Imperial College London
BSc/MSci EXAMINATION June 2012

This paper is also taken for the relevant Examination for the Associateship

FOUNDATIONS OF QUANTUM MECHANICS

For 3rd/4th Year Physics MSci Students and QFFF MSc Students

Thursday, 31st May 2012: 10:00 to 12:00

Answer THREE questions. All questions carry equal marks.
Marks shown on this paper are indicative of those the Examiners anticipate assigning.

General Instructions

Write your CANDIDATE NUMBER clearly on each of the 3 answer books provided.

If an electronic calculator is used, write its serial number in the box at the top right hand corner of the front cover of each answer book.

USE ONE ANSWER BOOK FOR EACH QUESTION.

Enter the number of each question attempted in the horizontal box on the front cover of its corresponding answer book.

Hand in 3 answer books even if they have not all been used.

You are reminded that Examiners attach great importance to legibility, accuracy and clarity of expression.

1. A point particle moving in one dimension along the real line is described by hermitian position operator $\hat{x}$ and hermitian momentum operator $\hat{p}$ obeying the canonical commutation relation $[\hat{x},\hat{p}] = i\hbar$.

(i) Write down the eigenvalue equations for $\hat{x}$ and $\hat{p}$. Write down the orthogonality relations and the completeness relations in each case. [2 marks]

(ii) Expand the arbitrary state $|\psi\rangle$ in terms of position eigenstates $|x\rangle$ and deduce an expression for the wave function $\psi(x)$ in terms of $|\psi\rangle$. [1 mark]

(iii) Show that the canonical commutation relation may be satisfied if the matrix elements of the momentum operator in the position representation are given by

$$\langle x|\hat{p}|y\rangle = -i\hbar\delta'(x-y)$$

where $\delta'(x)$ denotes the derivative of the delta-function. Hence show that

$$\langle x|\hat{p}|\psi\rangle = -i\hbar\frac{\partial\psi(x)}{\partial x}$$

[5 marks]

(iv) Use the eigenvalue equation for $\hat{p}$ together with the results of part (iii) to show that

$$\langle x|p\rangle = N\exp\left(\frac{i}{\hbar}xp\right)$$

where N is a constant. Assuming that N is real, use a completeness relation (in either $|x\rangle$ or $|p\rangle$) to determine its value. [4 marks]

(v) Under a constant shift a (where a is real), the position eigenstates change according to

$$|x+a\rangle = U(a)|x\rangle$$

where $U(a)$ is an operator. Using the completeness relation for the momentum eigenstates, show that

$$U(a) = \exp\left(-\frac{i}{\hbar}a\hat{p}\right)$$

Briefly outline how $U(a)$ is defined in terms of a power series and show that $U(a)$ is unitary. [4 marks]

(vi) Consider the unitary transformation on $\hat{x}$ given by

$$\hat{x}_\lambda = \exp\left(\frac{i}{\hbar}\lambda\hat{D}\right)\,\hat{x}\,\exp\left(-\frac{i}{\hbar}\lambda\hat{D}\right)$$

where the operator $\hat{D}$ is given by $\hat{D} = \frac{1}{2}(\hat{x}\hat{p}+\hat{p}\hat{x})$. By differentiating with respect to λ and solving the resulting differential equation, obtain an expression of $\hat{x}_\lambda$ in the form

$$\hat{x}_\lambda = f(\lambda)\hat{x} + g(\lambda)\hat{p}$$

where $f(\lambda)$ and $g(\lambda)$ are functions to be determined.

[4 marks]

[Total 20 marks]

2. The Hamiltonian for a quantum particle particle of mass m undergoing simple harmonic motion of frequency ω is

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 .$$

where $\hat{x}$ and $\hat{p}$ are the usual hermitian position and momentum operators. The operators a and $a^\dagger$ are given by

$$a = \frac{1}{\sqrt{2m\omega\hbar}}(m\omega\hat{x} + i\hat{p}) , \quad a^\dagger = \frac{1}{\sqrt{2m\omega\hbar}}(m\omega\hat{x} - i\hat{p}) . \tag{1}$$

In terms of these operators the Hamiltonian is

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

You are given that the number operator $a^\dagger a$ has orthonormal eigenstates $|n\rangle$ and eigenvalues n, where $n = 0, 1, 2, \cdots$ and therefore the eigenvalues of H are $E_n = \hbar\omega(n + 1/2)$.

