I.1 Atomic Structure

Civil Services 2016–2026: **26** parts, **240** marks · IFoS 2016–2025: **19** parts, **182** marks

Syllabus. Heisenberg's uncertainty principle, Schrodinger wave equation (time independent); interpretation of wave function, particle in one-dimensional box, quantum numbers, hydrogen atom wave functions; shapes of s, p and d orbitals.

Marks	2016	2017	2018	2019	2020	2021	2022	2023	2024	2025	2026
CSE	25	25	25	10	20	20	30	20	15	20	30
IFoS	15	10	23	10	30	15	18	23	18	20	

How to use this chapter. Read every question once and mark the ones that repeat. Pick three, write them by hand against the clock (about 7 minutes for 10 marks), then compare with the model answers on vkcscience.com.

2026

CSE 2026 · Q5(a) de Broglie wavelength of a baseball [5 marks]

What is the de Broglie wavelength for a baseball (140 g) moving at 40 m s^{-1}? Comment on your finding.

CSE 2026 · Q7(a) e^(α x) as an eigenfunction of dⁿ/dxⁿ; Why n=0 is not allowed for a particle in a box [10 marks]

(i) Show that $\psi(x) = e^{\alpha x}$ is an eigenfunction for the operator $\hat{A} = \frac{d^n}{dx^n}$. What is the eigenvalue?

(ii) The time-independent Schrödinger equation for a free particle (of mass m) in a box of length L (inside the box potential energy is zero, but outside the box is infinity) is

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi(x) = 0; \qquad 0 \leq x \leq L$$

The solution of the above equation is $\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$; where $n = 1, 2, 3, \ldots$. Why is $n = 0$ not allowed? Explain.

CSE 2026 · Q7(b) Uncertainty in momentum and speed of an electron, Δ x≈50 pm; Quantum numbers of the 2pz orbital [15 marks]

(i) Find the minimum uncertainty in momentum and speed if we wish to locate an electron within an atom so that $\Delta x \approx 50$ pm, using $\Delta p_x \times \Delta x \geq h$. Comment on your two findings.

(ii) What are the n, l and m_l values of $2p_z$ orbital? Explain.

2025

CSE 2025 · Q1(a) Probability of the 1s electron at a_o and at $10a_o$ [5 marks]

Calculate the ratio of probability of finding the 1s electron of hydrogen atom at $r = a_0$ and at $r = 10a_0$, where 'r' is the distance from the nucleus and a_0 = radius of the first Bohr orbit.

CSE 2025 · Q2(a) Particle in a box: probability in the first quarter [15 marks]

Find the probability of existence of a particle in a one-dimensional box of length 'a' in the region $0 \leq x \leq \frac{a}{4}$ for the states $n = 1$, 2 and 3.

IFoS 2025 · Q2(a) Hydrogen equation in spherical coordinates; Box length from an emission frequency [15 marks]

(i) Write down the time-independent Schrödinger equation for stationary states of hydrogen atom in spherical polar coordinates (r, θ, ϕ) considering origin at the nucleus of the atom and the proton to be stationary. Show pictorially the interrelation between the Cartesian and spherical polar coordinates. How are r, θ and ϕ called? 10

(ii) When a particle of mass 9.1×10^{-28} gram in a certain one-dimensional box goes from $n = 5$ level to $n = 2$ level, it emits a photon of frequency 6.0×10^{14} s^{-1}. Find the length of the box. [Given: $h = 6.626 \times 10^{-27}$ erg s] 5

IFoS 2025 · Q2(b)(i) Lifetime and spectral uncertainty [5 marks]

(i) The average time gap between the excitation of an atom and consequent emission of a photon is 10^{-8} s. Calculate the uncertainty in the (1) energy measurement and (2) frequency determination. [Given: $h = 6.626 \times 10^{-34}$ J s] 5

2024

CSE 2024 · Q1(a)(i) Most probable distance of the 1s electron [5 marks]

(i) Determine the distance from the nucleus at which the electron is most expected in the hydrogen atom in its ground state.

[Given: The normalized radial function for hydrogen-like systems is $R_{10}(1s) = 2\left(\frac{Z}{a_0}\right)^{3/2} \cdot e^{-\rho/2}$ where $\rho = \frac{2Zr}{na_0}$ and a_0 is the first Bohr orbit radius. Other notations have their usual meanings.] 5

CSE 2024 · Q2(a) Uncertainty principle; orthogonality of ψ_1 and ψ_2 in a box [10 marks]

State Heisenberg's uncertainty principle. Show that for a particle in a one-dimensional box having length from 0 to L, the two normalised eigen functions corresponding to the eigenvalues E_1 and E_2 (characterised by quantum numbers 1 and 2 respectively) are orthogonal to each other.

