<u>ONE HOUR THIRTY MINUTES</u>

A list of constants is enclosed.

UNIVERSITY OF MANCHESTER

Introduction to Quantum Mechanics

25 January 2017, 9.45 a.m. - 11.15 a.m.

Answer **ALL** parts of question 1 and **TWO** other questions

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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. a) A particle of mass m is moving in one dimension in a potential $\widehat{V}$. Write down the time-dependent Schrödinger equation of the particle for its wavefunction $\Psi(x,t)$.

[3 marks]

If $\widehat{V}$ is time independent, by substituting the stationary wavefunction with energy E,

$$\Psi(x,t) = \psi(x)\exp\left(-iEt/\hbar\right),$$

obtain the time-independent Schrödinger equation for the spatial wavefunction $\psi(x)$.

[2 marks]

b) Electrons with 2 eV kinetic energy are passing through a narrow slit of 8 Å width. Are the wave properties of the electrons important? Give your reason.

[3 marks]

c) For a particle of mass m moving in one dimension, write down the definition of the momentum operator $\hat{p}_x$ and derive the kinetic energy operator $\widehat{T}$.

[2 marks]

The particle is moving in a region of free space with a wavefunction

$$\psi(x) = A\cos kx,$$

where A and k are constants. Show that $\psi(x)$ is not an eigenfunction of $\hat{p}_x$ but is an eigenfunction of $\widehat{T}$. What are the possible outcomes of a measurement of the particle's momentum?

[5 marks]

d) In a scanning tunneling microscopic (STM) experiment, a metal tip is positioned about 3 Å from the sample surface. Use the wide-barrier approximation to estimate the probability for an electron with an energy deficit of 1.5 eV to tunnel through the vacuum gap.

[5 marks]

e) Specify the allowed values of the quantum numbers (n, l, m_l, m_s) of a hydrogen atom. Briefly state their physical meanings. If the energy of a hydrogen atom in an external field depends on (n, l) only, what is the degeneracy for each of the energy levels?

[5 marks]

2. A particle of mass m is confined by a one-dimensional infinite square well potential to a region $-L/2 < x < L/2$, where inside the well the potential is zero.

a) Write down the Hamiltonian $\hat{H}$ of the particle. Show that the wavefunction

$$f(x) = \begin{cases} \sqrt{\frac{2}{L}} \cos \frac{\pi x}{L}, & -\frac{L}{2} < x < \frac{L}{2} \\ 0, & \text{elsewhere} \end{cases}$$

is normalized and is an eigenfunction of $\hat{H}$. Determine the eigenvalue E.

[5 marks]

b) Find the uncertainties of position Δx and momentum Δp of the particle described by the wavefunction $f(x)$. Verify that $\Delta x \Delta p \geq \hbar/2$. You may use the following integral

$$\int_{-L/2}^{L/2} x^2 \cos \frac{2\pi x}{L} dx = -\frac{L^3}{2\pi^2}.$$

[10 marks]

c) Write down another eigenfunction, $g(x)$, of $\hat{H}$ and the corresponding eigenvalue, U. Show that $g(x)$ satisfies the boundary conditions of the system.

[3 marks]

d) Assume that at time $t = 0$, the particle is in the state

$$\psi(x) = \frac{1}{\sqrt{2}} \left[f(x) + g(x) \right].$$

Write down the particle wavefunction $\Psi(x, t)$ at time $t\,(> 0)$. Determine the probability of finding the particle in the interval $0 < x < L/2$. You may find the following identities useful:

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

[7 marks]

3. a) A particle of energy E is confined in one dimension to the region $x > 0$ with an impenetrable wall at $x = 0$. There is also a potential barrier of height V $(> E)$ as illustrated in the following figure. Sketch a possible energy eigenfunction of the particle.

[5 marks]

b) The Hamiltonian of a one-dimensional harmonic oscillator of mass m and angular frequency ω is written as

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

i) The operators $\hat{a}$ and $\hat{a}^\dagger$ are defined as

$$\hat{a} = \frac{1}{\sqrt{2}}\left(\frac{\hat{x}}{x_0} + \frac{ix_0\hat{p}_x}{\hbar}\right), \quad \hat{a}^\dagger = \frac{1}{\sqrt{2}}\left(\frac{\hat{x}}{x_0} - \frac{ix_0\hat{p}_x}{\hbar}\right),$$

with $x_0 = \sqrt{\hbar/m\omega}$. Show that

$$[\hat{a},\, \hat{a}^\dagger] = 1. \tag{1}$$

Show that $\hat{H}$ can be expressed as

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

[5 marks]

ii) Show that the ground-state wavefunction,

$$\psi_0(x) = A\exp\left(-\frac{x^2}{2x_0^2}\right)$$

with constant A, satisfies $\hat{a}\psi_0(x) = 0$. Hence find the ground-state energy E_0.

[5 marks]

iii) Use Eqs. (1) and (2) to show that $\psi_1(x) = \hat{a}^\dagger\psi_0(x)$ describes an excited state and find the corresponding energy E_1.

[5 marks]

iv) In a hydrogen iodide (HI) molecule, the spring constant of the covalent bond has a value of 310 N m^{-1}. Estimate the energy interval $\Delta E = E_1 - E_0$ in eV, of the vibrational motion. (The atomic masses of hydrogen and iodine are 1 and 130 respectively.)

[5 marks]

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

$$\begin{aligned} \psi_A(r,\theta,\phi) &= A\left(1-\frac{r}{2a_0}\right)e^{-r/2a_0}, \\ \psi_B(r,\theta,\phi) &= B\left(\frac{r}{3a_0}\right)^2 e^{-r/3a_0}\sin^2\theta e^{i2\phi}, \end{aligned}$$

where A, B and a_0 are constants.

i) Show that ψ_A and ψ_B are orthogonal to one another. State the values of the hydrogen quantum numbers (n, l, m) for both ψ_A and ψ_B.

[6 marks]

ii) Find the wavelength of the emitted (or absorbed) photon when the hydrogen atom makes a transition between these two states. What is the corresponding wavelength in the case of a lithium ion Li^{2+}?

[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.

[3 marks]

ii) Given the following commutation relation,

$$[\hat{L}_x,\, \hat{L}_y] = i\hbar\hat{L}_z,$$

use the cyclic rule to write down the other two commutation relations between the angular momentum component operators. Hence show that

$$[\hat{L}_z,\, \hat{L}^-] = -\hbar\hat{L}^-, \tag{3}$$

where $\hat{L}^- = \hat{L}_x - i\hat{L}_y$.

[5 marks]

iii) Use Eq. (3) to show that the wavefunction

$$\psi_C = \hat{L}^-\psi_B(r,\theta,\phi)$$

is also an eigenfunction of $\hat{L}_z$ and find the eigenvalue, where ψ_B is given in Part (a).

[5 marks]

END OF EXAMINATION PAPER