## ONE HOUR THIRTY MINUTES

A list of constants is enclosed.

## UNIVERSITY OF MANCHESTER

Introduction to Quantum Mechanics

26 January 2018, 09:45 - 11:15

Answer ALL parts of question 1 and TWO other questions

Electronic calculators may be used, provided that they cannot store text.

The numbers are given as a guide to the relative weights of the different parts of each question.

1 of 5 P.T.O

1. a) A particle of mass m is moving in three dimensions in a potential  $\hat{V}(x, y, z)$ . Write down the time-independent Schrödinger equation for the particle in Cartesian coordinates and explain any notation you have used.

[4 marks]

b) The normalized wavefunction of a particle moving in one dimension is  $\Psi$ . Write down the definition of the expectation value of a physical operator  $\hat{A}$  associated with a measurement of the particle. Briefly explain the physical meaning of this value.

[4 marks]

c) Calculate the kinetic energy in eV of a nonrelativistic electron which has a de Broglie wavelength of  $8.67 \times 10^{-10}$  m.

[3 marks]

d) Write down the definition of the commutator  $[\hat{A}, \hat{B}]$ . Briefly describe the physical meanings of (i)  $[\hat{A}, \hat{B}] = 0$  and (ii)  $[\hat{A}, \hat{B}] \neq 0$ . Give an example from quantum mechanics for each case without demonstration.

[5 marks]

- e) The wavefunction of a particle moving in the xy plane has the form  $\psi(x,y)=xf(r)$ , where  $r=\sqrt{x^2+y^2}$ .
  - i) Write down in polar coordinates the definition of the operator for the z-component of angular momentum,  $\hat{L}_z$ . Show that  $\psi(x,y)$  is not an eigenfunction of  $\hat{L}_z$ .
  - ii) What are the possible values of a measurement of  $L_z$  of the particle?

[5 marks]

f) A magnetic rotor has a moment of inertia I and is placed in a uniform magnetic field along the z direction of strength B. The Hamiltonian of the rotor is given by

$$\hat{H} = \frac{\hat{L}^2}{2I} + \alpha B \hat{L}_z,$$

where  $\alpha$  is a constant, and  $\hat{L}^2$  and  $\hat{L}_z$  are angular momentum operators in the usual notation. Write down the energy levels of the magnetic rotor.

[4 marks]

- 2. An electron is confined by a one-dimensional infinite square well potential to a region 0 < x < L. Inside the well the potential is zero.
  - a) Write down the Hamiltonian  $\hat{H}$  of the electron. Show that the wavefunctions,

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}, & 0 < x < L \\ 0, & \text{elsewhere} \end{cases},$$

where  $n=1,2,3,\cdots$ , are normalized and are eigenfunctions of  $\hat{H}$ . Determine the corresponding eigenvalues  $E_n$ .

[6 marks]

b) Calculate the ground-state energy in eV of the electron when L=1 Å and determine the wavelength in Å of the photon emitted by the electron when it makes a transition from the first excited state to the ground state.

4 marks

c) At time t = 0, the electron is in the state with the normalized wavefunction

$$\psi(x)=rac{1}{\sqrt{2}}\left[\psi_1(x)+\psi_2(x)
ight].$$

i) Write down the electron's wavefunction  $\Psi(x,t)$  at time t>0.

[2 marks]

ii) Determine the energy uncertainty  $\Delta E$  in the state  $\Psi(x,t)$ .

[4 marks]

iii) Show that the probability density  $|\Psi(x,t)|^2$  is an oscillatory function in time and find the period  $\tau$ . Show that the following uncertainty relation holds

$$\tau \Delta E > \frac{\hbar}{2}.$$

Calculate the maximum probability of finding the electron in the region 0 < x < L/2. You may find the following identity useful:

$$2\sin A\sin B = \cos(A - B) - \cos(A + B).$$

[6 marks]

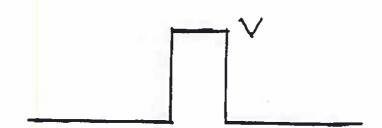
iv) In one measurement, the electron's energy is found to be  $E_1$ . What are the possible values of a subsequent measurement of the electron's momentum?

[3 marks]

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3. a) A particle of kinetic energy E is moving in one dimension towards a rectangular potential barrier of height V (> E). The barrier is illustrated in the following figure. Sketch a possible energy eigenfunction of the particle.

[4 marks]



b) Consider a one-dimensional quantum simple harmonic oscillator (SHO) of angular frequency  $\omega$ . Sketch its ground-state and first excited-state wavefunctions. Write down the full set of its energy eigenvalues. Calculate the value of the zero-point energy in eV of the oscillator if  $\omega = 2.5 \times 10^{14} \text{ rad s}^{-1}$ .

[8 marks]

c) Consider a three-dimensional quantum SHO of angular frequency  $\omega$ . Write down the full set of its energy eigenvalues. Find the first three energy levels and their corresponding degeneracy.

[7 marks]

d) Consider a one-dimensional quantum harmonic oscillator with Hamiltonian given by:

$$\hat{H} = \frac{\hat{p}^2}{2m} + V,$$

where V corresponds to an elastic spring which is extendable but incompressible. The potential of this spring is given by:

$$V(x) = \begin{cases} m\omega^2 x^2/2, & \text{if } x > 0, \\ \infty, & \text{if } x \le 0. \end{cases}$$

Write down the full set of energy eigenvalues of this oscillator and sketch the eigenfunction of the ground state. Find the first excitation energy (i.e., the difference between the energies of the ground state and first-excited state). Briefly state the reasoning behind your results.

[6 marks]

4. a) Consider the following wavefunctions of a hydrogen atom

$$\begin{array}{rcl} \psi_A(r,\theta,\phi) & = & Ae^{-r/a_0}, \\ \psi_B(r,\theta,\phi) & = & B\left(1-\frac{r}{2a_0}\right)e^{-r/2a_0}, \\ \psi_C(r,\theta,\phi) & = & C\left(\frac{r}{a_0}\right)e^{-r/2a_0}\sin\theta\,e^{-i\phi}, \end{array}$$

where A, B, C and  $a_0$  are constants.

i) Sketch the position probability density as a function of radial distance from the nucleus, r, for the electron described by the wavefunction  $\psi_B$ .

[4 marks]

ii) Show that  $\psi_B$  and  $\psi_C$  are orthogonal.

[3 marks]

iii) State the values of the hydrogen quantum numbers (n, l, m) corresponding to each of the wavefunctions  $\psi_A$ ,  $\psi_B$  and  $\psi_C$ .

[3 marks]

iv) Find the wavelength of the emitted photon when the hydrogen atom makes a transition from  $\psi_B$  to  $\psi_A$ . What is the corresponding wavelength in the case of a helium ion, He<sup>+</sup>?

[6 marks]

b) i) Write down the quantum operators for the angular momentum components,  $\hat{L}_x$ ,  $\hat{L}_y$  and  $\hat{L}_z$ , in terms of  $\hat{x}$  and  $\hat{p}_x$ , etc.

[4 marks]

ii) Given the following commutation relation,

$$[\hat{L}_z, \, \hat{L}^+] = \hbar \hat{L}^+,$$

where  $\hat{L}^+ = \hat{L}_x^+ + i\hat{L}_y$ , show that the wavefunction

$$\psi = \hat{L}^+ \psi_C(r, \theta, \phi)$$

is an eigenfunction of  $\hat{L}_z$  and find the corresponding eigenvalue, where  $\psi_C$  is given in part (a).

[5 marks]

## END OF EXAMINATION PAPER