(i) Use the canonical commutation relations $[\hat{x}, \hat{p}] = i\hbar$ to commute $[a, a^\dagger]$. [1 mark]

(ii) You are given that the operators a and $a^\dagger$ lower and raise the energy eigenstates, that is,

$$a|n\rangle = B_n|n-1\rangle, \quad a^\dagger|n\rangle = C_n|n+1\rangle$$

Use part (i) to deduce the values of the real constants B_n and C_n. [3 marks]

(iii) Express $\hat{x}$ and $\hat{p}$ in terms of a and $a^\dagger$. Show that

$$\langle n|\hat{x}|n\rangle = 0 = \langle n|\hat{p}|n\rangle$$

[3 marks]

(iv) Compute the average of $\hat{x}^2$ and $\hat{p}^2$ in the state $|n\rangle$. Hence show that

$$\Delta x \Delta p = \hbar\left(n + \frac{1}{2}\right)$$

in the state $|n\rangle$. [5 marks]

(v) The Hamiltonian for a pair of non-interacting harmonic oscillators with the same mass and frequency is

$$H_2 = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) + \hbar\omega\left(b^\dagger b + \frac{1}{2}\right)$$

where b and $b^\dagger$ are the lowering and raising oscillators for the second oscillator and they both commute with a and $a^\dagger$. Write down the eigenstates of H_2, in terms of the eigenstates $|n\rangle$, $|m\rangle$ of the first and second oscillator. Write down the eigenvalues E_{nm} of H_2. [2 marks]

(vi) Show that the operator

$$A = i(ab^\dagger - a^\dagger b)$$

commutes with H_2.

[2 marks]

(vii) Let $\hat{y}$ and $\hat{p}_y$ denote the position and momentum of the second oscillator, defined in terms of b and $b^\dagger$ analogously to Eq.(1). Derive an alternative expression for A in terms of the positions $\hat{x}, \hat{y}$ and momenta $\hat{p}, \hat{p}_y$. Without doing any calculation, write down the Hamiltonian H_2 in terms of the positions and momenta. Hence explain why on general mathematical grounds A must commute with H_2.

[4 marks]

[Total 20 marks]

3. (i) An operator A has eigenvalues λ_n and eigenvectors $|a_{ni}\rangle$, where $i = 1, 2, \cdots d_n$ is the degeneracy label for fixed n and $d_n > 1$ is the degeneracy. Suppose that there exists another operator B which commutes with A. Show that A and B have common eigenstates.

[5 marks]

(ii) Rigid rotations of position and momentum operators through angle θ about an axis $\mathbf{n}$ are described by the unitary operator

$$R(\mathbf{n}, \theta) = \exp\left(-\frac{i}{\hbar}\theta\mathbf{n}\cdot\mathbf{L}\right)$$

where $\mathbf{L} = \hat{\mathbf{x}} \times \hat{\mathbf{p}}$ is the angular momentum operator.

(a) Write down the action of R on $\hat{\mathbf{x}}$ and $\hat{\mathbf{p}}$. Show that, infinitesimally, the action of R on $\hat{\mathbf{x}}$ produces the change

$$\hat{\mathbf{x}} \to \hat{\mathbf{x}} - \theta\mathbf{n} \times \hat{\mathbf{x}}$$

[3 marks]

(b) Given only the tensor properties of the object $\mathbf{L}^2$, state how it transforms under rigid rotations. Use the result together with the above properties of the rotation operator to show that

$$[\mathbf{L}^2, L_i] = 0$$

[3 marks]

