Queen Mary
University of London

BSc EXAMINATION

PHY-413 Quantum Mechanics B

Time Allowed: 2 hours 15 minutes

Date: 4th May 2007

Time: 10:00-12:15

Answer ALL questions in section A. Answer ONLY TWO questions from section B. Section A carries 40 marks, each question in section B carries 30 marks. An indicative marking-scheme is shown in square brackets [ ] after each part of a question.

COMPLETE ALL ROUGH WORKINGS IN THE ANSWER BOOK AND CROSS THROUGH ANY WORK WHICH IS NOT TO BE ASSESSED. NUMERIC CALCULATORS ARE PERMITTED IN THIS EXAMINATION.

The following may be used without proof .

The adjoint $\hat{O}^\dagger$ of an operator $\hat{O}$ is defined by

$$\int_{-\infty}^{\infty} \psi_1^*(x)\hat{O}\psi_2(x)\,dx = \int_{-\infty}^{\infty} (\hat{O}^\dagger\psi_1(x))^*\psi_2(x)\,dx,$$

for any wave functions ψ_1, ψ_2.

YOU ARE NOT PERMITTED TO START READING THIS QUESTION PAPER UNTIL INSTRUCTED TO DO SO BY AN INVIGILATOR

Please turn over

Section A: All these questions must be answered by all candidates.

A1. Write down the Time Dependent Schrodinger Equation (TDSE) for a particle of mass m in a potential $V(x,t)$. [2]

A2. Complete this sentence: 'The Born interpretation is that $|\Psi(x,t)|^2 dx$ is ...' [2]

A3. A single-particle wave function is given as

$$\begin{aligned}\Psi_1(x,0) &= A\cos(\frac{\pi}{L}x) \text{ for } -L/2 \le x \le L/2 \\ &= 0 \text{ elsewhere}\end{aligned}$$

Determine the constant A. (You may assume $\cos^2\theta = (1+\cos 2\theta)/2$) [4]

A4. Write down a general expression for the expectation value of a quantum mechanical operator $\hat{O}$ for a particle in the quantum state $\Psi(x,t)$. [2]

A5. Write down a general expression (i.e. definition) for the uncertainty ΔO in terms of expectation values. [2]

A6. State Heisenberg's position-momentum uncertainty relation in mathematical form (ie. no words required). [2]

A7. In quantum mechanics, when using wave functions $\Psi(x,t)$, the momentum can be represented by an operator $\hat{p}$. Write down an expression for this opearator and calculate its commutator with the position operator. [4]

A8. Write down the Time Independent Schrodinger Equation (TISE). State under what conditions for the potential $V(x,t)$ the TISE may be derived from the TDSE. [2]

A9. If $\psi_n(x)$ are the eigenstates of the Hamiltonian corresponding to the eigenvalue E_n, write down this statement as an equation. [2]

A10. For a potential satisfying the conditions required in A8. the following are all possible wave functions. For each, determine whether it is a stationary state or not:

$$\begin{aligned}(i) \quad \Psi_n(x,t) &= \psi_n(x)e^{-iE_nt/\hbar} \\ (ii) \quad \Psi(x,t)_+ &= \sqrt{\frac{2}{5}}\psi_1(x)e^{-iE_1t/\hbar} + \sqrt{\frac{3}{5}}\psi_2(x)e^{-iE_2t/\hbar} \\ (iii) \quad \Psi(x,0)_- &= \frac{1}{\sqrt{2}}[\psi_1(x) - \psi_2(x)]\end{aligned}$$

[3]

A11. An ensemble measurement is made (at time t) of the energy for a system in the state

$$\Psi(x,t)_+ = \sqrt{\frac{2}{5}}\psi_1(x)e^{-iE_1t/\hbar} + \sqrt{\frac{3}{5}}\psi_2(x)e^{-iE_2t/\hbar}$$

($\psi_n(x)$ are normalised eigenstates). What are the possible outcomes of an individual energy measurement and what are their respective probabilities? [2]

A.12 What is meant by the expansion postulate and the measurement postulate (for the measurement of energy)? [4]

A.13 Sketch the wave functions $\psi(x)$ and the probability densities $|\psi(x)|^2$ for the *first excited state of both* the infinite square well and the finite square well potentials. [4]

A.14 Given the expressions for the x, y and z components of the angular momentum operators:- $\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y$, $\hat{L}_y = -\hat{x}\hat{p}_z + \hat{z}\hat{p}_x$, $\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$, prove the commutation relation $[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z$ [5]

Section B: Answer TWO questions from this section.

B1.

(i) By considering the quantity,

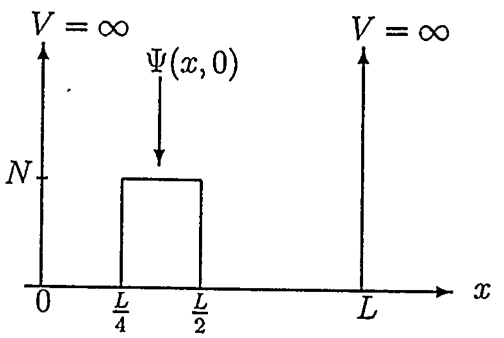
$$\int_{-\infty}^{+\infty} \psi_i^* \widehat{H} \psi_j \, dx,$$

and assuming that the Hamiltonian is hermitian, prove that its eigenvalues are real and that its eigenfunctions, $\psi_n(x)$, corresponding to different eigenvalues, are orthogonal. You may assume that the states are non-degenerate. [8]

