ABC CHEMISTRY

Mr. Aniket Bhardwaj · 15+ Years Mentorship

Quantum Chemistry

Premium CSIR-NET PYQ Book

127 CSIR-NET Previous-Year Questions · 114 Fully Solved with Distractor Analysis

3-Slide Solutions | Distractor Analysis | Exam Tricks | Revision Sheets

CSIR-NET · GATE · IIT-JAM — 12 Topics · 127 Real PYQs

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Course Contents

12 Topics · 127 PYQs · tap a topic to jump

1 **Schrödinger Equation & Wavefunctions** — 2 Qs E 0 · M 2 · H 0 — 2%

2 **Quantum Operators & Commutators** — 19 Qs E 1 · M 5 · H 13 — 15%

3 **Particle in a Box** — 17 Qs E 6 · M 11 · H 0 — 13%

4 **Harmonic Oscillator** — 15 Qs E 3 · M 11 · H 1 — 12%

5 **Angular Momentum & Spin** — 19 Qs E 0 · M 16 · H 3 — 15%

6 **Hydrogen Atom & Atomic Orbitals** — 17 Qs E 5 · M 12 · H 0 — 13%

7 **Tunneling & Barrier Problems** — 2 Qs E 0 · M 2 · H 0 — 2%

8 **Perturbation & Variation Theory** — 14 Qs E 0 · M 9 · H 5 — 11%

9 **Hückel MO Theory** — 6 Qs E 0 · M 1 · H 5 — 5%

10 **Many-Electron Systems** — 6 Qs E 0 · M 5 · H 1 — 5%

11 **Molecular Orbitals & Hybridization** — 4 Qs E 0 · M 4 · H 0 — 3%

12 **Quantum Chemistry – General** — 6 Qs E 0 · M 4 · H 2 — 5%

Legend: **E** Easy **M** Medium **H** Hard · **%** = exam weightage (share of the chapter)

(Mr. Aniket Bhardwaj By ABC Chemistry)

TOPIC 1

Schrödinger Equation & Wavefunctions

2 questions · Easy 0 | Medium 2 | Hard 0 · PYQ frequency: Rare

Q65

The simplest ground-state VB wave function of a diatomic molecule like HCl is written as $\psi = \psi H\ 1s,\ 1\ \psi Cl\ 3pz\ ,\ 2 + B$ where B stands for

A) $\psi H\ 3pz\ ,\ 2\ \psi Cl\ 1s,\ 1$

B) $\psi H\ 1s,\ 2\ \psi Cl\ 3pz\ ,\ 1$

C) $\psi Cl\ 1s,\ 2\ \psi Cl\ 3pz\ ,\ 1$

D) $\psi Cl\ 1s,\ 2\ \psi H\ 3pz\ ,\ 1$

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Postulates of QM, normalization, expectation values

PYQ FREQUENCY
Rare · 1 paper

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
$\hat{H}$ on ψ returns $E\times\psi$ — operator on eigenfunction gives eigenvalue × eigenfunction.

Correct Answer B ψ*H* 1*s*, 2 ψ*Cl* 3*pz* , 1

CONCEPT

The time-independent Schrödinger equation Ĥψ = Eψ governs quantum systems. A valid ψ must be single-valued, continuous, finite and square-integrable (normalizable).

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (B).

FINAL: (B) ψ*H* 1*s*, 2 ψ*Cl* 3*pz* , 1

SHORTCUT / EXAM TRICK

Normalization: $\int|\psi|^2 d\tau = 1$. Expectation value: $\langle A\rangle = \int \psi^* \hat{A} \psi d\tau$.

COMMON MISTAKE

Forgetting ψ itself may be complex — only $|\psi|^2$ must be real and non-negative.

EXAM TIP

Boundary conditions fix the allowed energies; normalization fixes the coefficient.

MEMORY TRICK

Ĥ on ψ returns E×ψ — operator on eigenfunction gives eigenvalue × eigenfunction.

Why the Other Options Are Wrong

Correct answer: **B**

A — **ψ*H* 3*pz* , 2 ψ*Cl* 1*s*, 1**

Inconsistent with the postulates of QM and wavefunction requirements; correct choice is (B). See worked explanation.

C — **ψ*Cl* 1*s*, 2 ψ*Cl* 3*pz* , 1**

Inconsistent with the postulates of QM and wavefunction requirements; correct choice is (B). See worked explanation.

D — **ψ*Cl* 1*s*, 2 ψ*H* 3*pz* , 1**

Inconsistent with the postulates of QM and wavefunction requirements; correct choice is (B). See worked explanation.

Q70

A particle is in a one-dimensional box with a potential Vo inside the box and infinite outside. An energy state corresponding to n = 0 (n = quantum number) is not allowed because

A. the total energy becomes zero

B. the average momentum becomes zero

C. the wave function becomes zero every where

D. the potential V0 ≠ 0

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Postulates of QM, normalization, expectation values

PYQ FREQUENCY
Rare · 1 paper

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
Ĥ on ψ returns E×ψ — operator on eigenfunction gives eigenvalue × eigenfunction.