IFoS 2024 · Q1(a) Free-particle waves and de Broglie relation [8 marks]

For a free particle, show how the time-independent Schrodinger equation gives a solution to explain de Broglie relation.

IFoS 2024 · Q2(a) Most probable radius in Li^{2+} [10 marks]

Determine the most probable radius at which electron will be found when it occupies 1s orbital of Li^{2+} ion.

2023

CSE 2023 · Q1(a) Light emitted by a particle in a box; the uncertainty principle [10 marks]

(i) Find the wavelength of the emitted light when 1.0×10^{-27} g particle in a one-dimensional box of length 3 Å goes from $n_x = 2$ to $n_x = 1$ level.

(ii) Explain the Heisenberg uncertainty principle.

CSE 2023 · Q2(b) Continuous energy of a free particle, quantised energy in a box [10 marks]

Explain why the energy of a free particle can vary continuously but the energy of a particle in a box is quantized.

IFoS 2023 · Q1(a) Quantum numbers of oxygen electrons [8 marks]

An oxygen atom has a total of eight electrons. Write the four quantum numbers (in tabular form) for each of the eight electrons in the ground state.

IFoS 2023 · Q2(a) Emission and eigenvalues in a box [15 marks]

(i) Find the wavelength of light emitted when 5×10^{-28} g particles in a 3 Å one-dimensional box goes from $n = 2$ to $n = 1$ level.
(ii) Verify $H\psi = E\psi$ for the particle in a one-dimensional box.

2022

CSE 2022 · Q1(a) Average and most probable distance of the 1s electron [10 marks]

Compare average and most probable values of position of an electron in the ground state of hydrogen atom. Explain with the help of drawing, why two values differ.

CSE 2022 · Q2(b) Particle in a box: probability in the first 1/a of the width [20 marks]

A particle is in the nth energy state, $\phi_n(x)$, of an infinite square well potential with width L (box size from O to L). Calculate the probability that the particle is confined to the first $1/a$ of the width of the well.

IFoS 2022 · Q1(a) Continuity of the wavefunction [8 marks]

For an acceptable solution, the wavefunction, $\phi(x)$ and its derivative, $d\phi(x)/dx$, has to be continuous. Why is this condition imposed on the wavefunction?

IFoS 2022 · Q2(a) Nodes in hydrogen 3p orbitals [10 marks]

Find the radial and angular nodes in H-orbitals, $\psi_{3p_z}(r, \theta, \phi)$ and $\psi_{3p_x}(r, \theta, \phi)$.

2021

CSE 2021 · Q1(a) Expectation value of position in the ground state of a box [10 marks]

Calculate $\langle x \rangle$, the expectation value of position of a particle, in the ground state of one-dimensional box having length from 0 to l.

CSE 2021 · Q2(a) Hydrogen atom: the transition n = 101 → 100 [10 marks]

Hydrogen atoms are observed to have radiative transitions from $n = 101$ to $n = 100$ to occur.
(i) What are the frequency and wavelength of the radiation emitted in this transition?
(ii) Why is it difficult to observe this transition?

IFoS 2021 · Q2(a) Particle in a one-dimensional box [15 marks]

Prove that for a particle in the box, the total energy eigenfunctions,

$$\phi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

where $\phi(x)$ is a continuous function at the edges of the box. Is $d\phi_{(x)}$ a continuous function of x at the edges of the box? The dimensions of the box are from $x = 0$ to $x = L$.

2020

CSE 2020 · Q3(a) Most probable distance of the 1s electron of hydrogen [10 marks]

The wave function of the hydrogen atom is given by $R_{1s} = \frac{1}{\sqrt{\pi}} e^{-r}$ (in atomic units). What will be the most probable distance of an electron from the nucleus in its ground state (in unit of a_0, the Bohr radius and in Å unit)?

CSE 2020 · Q5(a) Degeneracy of the hydrogenic level with E=-RH/36 [10 marks]

What do you mean by degeneracy of energy level? Find the number of degeneracy of hydrogenic orbital having energy $-R_H/36$. R_H = Rydberg constant.

IFoS 2020 · Q2(b) Particle in a box from −L/2 to L/2: ground and first excited states [15 marks]

Obtain an expression of wave function for the ground state and first excited state for a particle confined in a one-dimensional box of length L with infinitely hard walls between $x = -\frac{L}{2}$ to $x = +\frac{L}{2}$.