(ii) Given the energy eigenstates, $\psi_n(x)$, and eigenvalues, E_n, for a quantum mechanical system, write down an expression for the most general wave function $\Psi(x,t)$ for this system. Derive a formula for the expansion coefficients, justifying clearly all the steps in your derivation. [8]

(iii) Hence explain how a knowledge of the wave function at $t = 0$ determines the wave function for all subsequent times, provided the system is not disturbed. [4]

(iv) At $t = 0$ a particle in an infinite square well is prepared in a state corresponding to the normalised top-hat wave function, $\Psi(x, 0)$, illustrated:



For this infinite square well potential the energy eigenstates are, for $n = 1, 2, \ldots$,

$$\psi_n(x) = \sqrt{\tfrac{2}{L}} \sin(\tfrac{n\pi}{L}x) \quad \text{for} \quad 0 \le x \le L$$
$$= 0 \quad \text{elsewhere}$$

Calculate the constant N (see figure). [2]

Obtain an expression for the probability that the result of an energy measurement is E_n, showing that it depends on $1/n^2$. [8]

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B2.

In answering this question you may use any commutators derived in Section A without repeating your proof.

(i) For a particle of mass m moving in one dimension in a potential, $V(x,t)$, use Heisenberg's equation of motion,

$$\frac{d\langle\hat{O}\rangle}{dt} = \frac{i}{\hbar}\langle[\hat{H},\hat{O}]\rangle + \langle\frac{\partial\hat{O}}{\partial t}\rangle$$

to show that [6]

$$\langle\hat{p}_x\rangle = m\frac{d\langle x\rangle}{dt}$$

(ii) Use Heisenberg's equation to derive Ehrenfest's theorem for the quantity [6]

$$\frac{d\langle\hat{p}_x\rangle}{dt}$$

Hence show that in quantum mechanics the *average* momentum is conserved for a *free* particle. [4]

(iii) An electron moves in an oscillating electric field of strength $E_0\cos\omega t$ with potential:

$$V(x,t) = -eE_0 x\cos\omega t$$

Use Heisenberg's equation of motion, to obtain the equations of motion for $\langle\hat{p}\rangle_t$ and $\langle\hat{x}\rangle_t$. Solve for $\langle\hat{p}\rangle_t$ and $\langle\hat{x}\rangle_t$ subject to the initial conditions that $\langle\hat{p}\rangle_0 = 0$ and $\langle\hat{x}\rangle_0 = 0$. [14]

B3.

(i) A two-particle system has reduced mass μ; with the vector $\mathbf{r}$ joining the two particles and with a potential $V = 0$ the Hamiltonian takes the form,

$$\hat{H} = -\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) + \frac{\hat{L}^2}{2\mu r^2}$$

Use this result to obtain the time independent Schrödinger equation for the *rigid* rotator with equilibrium atomic separation a and moment of inertia I. Hence, using the known eigenvalues of the orbital angular momentum operators, obtain its energy eigenvalues.

[12]

(ii) Describe briefly, and in outline only, the physical basis of a simple quantum mechanical model for the vibrations and rotations of a diatomic molecule. Use the results obtained in (i) and (ii) to obtain expressions for the frequencies of the infrared rotation-vibration *absorption* spectrum of the diatomic molecule, explaining why it breaks up into distinct branches.
In your discussion you should explicitly state the selection rules for the emission and absorption of a photon, explaining clearly the role they play in the argument. Illustrate your discussion with a diagram of the relevant energy levels of the molecule, indicating by arrows the quantum number changes involved for 3 of the lowest transitions of *each* branch of the *absorption* spectrum. Sketch the spectrum and indicate the P(1) and R(0) lines. [18]

B4.

(i) What is the condition for two operators to have a common eigenstate? Explain briefly why, for a spherically symmetric potential, eigenstates of energy are also eigenstates of some, but not all, of the orbital angular momentum operators $\hat{L}_x$, $\hat{L}_y$, $\hat{L}_z$, $\hat{L}^2$; state which and list their allowed eigenvalues. [7]

(ii) An ensemble of isolated quantum rotators is prepared, each one in a state with orbital angular momentum $\hbar\sqrt{56}$. If β is defined as the angle between the angular momentum vector and the positive z−axis, what is the minimum allowed value of β? [6]

(iii) The raising and lowering angular momentum operators are defined as:

$$\hat{L}_\pm \equiv \hat{L}_x \pm i\hat{L}_y$$

Show by using only the commutation relations of the $\hat{L}_i, i = x, y, z$ that [6]

$$[\hat{L}_z, \hat{L}_\pm] = \pm\hbar\hat{L}_\pm$$

(iv) Hence show that $\hat{L}_\pm Y_{\ell,m}(\theta,\varphi)$ are both eigenstates of $\hat{L}_z$ with eigenvalues $\hbar(m \pm 1)$. [5]

(v) Use appropriate properties of the spherical harmonics to show that the raising and lowering operators $\hat{L}_\pm \equiv \hat{L}_x \pm i\hat{L}_y$ have zero expectation values for a system in the angular momentum eigenstate $Y_{\ell,m}(\theta,\varphi)$. Hence find the expectation values for the operators $\hat{L}_x$ and $\hat{L}_y$. [6]

End of Examination Paper

Prof. S. Thomas