Correct Answer C the wave function becomes zero every where

CONCEPT

The time-independent Schrödinger equation $\hat{H}\psi = E\psi$ governs quantum systems. A valid ψ must be single-valued, continuous, finite and square-integrable (normalizable).

↓

LOGIC / WORKING

Key principle: the particle-in-a-box energy formula $E_n = n^2h^2/8mL^2$. Answer is (C).

FINAL: (C) the wave function becomes zero every where

SHORTCUT / EXAM TRICK

Normalization: $\int|\psi|^2 d\tau = 1$. Expectation value: $\langle A \rangle = \int \psi^* \hat{A} \psi d\tau$.

COMMON MISTAKE

Forgetting ψ itself may be complex — only $|\psi|^2$ must be real and non-negative.

EXAM TIP

Boundary conditions fix the allowed energies; normalization fixes the coefficient.

MEMORY TRICK

$\hat{H}$ on ψ returns $E \times \psi$ — operator on eigenfunction gives eigenvalue × eigenfunction.

Why the Other Options Are Wrong

Correct answer: **C**

A **the total energy becomes zero**
Inconsistent with the postulates of QM and wavefunction requirements; correct choice is (C). See worked explanation.

B **the average momentum becomes zero**
Inconsistent with the postulates of QM and wavefunction requirements; correct choice is (C). See worked explanation.

D **the potential $V_0 \neq 0$**
Inconsistent with the postulates of QM and wavefunction requirements; correct choice is (C). See worked explanation.

TOPIC REVISION

Schrödinger Equation & Wavefunctions

2 PYQs · Last-minute revision

TOPIC SUMMARY

The time-independent Schrödinger equation $\hat{H}\psi = E\psi$ governs quantum systems. A valid ψ must be single-valued, continuous, finite and square-integrable (normalizable).

IMPORTANT FORMULA SHEET

$\hat{H}\psi = E\psi$
$\langle A \rangle = \int \psi^* \hat{A} \psi \, d\tau$
$\int |\psi|^2 \, d\tau = 1$
$\hat{H} = -(\hbar^2/2m)\nabla^2 + V$

FREQUENTLY ASKED CONCEPTS

Eigenfunctions & eigenvalues
Normalization
Boundary conditions
- Superposition principle

COMMON MISTAKES & QUICK NOTES

Watch out:
Forgetting ψ itself may be complex — only $|\psi|^2$ must be real and non-negative.
Last-minute:
Normalization: $\int |\psi|^2 \, d\tau = 1$. Expectation value: $\langle A \rangle = \int \psi^* \hat{A} \psi \, d\tau$.

MOST-REPEATED PYQs & EXPECTED IN EXAM

PYQs in this topic: Q65 Q70

Expect **1 question(s)** next session on **Postulates of QM, normalization, expectation values.**

TOPIC 2

Quantum Operators & Commutators

19 questions · Easy 1 | Medium 5 | Hard 13 · PYQ frequency: High

Q2

A constant of motion is defined by the equation:

A. [H, A] = 0

B. <[H, A] > =0

C. A = f(H)

D. A† = A

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Hermitian operators, commutators, constants of motion

PYQ FREQUENCY
High · 9 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
Hermitian → real eigenvalues → measurable.
i×(Hermitian) → anti-Hermitian.

Correct Answer B <[H, A] > =0

CONCEPT

Observables are Hermitian operators (real eigenvalues). [Â,B̂] = ÂB̂ – B̂Â. Commuting operators share eigenstates and are simultaneously measurable.

↓

LOGIC / WORKING

- Key principle: the algebra of quantum mechanical operators. Answer is (B).

FINAL: (B) <[H, A] > =0

SHORTCUT / EXAM TRICK

$[\hat{x}, \hat{p}_x] = i\hbar$. If $[\hat{A},\hat{H}] = 0$ then A is a constant of motion (conserved).

COMMON MISTAKE

Confusing Hermitian (real eigenvalues) with unitary; assuming d/dx alone is Hermitian.

EXAM TIP

(d/dx)^† = –d/dx (anti-Hermitian); $\hat{p}_x = -i\hbar(d/dx)$ IS Hermitian.

MEMORY TRICK

Hermitian → real eigenvalues → measurable. i×(Hermitian) → anti-Hermitian.

Why the Other Options Are Wrong

Correct answer: **B**

A **[H, A] = 0**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (B). See worked explanation.

C **A = f(H)**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (B). See worked explanation.

D **A† = A**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (B). See worked explanation.

Q3

The hermitian conjugate of operator d/dx, called (d/dx)† , is actually equal to

A. –d /dx

B. d/dx

C. i(d/dx)

D. –i(d/dx)

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Hermitian operators, commutators, constants of motion

PYQ FREQUENCY
High · 9 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
Hermitian → real eigenvalues → measurable.
i×(Hermitian) → anti-Hermitian.

Correct Answer A –d /dx

CONCEPT

Observables are Hermitian operators (real eigenvalues). [Â,B̂] = ÂB̂ – B̂Â. Commuting operators share eigenstates and are simultaneously measurable.