(iii) You are now given that the angular momentum operators, which we now denote J_i, satisfy

$$\left[\mathbf{J}^2, J_i\right] = 0\,,$$

and also that

$$[J_z, J_\pm] = \pm\hbar J_\pm$$

where $J_\pm = J_x \pm iJ_y$. Choosing $\mathbf{J}^2$ and J_z as a complete set of commuting observables, let the normalised simultaneous eigenvectors be $|\lambda\, m\rangle$ where

$$\mathbf{J}^2|\lambda\, m\rangle = \hbar^2\lambda|\lambda\, m\rangle\,,$$
$$J_z|\lambda\, m\rangle = \hbar m|\lambda\, m\rangle\,.$$

(a) Show that $J_\pm|\lambda\, m\rangle$ is an eigenvector of $\mathbf{J}^2$ with eigenvalue $\hbar^2\lambda$ and an eigenvector of J_z with eigenvalue $(m \pm 1)\hbar$. [3 marks]

(b) Now set

$$J_\pm|\lambda, m\rangle = N_m^\pm|\lambda, m \pm 1\rangle$$

and derive expressions for the real constants $N_m^\pm$. You may use without proof the formulas

$$J_\mp J_\pm = \mathbf{J}^2 - (J_z^2 \pm \hbar J_z).$$

Show also that m is bounded from above and below. [3 marks]

(c) Using the results of (a) and (b), prove that the possible values of λ are $\lambda = j(j+1)$ where j is any non-negative half-integer: $j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$. What are the possible values of m for each j? [3 marks]

[Total 20 marks]

4. The state of a pair of spin 1/2 particles, denoted A and B, lives in the Hilbert space $\mathscr{H}_A \otimes \mathscr{H}_B$. The EPRB state for such a pair is

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle \otimes |\downarrow\rangle - |\downarrow\rangle \otimes |\uparrow\rangle\right)$$

where $|\uparrow\rangle$ and $|\downarrow\rangle$ are eigenstates of the Pauli matrix σ_z with eigenvalues $+1$ and -1 respectively.

(i) Compute the action of $\sigma_z \otimes \mathbf{1} + \mathbf{1} \otimes \sigma_z$ on the EPRB state $|\psi\rangle$. Deduce from this result the action of $\sigma_z \otimes \sigma_z$ on $|\psi\rangle$. You may quote without proof any properties of σ_z you require. [2 marks]

(ii) The rotation operator for a single spin $1/2$ system for rotation through angle θ about axis defined by normal vector $\mathbf{n}$ is given by

$$R(\mathbf{n},\theta) = \exp\left(-\frac{i}{2}\theta\mathbf{n}\cdot\sigma\right)$$

where σ_i denotes the three Pauli matrices. Write down the rotation operator R^{AB} acting on the Hilbert space $\mathscr{H}_A \otimes \mathscr{H}_B$. State the result of acting on the EPRB state $|\psi\rangle$ with R^{AB}. Briefly explain the reason for your answer. [2 marks]

(iii) You are now given that the rotation operator on a single spin 1/2 system has the property

$$R(\mathbf{n},\theta)\mathbf{a}\cdot\sigma R^{\dagger}(\mathbf{n},\theta) = \mathbf{a}(\theta)\cdot\sigma$$

where $\mathbf{a}(\theta)$ is a rotation of the vector $\mathbf{a}$ (whose explicit form is not needed). The correlation function for spin measurements in direction $\mathbf{a}$ on particle A and direction $\mathbf{b}$ on particle B is defined by

$$C(\mathbf{a},\mathbf{b}) = \langle\psi|\mathbf{a}\cdot\sigma\otimes\mathbf{b}\cdot\sigma|\psi\rangle$$

where $|\psi\rangle$ is the EPRB state. Use the result of part (ii) to show that

$$C(\mathbf{a},\mathbf{b}) = C(\mathbf{a}(-\theta),\mathbf{b}(-\theta))$$

Give a simple argument to show that

$$C(\mathbf{a},\mathbf{b}) = K\mathbf{a}\cdot\mathbf{b} \tag{2}$$

where K is a constant. Use part (i) to determine the value of K. [5 marks]

