ONE HOUR THIRTY MINUTES

A list of constants is enclosed.

UNIVERSITY OF MANCHESTER

Introduction to Quantum Mechanics

24 January 2019, 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 moves in two dimensions in a potential $\widehat{V}$. Write down the time-dependent Schrödinger equation (TDSE) for the particle's wavefunction $\Psi(\mathbf{r},t)$. Assume that $\widehat{V}$ is time independent, substitute the stationary wavefunction with energy E,

$$\Psi(\mathbf{r},t) = \psi(\mathbf{r}) \exp\left(-iEt/\hbar\right),$$

to obtain the time-independent Schrödinger equation for the spatial wavefunction $\psi(\mathbf{r})$.

[4 marks]

Given that $\Psi_1(\mathbf{r},t) = \psi_1(\mathbf{r}) \exp\left(-iE_1t/\hbar\right)$ and $\Psi_2(\mathbf{r},t) = \psi_2(\mathbf{r}) \exp\left(-iE_2t/\hbar\right)$ are two solutions of the TDSE of the particle where ψ_1 and ψ_2 are real, show that their linear combination,

$$\Phi = \frac{1}{\sqrt{2}}\left(\Psi_1 + \Psi_2\right),$$

is also a solution. Show also that the probability density $|\Phi|^2$ is an oscillatory function of time and find the period in terms of the energies E_1 and E_2.

[5 marks]

b) A particle is moving in two-dimensions. Show that the function

$$\psi(\mathbf{r}) = Ae^{i\mathbf{k}\cdot\mathbf{r}},$$

where A is a constant and $\mathbf{k}$ is a constant wavevector, is an eigenfunction of the momentum operator $\hat{\mathbf{p}}$. Find the eigenvalue.

[2 marks]

The particle is in a state described by a wavefunction

$$\psi(x,y) = \frac{2}{a}\sin\frac{\pi x}{a}\sin\frac{2\pi y}{a},$$

where a is a constant. What are the possible values of a measurement of the particle's momentum vector? What are the corresponding probabilities?

[4 marks]

c) In the usual notation the quantum numbers of hydrogen are (n, l, m_l, m_s). Briefly state their meanings and give their allowed values.

[3 marks]

Explain what is meant by the parity of an electron state. For a given wavefunction ψ_{n,l,m_l,m_s} of hydrogen, what is its parity?

[2 marks]

d) Write down the ground-state electronic configurations of oxygen ($Z = 8$) and selenium ($Z = 34$). Determine the total S, L and J of the ground state of oxygen and write down the corresponding spectroscopic term symbol.

[5 marks]

2. a) A strong magnetic field of magnitude B is applied to a hydrogen atom in the $2p$ state. The magnetic interaction operator $\hat{V}_{\text{mag}}$ is given, in the usual notation, as

$$\hat{V}_{\text{mag}} = \frac{e}{2m_e}\left(\hat{\mathbf{L}} + 2\hat{\mathbf{S}}\right) \cdot \mathbf{B}.$$

Determine the energy splitting due to the magnetic field and sketch the energy levels with appropriate quantum numbers.

[6 marks]

b) The Hamiltonian of a one-dimensional simple harmonic oscillator (SHO) 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 $[\hat{a}, \hat{a}^\dagger] = 1$. Also show that $\hat{H}$ can be expressed as

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

[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.

[4 marks]

iii) The oscillator carries a charge q. The recurrence relation of the eigenfunctions of the SHO is

$$x\psi_n(x) = A_n\psi_{n+1}(x) + B_n\psi_{n-1}(x), \quad n \geq 1$$

where A_n and B_n are coefficients independent of x. Use this recurrence relation to find the selection rule for an electric dipole transition for the oscillator.

[5 marks]

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

[5 marks]

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

[3 marks]

ii) Show that in spherical coordinates (r, θ, ϕ), $\hat{L}_z$ can be expressed as $\hat{L}_z = -i\hbar\partial/\partial\phi$.

[3 marks]

iii) Given the angular momentum squared operator in spherical coordinates,

$$\hat{L}^2 = -\hbar^2 \left(\frac{\partial^2}{\partial\theta^2} + \cot\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right),$$

show that

$$\psi(\theta, \phi) = A \sin\theta \, e^{-i\phi}$$

with constant A, is an eigenfunction of both $\hat{L}_z$ and $\hat{L}^2$ and find the corresponding eigenvalues.

[5 marks]

b) The following wavefunctions are energy eigenfunctions of the hydrogen atom:

$$\begin{aligned}
\psi_1(r, \theta, \phi) &= A_1 e^{-r/a_0}, \\
\psi_2(r, \theta, \phi) &= \frac{1}{\sqrt{32\pi a_0^3}} \left(2 - \frac{r}{a_0}\right) e^{-r/2a_0}, \\
\psi_3(r, \theta, \phi) &= A_3 \left(\frac{r}{a_0}\right)^2 e^{-r/3a_0} \sin^2\theta \, e^{-2i\phi},
\end{aligned}$$

where A_1 and A_3 are normalization constants and a_0 is the Bohr radius.

i) Determine the normalization constant A_1.

[3 marks]

ii) Consider the approximation that, over the small volume of the nucleus, the wavefunction ψ_2 is constant and equal to its value at $r = 0$. Estimate the probability that an electron in state ψ_2 would be found within the nucleus, which has a radius of 1 fm.

[5 marks]

iii) Show that ψ_1 and ψ_3 are orthogonal.

[2 marks]

iv) Write down the formula for the hydrogen energy levels in terms of the principle quantum number n. Calculate the wavelength of the emitted photon when the hydrogen atom makes a transition from ψ_3 to ψ_1. Comment on the likelihood of this transition.

[4 marks]

4. a) Give the definition of an Hermitian operator in one dimension. Show that the eigenvalues of an Hermitian operator are real.

[5 marks]

b) The ground-state electronic configuration of a helium atom is $(1s)^2$.

i) Write down the corresponding wavefunction in terms of the $1s$ orbital ψ_{1s} and spin-1/2 wavefunctions $\chi_{\pm}$. Discuss the symmetry of the wavefunction.

[6 marks]

ii) Ignoring the Coulomb repulsion between the electrons, estimate the ground-state energy of helium in units of eV. By comparing your result with the observed value of -79 eV, estimate the Coulomb repulsion energy of the two electrons in the ground state and comment on your result.

[4 marks]

c) The spin-orbit coupling operator $\hat{V}_{\mathrm{SO}}$ for a hydrogen atom is given by

$$\hat{V}_{\mathrm{SO}} = f(r)\hat{\mathbf{S}} \cdot \hat{\mathbf{L}}$$

with the function $f(r)$ defined as

$$f(r) = \frac{\alpha\hbar}{2m_e^2 c} \cdot \frac{1}{r^3},$$

where $\alpha = 1/137$ and all other symbols have their usual meaning.

i) The hydrogen atom is in the $2p$ state. Determine the possible values of the total angular momentum quantum number j. Hence determine the eigenvalues of the operator $\hat{\mathbf{S}} \cdot \hat{\mathbf{L}}$.

[6 marks]

ii) Estimate the spin-orbit energy splitting between the states with these j values. You may use the result that the expectation value for the $2p$ state of hydrogen is

$$\left\langle \frac{1}{r^3} \right\rangle = \frac{1}{(3a_0)^3},$$

where a_0 is the Bohr radius.

[4 marks]

END OF EXAMINATION PAPER