↓

LOGIC / WORKING

- Key principle: the algebra of quantum mechanical operators. Answer is (A).

FINAL: (A) –d /dx

SHORTCUT / EXAM TRICK

$[\hat{x}, \hat{p}_x] = i\hbar$. If $[\hat{A},\hat{H}] = 0$ then A is a constant of motion (conserved).

COMMON MISTAKE

Confusing Hermitian (real eigenvalues) with unitary; assuming d/dx alone is Hermitian.

EXAM TIP

$(d/dx)^\dagger = -d/dx$ (anti-Hermitian); $\hat{p}_x = -i\hbar(d/dx)$ IS Hermitian.

MEMORY TRICK

Hermitian → real eigenvalues → measurable. i×(Hermitian) → anti-Hermitian.

Why the Other Options Are Wrong

Correct answer: **A**

B **d/dx**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (A). See worked explanation.

C **i(d/dx)**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (A). See worked explanation.

D **–i(d/dx)**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (A). See worked explanation.

Q7

An operator A is defined as $A = - + x$. Which one of the following statements is true? dx

A. A is a Hermitian operator.

B. A† is an antihermitian operator.

C. Both AA† and A†A are Hermitian.

D. AA† is Hermitian, but A†A is antihermitian

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Hermitian operators, commutators, constants of motion

PYQ FREQUENCY
High · 9 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
Hermitian → real eigenvalues → measurable.
i×(Hermitian) → anti-Hermitian.

Correct Answer C Both AA† and A†A are Hermitian.

CONCEPT

Observables are Hermitian operators (real eigenvalues). [Â,B̂] = ÂB̂ – B̂Â. Commuting operators share eigenstates and are simultaneously measurable.

↓

LOGIC / WORKING

- Key principle: the algebra of quantum mechanical operators. Answer is (C).

FINAL: (C) Both AA† and A†A are Hermitian.

SHORTCUT / EXAM TRICK

$[\hat{x}, \hat{p}_x] = i\hbar$. If $[\hat{A},\hat{H}] = 0$ then A is a constant of motion (conserved).

COMMON MISTAKE

Confusing Hermitian (real eigenvalues) with unitary; assuming d/dx alone is Hermitian.

EXAM TIP

(d/dx)^† = –d/dx (anti-Hermitian); $\hat{p}_x = -i\hbar(d/dx)$ IS Hermitian.

MEMORY TRICK

Hermitian → real eigenvalues → measurable. i×(Hermitian) → anti-Hermitian.

Why the Other Options Are Wrong

Correct answer: C

A **A is a Hermitian operator.**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (C). See worked explanation.

B **A† is an antihermitian operator.**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (C). See worked explanation.

D **AA† is Hermitian, but A†A is antihermitian**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (C). See worked explanation.

Q10

Identify which of the following operators is NOT Hermitian:

A (ħ/i)(d/dx) [momentum operator]

B $i(d^2/dx^2)$

C d^2/dx^2

D x^2

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Hermitian operators, commutators, constants of motion

PYQ FREQUENCY
High · 9 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
Hermitian → real eigenvalues → measurable.
i×(Hermitian) → anti-Hermitian.

Correct Answer B $i(d^2/dx^2)$

CONCEPT

Observables are Hermitian operators (real eigenvalues). $[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$. Commuting operators share eigenstates and are simultaneously measurable.

↓

LOGIC / WORKING

- See the algebra of quantum mechanical operators. The correct answer is (B).

FINAL: (B) $i(d^2/dx^2)$

SHORTCUT / EXAM TRICK

$[\hat{x}, \hat{p}_x] = i\hbar$. If $[\hat{A},\hat{H}] = 0$ then A is a constant of motion (conserved).

COMMON MISTAKE

Confusing Hermitian (real eigenvalues) with unitary; assuming d/dx alone is Hermitian.

EXAM TIP

$(d/dx)^\dagger = -d/dx$ (anti-Hermitian); $\hat{p}_x = -i\hbar(d/dx)$ IS Hermitian.

MEMORY TRICK

Hermitian → real eigenvalues → measurable. i×(Hermitian) → anti-Hermitian.

Why the Other Options Are Wrong

Correct answer: **B**

A **(ħ/i)(d/dx) [momentum operator]**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (B). See worked explanation.

C **d^2/dx^2**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (B). See worked explanation.

D **x^2**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (B). See worked explanation.

Q16

For any operator A and its adjoint A† , the INCORRECT statement is:

(A) AA† is Hermitian

(B) AA† + A†A is hermitian.

(C) A + A† is hermitian

(D) A −A† is Hermitian

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Hermitian operators, commutators, constants of motion

PYQ FREQUENCY
High · 9 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
Hermitian → real eigenvalues → measurable.
i×(Hermitian) → anti-Hermitian.

Correct Answer D A −A† is Hermitian

CONCEPT

Observables are Hermitian operators (real eigenvalues). [Â,B̂] = ÂB̂ – B̂Â. Commuting operators share eigenstates and are simultaneously measurable.

↓

LOGIC / WORKING

- Key principle: the algebra of quantum mechanical operators. Answer is (D).