(iv) Now suppose that the results of spin measurements on the EPRB state may be described by a hidden variables theory. The spin of A in directions $\mathbf{a}$, $\mathbf{a}'$ takes values $a, a' = \pm 1$, and the spin of B in directions $\mathbf{b}$, $\mathbf{b}'$ takes values $b, b' = \pm 1$, and their exists an underlying probability distribution $p(a,a',b,b')$ for all four variables. Consider the quantity Q defined by

$$Q = \sum_{aa'bb'}(ab + ab' + a'b - a'b')p(a,a',b,b')$$

By considering all possible values of the quantity $ab + ab' + a'b - a'b'$, show that

$$|Q| \leq 2 \tag{3}$$

[5 marks]

(v) Briefly explain why, in the hidden variables theory of part (iv), it is reasonable to take the quantum-mechanical correlation function to be equal to

$$C(\mathbf{a},\mathbf{b}) = \sum_{aa'bb'} ab\,p(a,a',b,b')$$

Hence deduce the form of the inequality Eq.(3) when the correlation functions are given by Eq.(2). [3 marks]

(vi) Suppose now that all four vectors $\mathbf{a},\mathbf{a}',\mathbf{b},\mathbf{b}'$ are coplanar. Find a set of choices of these vectors for which the inequality is violated by a factor of $\sqrt{2}$.

[3 marks]

[Total 20 marks]

5. (i) State the three properties an operator ρ must satisfy in order to be a density operator. Deduce from these properties the conditions under which the operator

$$\rho = \sum_n p_n |\psi_n\rangle\langle\psi_n|$$

is a density operator, where the set of states $\{|\psi_n\rangle\}$ are orthonormal.

[3 marks]

(ii) Explain in terms of a density operator ρ the meaning of the terms *pure state* and *mixed state*. Explain how $\mathrm{Tr}(\rho^2)$ may be used to discriminate between pure and mixed states. [3 marks]

(iii) A composite system consisting of components A, B has Hilbert space $\mathscr{H}_A \otimes \mathscr{H}_B$ and its state is

$$|\psi\rangle = \sum_n \alpha_n |a_n\rangle \otimes |b_n\rangle$$

where $\{|a_n\rangle\}$ and $\{|b_n\rangle\}$ are orthonormal sets of states. Compute ρ_A, the reduced density operator of system A obtained by tracing over B. Compute ρ_B, defined similarly. Hence show that

$$\mathrm{Tr}(\rho_A^2) = \mathrm{Tr}(\rho_B^2)$$

[4 marks]

(iv) Write down the spectral expansion formula for a non-degenerate hermitian operator A. Given a function $f(x)$ which may be expanded in a power series, briefly explain how to compute $f(A)$. [3 marks]

(v) The entropy of a density operator is defined by the function

$$S(\rho) = -\mathrm{Tr}(\rho \ln \rho)$$

Use the form of ρ in part (i) and the results of part (iv) to write down an expression for $S(\rho)$ entirely in terms of p_n. Explain how the resulting expression for S may be used to distinguish between pure and mixed states. [4 marks]

(vi) Show that the reduced density operators defined in part (iii) satisfy $S(\rho_A) = S(\rho_B)$. [1 mark]

(vii) A thermal state is defined to be a density operator of the form

$$\rho = \frac{1}{Z} \sum_n e^{-\beta E_n} |\psi_n\rangle\langle\psi_n|$$

where $H|\psi_n\rangle = E_n|\psi_n\rangle$, for some non-degenerate hermitian Hamiltonian H, and $Z = \sum_n e^{-\beta E_n}$ where β is a constant (the inverse temperature) and $E_n \geq 0$. Show that ρ may be written in such a way that it is a function only of the operator βH and is basis independent. [2 marks]

[Total 20 marks]