IFoS 2020 · Q4(c) Degeneracy of the hydrogen level with E = $-e^2/72\pi\varepsilon_0 a_0$; lifetime broadening [15 marks]

(i) The total energy eigenvalues for the hydrogen atom are given by

$$E_n = \frac{-e^2}{8\pi\varepsilon_0 a_0 n^2}$$

List all the eigenfunctions that have the following total energy eigenvalue :

$$E = \frac{-e^2}{72\pi\varepsilon_0 a_0}$$

What is the degeneracy of energy level? 10

(ii) An atom exists in an excited state for about $\Delta t = 10^{-8}$ second. Estimate the uncertainty, Δf in the frequency of emitted photons when an atom makes a transition from an excited state with the emission of photon. 5

2019

CSE 2019 · Q1(d) Uncertainty in the position of a honeybee [10 marks]

Use the Heisenberg uncertainty principle to calculate the uncertainty (in metres) in the position of a honeybee weighing 0.68 g and travelling at a velocity of 0.85 m/s. Assume that the uncertainty in the velocity is 0.1 m/s.

IFoS 2019 · Q4(c) Orbits versus orbitals; the Hamiltonian and acceptable ψ [10 marks]

(i) Justify the statement : Instead of being able to describe precise "orbits" of electrons, we can only describe "orbitals". 5

(ii) Define Hamiltonian Operator. Write the conditions for a physically realistic solution for wave function ψ. 5

2018

CSE 2018 · Q1(a) Particle in a box: probability in the centre half [10 marks]

A particle in a rigid box of length 'L' is in its ground state. What is the probability of finding the particle in the centre half of the box?

CSE 2018 · Q2(a)(i) Orbital and probability density [5 marks]

What is an orbital and how is it related to the probability density?

CSE 2018 · Q2(a)(ii) Radial, angular and total nodes [5 marks]

Determine the number of radial nodes, angular nodes and total number of nodes in the following orbitals: 2p, 3s, 3p, 4d, 5f.

CSE 2018 · Q2(a)(iii) If Planck's constant were zero [5 marks]

Would it be possible to determine the position and momentum of an electron simultaneously and accurately if the value of Plank's constant is zero?

IFoS 2018 · Q1(a) Is Be^{-ax} an eigenfunction of $\mathrm{d}^2/\mathrm{d}x^2$? [8 marks]

Is the function, $\psi(x)$ = Be^{-mx} an eigenfunction for the operator $\hat{A} = \frac{d^2}{dx^2}$? If so, what is the eigenvalue?

IFoS 2018 · Q2(a) de Broglie wavelengths of an electron and a baseball [15 marks]

Using de Broglie wave-particle dual relationship, $\lambda \times p = h$; calculate the wavelength (in SI units) of (i) an electron travelling 1·00% of the speed of light, and (ii) a baseball (mass = 140 g) travelling at 40 ms^{-1}. Comment on your findings.

2017

CSE 2017 · Q4(a)(i) Particle in a box: probability between 0 and a/2 [15 marks]

For a particle in one-dimensional box of length a calculate the probability of its locating between zero and $a/2$.

CSE 2017 · Q4(a)(ii) Complete 1s wavefunction and its spherical shape [10 marks]

Write the complete wave function for 1s-orbital and deduce its shape.

IFoS 2017 · Q1(c) Principal quantum number from the orbital energy [5 marks]

What would be the value of the principal quantum number, if an electron in a hydrogen atom was in the orbital of energy $-0{\cdot}242 \times 10^{-18}$ J? Given : $k = 2{\cdot}179 \times 10^{-18}$ J.

IFoS 2017 · Q2(a) Uncertainty in momentum of an electron [5 marks]

If uncertainty in position is written as Δx and in momentum as Δp, then Heisenberg Uncertainty principle is $\Delta p\, \Delta x \geq h/4\pi$. If the position of an electron is known to within 10^{-12} m, what is the uncertainty in its momentum? Given $h = 6{\cdot}626 \times 10^{-34}$ Js and $\pi = 3{\cdot}14$.

2016

CSE 2016 · Q3(c) Angular wave functions of the d orbitals and their signs [10 marks]

What are the angular wave functions of d-orbitals? Explain them, including their geometric signs, with the help of neat and labelled diagrams.

CSE 2016 · Q4(b) Schrödinger wave equation in three dimensions; meaning of ψ and ψ² [15 marks]

Set up the Schrödinger's wave equation in 3-dimension. Comment on the nature of the equation and various terms involved. Explain the significance of ψ and ψ^2.

IFoS 2016 · Q4(c) Schrödinger wave equation in three dimensions; meaning of ψ and ψ² [10 marks]

Set up the Schrödinger wave equation (three dimensions). Comment on the nature of the equation and various terms involved. Explain the significance of ψ and ψ^2.

IFoS 2016 · Q5(d)(i) Shapes of the d orbitals [5 marks]

Draw neat diagrams of the shapes of *d*-orbitals.