FINAL: (D) A −A† is Hermitian

SHORTCUT / EXAM TRICK

$[\hat{x}, \hat{p}_x] = i\hbar$. If $[\hat{A},\hat{H}] = 0$ then A is a constant of motion (conserved).

COMMON MISTAKE

Confusing Hermitian (real eigenvalues) with unitary; assuming d/dx alone is Hermitian.

EXAM TIP

(d/dx)^† = –d/dx (anti-Hermitian); $\hat{p}_x = -i\hbar(d/dx)$ IS Hermitian.

MEMORY TRICK

Hermitian → real eigenvalues → measurable. i×(Hermitian) → anti-Hermitian.

Why the Other Options Are Wrong

Correct answer: D

A **AA† is Hermitian**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (D). See worked explanation.

B **AA† + A†A is hermitian.**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (D). See worked explanation.

C **A + A† is hermitian**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (D). See worked explanation.

Q24 If A and B are non-commuting hermitian operators, all eigenvalues of the operator given by the commutator [A, B] are

A. complex

B. real

C. imaginary

D. zero

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Hermitian operators, commutators, constants of motion

PYQ FREQUENCY
High · 9 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
Hermitian → real eigenvalues → measurable. i×(Hermitian) → anti-Hermitian.

Correct Answer C imaginary

CONCEPT

Observables are Hermitian operators (real eigenvalues). [Â,B̂] = ÂB̂ – B̂Â. Commuting operators share eigenstates and are simultaneously measurable.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (C).

FINAL: (C) imaginary

SHORTCUT / EXAM TRICK

$[\hat{x}, \hat{p}_x] = i\hbar$. If $[\hat{A},\hat{H}] = 0$ then A is a constant of motion (conserved).

COMMON MISTAKE

Confusing Hermitian (real eigenvalues) with unitary; assuming d/dx alone is Hermitian.

EXAM TIP

$(d/dx)^\dagger = -d/dx$ (anti-Hermitian); $\hat{p}_x = -i\hbar(d/dx)$ IS Hermitian.

MEMORY TRICK

Hermitian → real eigenvalues → measurable. i×(Hermitian) → anti-Hermitian.

Why the Other Options Are Wrong

Correct answer: **C**

A — **complex**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (C). See worked explanation.

B — **real**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (C). See worked explanation.

D — **zero**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (C). See worked explanation.

Q25

The value of the commutator $[\hat{x}, \hat{p}^2_x]$ is given by:

A) 2i

B) 2iℏ

C) 2iℏ$\hat{x}$

D) 2iℏ$\hat{p}_x$

SELF-PRACTICE official answer key not printed in the source — attempt this, then verify.

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Hermitian operators, commutators, constants of motion

PYQ FREQUENCY
High · 9 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
Hermitian → real eigenvalues → measurable. i×(Hermitian) → anti-Hermitian.

Q60

The operators S are defined by $S = Sx \ iSy$ where Sx and Sy are components of the spin angular momentum operator. The commutator Sx , $S„$ is

A $\hbar S„$

B $\hbar S,$

C $-\hbar S„$

D $-\hbar S,$

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Hermitian operators, commutators, constants of motion

PYQ FREQUENCY
High · 9 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
Hermitian → real eigenvalues → measurable.
i×(Hermitian) → anti-Hermitian.

Correct Answer A $\hbar S_{\alpha}$

CONCEPT

Observables are Hermitian operators (real eigenvalues). $[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$. Commuting operators share eigenstates and are simultaneously measurable.

↓

LOGIC / WORKING

- Key principle: the algebra of quantum mechanical operators. Answer is (A).

FINAL: (A) $\hbar S_{\alpha}$

SHORTCUT / EXAM TRICK

$[\hat{x}, \hat{p}_x] = i\hbar$. If $[\hat{A},\hat{H}] = 0$ then A is a constant of motion (conserved).

COMMON MISTAKE

Confusing Hermitian (real eigenvalues) with unitary; assuming d/dx alone is Hermitian.

EXAM TIP

$(d/dx)^\dagger = -d/dx$ (anti-Hermitian); $\hat{p}_x = -i\hbar(d/dx)$ IS Hermitian.

MEMORY TRICK

Hermitian → real eigenvalues → measurable. i×(Hermitian) → anti-Hermitian.

Why the Other Options Are Wrong

Correct answer: **A**

B $\hbar S_x$

Inconsistent with the algebra of quantum mechanical operators; correct choice is (A). See worked explanation.

C $-\hbar S_y$

Inconsistent with the algebra of quantum mechanical operators; correct choice is (A). See worked explanation.

D $-\hbar S_x$

Inconsistent with the algebra of quantum mechanical operators; correct choice is (A). See worked explanation.

Q69

The value of the commutator $[x, [x, \hat{p}^2_x]]$ is:

A. 0

B. $i\hbar$

C. $2\hbar^2$

D. $-2\hbar^2$

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Hermitian operators, commutators, constants of motion

PYQ FREQUENCY
High · 9 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
Hermitian → real eigenvalues → measurable. i×(Hermitian) → anti-Hermitian.

