto r of the system is equal to $\mid 1\rangle$ again is $t = 1.2 \times 10^{-9}s$, calculate the difference (in eV) between the two energy eigenvalues.

B2. Show that the most general Hermitian Hamiltonian matrix for a 2-state system can be written in the form

$$\mathbf{H} = \sum_{i=0}^{3} a_i \sigma_i$$

where the a_i are real numbers and

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Calculate the commutator

$$\left[\frac{1}{2}\sigma_1, \frac{1}{2}\sigma_2\right]$$

and the quantity $\frac{1}{4}(\sigma_1^2 + \sigma_2^2 + \sigma_3^2)$. What do these results suggest physically?

B3. The Hamiltonian for a two-state system using normalised basis states $\mid 1\rangle$ and $\mid 2\rangle$ is

$$\begin{pmatrix} \langle 1 \mid H \mid 1\rangle & \langle 1 \mid H \mid 2\rangle \\ \langle 2 \mid H \mid 1\rangle & \langle 2 \mid H \mid 2\rangle \end{pmatrix} = \begin{pmatrix} 3a\cos 2\theta & a\sin 2\theta \\ a\sin 2\theta & a\cos 2\theta \end{pmatrix}$$

where a and θ are real and positive. Find the eigenvalues E_+ and E_-, and express the corresponding normalised eigenstates $\mid +\rangle$ and $\mid -\rangle$ of the Hamiltonian in terms of $\mid 1\rangle$ and $\mid 2\rangle$.

At time $t = 0$ the system is in state $\mid 1\rangle$. Show that the probability that it will be found to be in state $\mid 2\rangle$ at a later time t is $\sin^2 2\theta \ \sin^2(at/\hbar)$.

B4. The Hamiltonian of a system is expressed in terms of a basis set of three (orthogonal) wavefunctions ϕ_1, ϕ_2, ϕ_3 as follows:

$$\mathbf{H} = \begin{pmatrix} \epsilon_0 & -\lambda & -\lambda \\ -\lambda & \epsilon_0 & -\lambda \\ -\lambda & -\lambda & \epsilon_0 \end{pmatrix}.$$

Find the eigenvalues and eigenfunctions. At $t = 0$ the system is known to be in state ϕ_1; show that the state vector at a later time t may be written as

$$\psi(t) = e^{-i\mathbf{H}t/\hbar} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \frac{1}{3} e^{-i(\epsilon_0 - 2\lambda)t/\hbar} \begin{pmatrix} 1 + 2e^{-i\gamma} \\ 1 - e^{-i\gamma} \\ 1 - e^{-i\gamma} \end{pmatrix}$$

where $\gamma = 3t\lambda/\hbar$.

Find the probabilities $p_i(t), i = 1, 2, 3$, that the system will be found in the ith state at a later time.

[A state vector $\begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix}$ means that the wave function is $\Phi = \alpha_1\phi_1 + \alpha_2\phi_2 + \alpha_3\phi_3$.]