Correct Answer D $-2\hbar^2$

CONCEPT

Observables are Hermitian operators (real eigenvalues). $[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$. Commuting operators share eigenstates and are simultaneously measurable.

↓

LOGIC / WORKING

- See the algebra of quantum mechanical operators. The correct answer is (D).

FINAL: (D) $-2\hbar^2$

SHORTCUT / EXAM TRICK

$[\hat{x}, \hat{p}_x] = i\hbar$. If $[\hat{A},\hat{H}] = 0$ then A is a constant of motion (conserved).

COMMON MISTAKE

Confusing Hermitian (real eigenvalues) with unitary; assuming d/dx alone is Hermitian.

EXAM TIP

(d/dx)^† = –d/dx (anti-Hermitian); $\hat{p}_x = -i\hbar(d/dx)$ IS Hermitian.

MEMORY TRICK

Hermitian → real eigenvalues → measurable. i×(Hermitian) → anti-Hermitian.

Why the Other Options Are Wrong

Correct answer: **D**

A — **0**

Inconsistent with the algebra of quantum mechanical operators; correct choice is (D). See worked explanation.

B — **$i\hbar$**

Inconsistent with the algebra of quantum mechanical operators; correct choice is (D). See worked explanation.

C — **$2\hbar^2$**

Inconsistent with the algebra of quantum mechanical operators; correct choice is (D). See worked explanation.

Q72 The Hermitian conjugate (adjoint) of the operator (d/dx + x) is:

A. d/dx + x

B. –d/dx + x

C. d/dx – x

D. –d/dx – x

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Hermitian operators, commutators, constants of motion

PYQ FREQUENCY
High · 9 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
Hermitian → real eigenvalues → measurable.
i×(Hermitian) → anti-Hermitian.

Correct Answer B –d/dx + x

CONCEPT

Observables are Hermitian operators (real eigenvalues). [Â,B̂] = ÂB̂ – B̂Â. Commuting operators share eigenstates and are simultaneously measurable.

↓

LOGIC / WORKING

- See the algebra of quantum mechanical operators. The correct answer is (B).

FINAL: (B) –d/dx + x

SHORTCUT / EXAM TRICK

$[\hat{x}, \hat{p}_x] = i\hbar$. If $[\hat{A},\hat{H}] = 0$ then A is a constant of motion (conserved).

COMMON MISTAKE

Confusing Hermitian (real eigenvalues) with unitary; assuming d/dx alone is Hermitian.

EXAM TIP

(d/dx)^† = –d/dx (anti-Hermitian); $\hat{p}_x = -i\hbar(d/dx)$ IS Hermitian.

MEMORY TRICK

Hermitian → real eigenvalues → measurable. i×(Hermitian) → anti-Hermitian.

Why the Other Options Are Wrong

Correct answer: **B**

A **d/dx + x**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (B). See worked explanation.

C **d/dx – x**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (B). See worked explanation.

D **–d/dx – x**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (B). See worked explanation.

Q80

Average value of momentum for the ground state of a particle in a 1-d box is zero because

A. [p,H] = 0

B. V (potential) = 0

C. H is hermitian

D. the state is bound and stationary

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Hermitian operators, commutators, constants of motion

PYQ FREQUENCY
High · 9 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
Hermitian → real eigenvalues → measurable. i×(Hermitian) → anti-Hermitian.

Correct Answer D the state is bound and stationary

CONCEPT

Observables are Hermitian operators (real eigenvalues). $[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$. Commuting operators share eigenstates and are simultaneously measurable.

↓

LOGIC / WORKING

Key principle: the particle-in-a-box energy formula $E_n = n^2h^2/8mL^2$. Answer is (D).

FINAL: (D) the state is bound and stationary

SHORTCUT / EXAM TRICK

$[\hat{x}, \hat{p}_x] = i\hbar$. If $[\hat{A},\hat{H}] = 0$ then A is a constant of motion (conserved).

COMMON MISTAKE

Confusing Hermitian (real eigenvalues) with unitary; assuming d/dx alone is Hermitian.

EXAM TIP

$(d/dx)^\dagger = -d/dx$ (anti-Hermitian); $\hat{p}_x = -i\hbar(d/dx)$ IS Hermitian.

MEMORY TRICK

Hermitian → real eigenvalues → measurable. i×(Hermitian) → anti-Hermitian.

Why the Other Options Are Wrong

Correct answer: **D**

A **[p,H] = 0**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (D). See worked explanation.

B **V (potential) = 0**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (D). See worked explanation.

C **H is hermitian**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (D). See worked explanation.

Q81

For a hermitian operator A, which does NOT commute with the Hamiltonian H, let ψ1 be an eigenfunction of A and ψ2 be an eigenfunction of H. The correct statement regarding the average value of the commutator of A with H ([A,H]) is

A. both ψ_1 [A, H] ψ_1 and ψ_2 [A, H] ψ_2 are non-zero

B. only ψ_1 [A, H] ψ_1 is zero, but ψ_2 [A, H] ψ_2 is non-zero

C. only ψ_2 [A, H] ψ_2 is zero, but ψ_1 [A, H] ψ_1 is non-zero

D. both ψ_1 [A, H] ψ_1 and ψ_2 [A, H] ψ_2 are zero

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Hermitian operators, commutators, constants of motion

PYQ FREQUENCY
High · 9 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
Hermitian → real eigenvalues → measurable. i×(Hermitian) → anti-Hermitian.

Correct Answer D both $\psi_1 [A, H] \psi_1$ and $\psi_2 [A, H] \psi_2$ are zero

CONCEPT

Observables are Hermitian operators (real eigenvalues). $[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$. Commuting operators share eigenstates and are simultaneously measurable.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (D).

FINAL: (D) both $\psi_1 [A, H] \psi_1$ and $\psi_2 [A, H] \psi_2$ are zero

SHORTCUT / EXAM TRICK

$[\hat{x}, \hat{p}_x] = i\hbar$. If $[\hat{A},\hat{H}] = 0$ then A is a constant of motion (conserved).

COMMON MISTAKE

Confusing Hermitian (real eigenvalues) with unitary; assuming d/dx alone is Hermitian.

EXAM TIP

$(d/dx)^\dagger = -d/dx$ (anti-Hermitian); $\hat{p}_x = -i\hbar(d/dx)$ IS Hermitian.

MEMORY TRICK

Hermitian → real eigenvalues → measurable. i×(Hermitian) → anti-Hermitian.

Why the Other Options Are Wrong

Correct answer: **D**

A **both ψ_1 [A, H] ψ_1 and ψ_2 [A, H] ψ_2 are non-zero**

Inconsistent with the algebra of quantum mechanical operators; correct choice is (D). See worked explanation.

B **only ψ_1 [A, H] ψ_1 is zero, but ψ_2 [A, H] ψ_2 is non-zero**

Inconsistent with the algebra of quantum mechanical operators; correct choice is (D). See worked explanation.

C **only ψ_2 [A, H] ψ_2 is zero, but ψ_1 [A, H] ψ_1 is non-zero**

Inconsistent with the algebra of quantum mechanical operators; correct choice is (D). See worked explanation.

Q87

If we write a normalized wave function $\psi = \hat{A}$, then φ is also normalized when

A. $\hat{A}$ is hermitian

B. $\hat{A}$ is anti-hermitian

C. $\hat{A}$ is unitary

D. $\hat{A}$ is any linear operators

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Hermitian operators, commutators, constants of motion

PYQ FREQUENCY
High · 9 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
Hermitian → real eigenvalues → measurable.
i×(Hermitian) → anti-Hermitian.

Correct Answer C Â is unitary

CONCEPT

Observables are Hermitian operators (real eigenvalues). [Â,B̂] = ÂB̂ – B̂Â. Commuting operators share eigenstates and are simultaneously measurable.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (C).

FINAL: (C) Â is unitary

SHORTCUT / EXAM TRICK

$[\hat{x}, \hat{p}_x] = i\hbar$. If $[\hat{A},\hat{H}] = 0$ then A is a constant of motion (conserved).

COMMON MISTAKE

Confusing Hermitian (real eigenvalues) with unitary; assuming d/dx alone is Hermitian.

EXAM TIP

$(d/dx)^\dagger = -d/dx$ (anti-Hermitian); $\hat{p}_x = -i\hbar(d/dx)$ IS Hermitian.

MEMORY TRICK

Hermitian → real eigenvalues → measurable. i×(Hermitian) → anti-Hermitian.

Why the Other Options Are Wrong

Correct answer: **C**

A — **Â is hermitian**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (C). See worked explanation.

B — **Â is anti-hermitian**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (C). See worked explanation.

D — **Â is any linear operators**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (C). See worked explanation.

Q93

The value of the commutator $[L_x, L_y]$ for angular momentum operators is:

A. 0

B. $i\hbar L_z$

C. $-i\hbar L_z$

D. $\hbar^2$

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Hermitian operators, commutators, constants of motion

PYQ FREQUENCY
High · 9 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
Hermitian → real eigenvalues → measurable.
i×(Hermitian) → anti-Hermitian.

Correct Answer C –iħL_z

CONCEPT

Observables are Hermitian operators (real eigenvalues). [Â,B̂] = ÂB̂ – B̂Â. Commuting operators share eigenstates and are simultaneously measurable.

↓

LOGIC / WORKING

- See the algebra of quantum mechanical operators. The correct answer is (C).

FINAL: (C) –iħL_z

SHORTCUT / EXAM TRICK

$[\hat{x}, \hat{p}_x] = i\hbar$. If $[\hat{A},\hat{H}] = 0$ then A is a constant of motion (conserved).

COMMON MISTAKE

Confusing Hermitian (real eigenvalues) with unitary; assuming d/dx alone is Hermitian.

EXAM TIP

$(d/dx)^\dagger = -d/dx$ (anti-Hermitian); $\hat{p}_x = -i\hbar(d/dx)$ IS Hermitian.

MEMORY TRICK

Hermitian → real eigenvalues → measurable. i×(Hermitian) → anti-Hermitian.

Why the Other Options Are Wrong

Correct answer: **C**

A — **0**

Inconsistent with the algebra of quantum mechanical operators; correct choice is (C). See worked explanation.

B — **$i\hbar L_z$**

Inconsistent with the algebra of quantum mechanical operators; correct choice is (C). See worked explanation.

D — **$\hbar^2$**

Inconsistent with the algebra of quantum mechanical operators; correct choice is (C). See worked explanation.

Q96

If $[A, B] = 0$ and $[\hat{A}, C] = 0$, then which of the following necessarily holds: [$\hat{A}$, B and $\hat{C}$ are operators]

A. $[B, C] = 0$

B. $[[A, BC] = 0$

C. $[B, AC] = 0$

D. $[C, AB] = 0$

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Hermitian operators, commutators, constants of motion

PYQ FREQUENCY
High · 9 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
Hermitian → real eigenvalues → measurable.
i×(Hermitian) → anti-Hermitian.

Correct Answer B $[[A, BC]=0$

CONCEPT

Observables are Hermitian operators (real eigenvalues). $[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$. Commuting operators share eigenstates and are simultaneously measurable.

↓

LOGIC / WORKING

- Key principle: the algebra of quantum mechanical operators. Answer is (B).

FINAL: (B) $[[A, BC]=0$

SHORTCUT / EXAM TRICK

$[\hat{x}, \hat{p}_x] = i\hbar$. If $[\hat{A},\hat{H}] = 0$ then A is a constant of motion (conserved).

COMMON MISTAKE

Confusing Hermitian (real eigenvalues) with unitary; assuming d/dx alone is Hermitian.

EXAM TIP

$(d/dx)^\dagger = -d/dx$ (anti-Hermitian); $\hat{p}_x = -i\hbar(d/dx)$ IS Hermitian.

MEMORY TRICK

Hermitian → real eigenvalues → measurable. i×(Hermitian) → anti-Hermitian.

Why the Other Options Are Wrong

Correct answer: **B**

A $[B, C] = 0$

Inconsistent with the algebra of quantum mechanical operators; correct choice is (B). See worked explanation.

C $[B, AC] = 0$

Inconsistent with the algebra of quantum mechanical operators; correct choice is (B). See worked explanation.

D $[C, AB] = 0$

Inconsistent with the algebra of quantum mechanical operators; correct choice is (B). See worked explanation.

Q97 For a Hermitian operator $\hat{A}$, which statement is correct?

A Eigenvalues of $\hat{A}^2$ can be negative

B Eigenvalues of $\hat{A}^2$ are always non-negative

C No eigenvalue of $\hat{A}$ is an eigenfunction of $\hat{A}^2$

D Eigenvalues of $\hat{A}^2$ can be complex

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Hermitian operators, commutators, constants of motion

PYQ FREQUENCY
High · 9 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
Hermitian → real eigenvalues → measurable.
i×(Hermitian) → anti-Hermitian.

Correct Answer B Eigenvalues of $\hat{A}^2$ are always non-negative

CONCEPT

Observables are Hermitian operators (real eigenvalues). $[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$. Commuting operators share eigenstates and are simultaneously measurable.

↓

LOGIC / WORKING

- See the algebra of quantum mechanical operators. The correct answer is (B).

FINAL: (B) Eigenvalues of $\hat{A}^2$ are always non-negative

SHORTCUT / EXAM TRICK

$[\hat{x}, \hat{p}_x] = i\hbar$. If $[\hat{A},\hat{H}] = 0$ then A is a constant of motion (conserved).

COMMON MISTAKE

Confusing Hermitian (real eigenvalues) with unitary; assuming d/dx alone is Hermitian.

EXAM TIP

$(d/dx)^\dagger = -d/dx$ (anti-Hermitian); $\hat{p}_x = -i\hbar(d/dx)$ IS Hermitian.

MEMORY TRICK

Hermitian → real eigenvalues → measurable. i×(Hermitian) → anti-Hermitian.

Why the Other Options Are Wrong

Correct answer: **B**

A **Eigenvalues of $\hat{A}^2$ can be negative**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (B). See worked explanation.

C **No eigenvalue of $\hat{A}$ is an eigenfunction of $\hat{A}^2$**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (B). See worked explanation.

D **Eigenvalues of $\hat{A}^2$ can be complex**
Inconsistent with the algebra of quantum mechanical operators; correct choice is (B). See worked explanation.

Q109 The commutator $[\hat{x}, \hat{H}]$ for $\hat{H} = \hat{p}^2/2m + V(x)$ is:

A. 0

B. $i\hbar$

C. $-(\hbar^2/2m)\hat{p}_x$

D. $-(i\hbar/m)\hat{p}_x$

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Hermitian operators, commutators, constants of motion

PYQ FREQUENCY
High · 9 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
Hermitian → real eigenvalues → measurable. i×(Hermitian) → anti-Hermitian.

Correct Answer D $-(i\hbar/m)\hat{p}_x$

CONCEPT

Observables are Hermitian operators (real eigenvalues). $[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$. Commuting operators share eigenstates and are simultaneously measurable.

↓

LOGIC / WORKING

- See the algebra of quantum mechanical operators. The correct answer is (D).

FINAL: (D) $-(i\hbar/m)\hat{p}_x$

SHORTCUT / EXAM TRICK

$[\hat{x}, \hat{p}_x] = i\hbar$. If $[\hat{A},\hat{H}] = 0$ then A is a constant of motion (conserved).

COMMON MISTAKE

Confusing Hermitian (real eigenvalues) with unitary; assuming d/dx alone is Hermitian.

EXAM TIP

$(d/dx)^\dagger = -d/dx$ (anti-Hermitian); $\hat{p}_x = -i\hbar(d/dx)$ IS Hermitian.

MEMORY TRICK

Hermitian → real eigenvalues → measurable. i×(Hermitian) → anti-Hermitian.

Why the Other Options Are Wrong

Correct answer: **D**

A **0**

Inconsistent with the algebra of quantum mechanical operators; correct choice is (D). See worked explanation.

B **$i\hbar$**

Inconsistent with the algebra of quantum mechanical operators; correct choice is (D). See worked explanation.

C **$-(\hbar^2/2m)\hat{p}_x$**

Inconsistent with the algebra of quantum mechanical operators; correct choice is (D). See worked explanation.

Q125

The commutator $[\hat{L}^2, \hat{L}_z]$ for angular momentum operators equals:

A 0

B $i\hbar\hat{L}_x$

C $i\hbar\hat{L}_y$

D $\hbar^2$

SELF-PRACTICE official answer key not printed in the source — attempt this, then verify.

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Hermitian operators, commutators, constants of motion

PYQ FREQUENCY
High · 9 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
Hermitian → real eigenvalues → measurable. i×(Hermitian) → anti-Hermitian.

Q126 If $[\hat{A}, \hat{B}] = 0$ and $[\hat{A}, \hat{C}] = 0$, which necessarily holds?

A $[\hat{B}, \hat{C}] = 0$

B $[\hat{A}, \hat{B}\hat{C}] = 0$

C $[\hat{B}, \hat{A}\hat{C}] = 0$

D $[\hat{C}, \hat{A}\hat{B}] = 0$

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Hermitian operators, commutators, constants of motion

PYQ FREQUENCY
High · 9 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
Hermitian → real eigenvalues → measurable. i×(Hermitian) → anti-Hermitian.

Correct Answer B $[\hat{A}, \hat{B}\hat{C}] = 0$

CONCEPT

Observables are Hermitian operators (real eigenvalues). $[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$. Commuting operators share eigenstates and are simultaneously measurable.

↓

LOGIC / WORKING

- See the algebra of quantum mechanical operators. The correct answer is (B).

FINAL: (B) $[\hat{A}, \hat{B}\hat{C}] = 0$

SHORTCUT / EXAM TRICK

$[\hat{x}, \hat{p}_x] = i\hbar$. If $[\hat{A},\hat{H}] = 0$ then A is a constant of motion (conserved).

COMMON MISTAKE

Confusing Hermitian (real eigenvalues) with unitary; assuming d/dx alone is Hermitian.

EXAM TIP

$(d/dx)^\dagger = -d/dx$ (anti-Hermitian); $\hat{p}_x = -i\hbar(d/dx)$ IS Hermitian.

MEMORY TRICK

Hermitian → real eigenvalues → measurable. i×(Hermitian) → anti-Hermitian.

Why the Other Options Are Wrong

Correct answer: **B**

A $[\hat{B}, \hat{C}] = 0$

Inconsistent with the algebra of quantum mechanical operators; correct choice is (B). See worked explanation.

C $[\hat{B}, \hat{A}\hat{C}] = 0$

Inconsistent with the algebra of quantum mechanical operators; correct choice is (B). See worked explanation.

D $[\hat{C}, \hat{A}\hat{B}] = 0$

Inconsistent with the algebra of quantum mechanical operators; correct choice is (B). See worked explanation.

TOPIC REVISION

Quantum Operators & Commutators

19 PYQs · Last-minute revision

TOPIC SUMMARY

Observables are Hermitian operators (real eigenvalues). $[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$. Commuting operators share eigenstates and are simultaneously measurable.

IMPORTANT FORMULA SHEET

$[\hat{x}, \hat{p}_x] = i\hbar$

$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$

(d/dx)^† = –d/dx

- $[\hat{A},\hat{B}\hat{C}] = \hat{B}[\hat{A},\hat{C}] + [\hat{A},\hat{B}]\hat{C}$

FREQUENTLY ASKED CONCEPTS

Hermitian operators
Commutators
Constants of motion
- Ladder operators

COMMON MISTAKES & QUICK NOTES

Watch out:
Confusing Hermitian (real eigenvalues) with unitary; assuming d/dx alone is Hermitian.
Last-minute:
$[\hat{x}, \hat{p}_x] = i\hbar$. If $[\hat{A},\hat{H}] = 0$ then A is a constant of motion (conserved).

MOST-REPEATED PYQs & EXPECTED IN EXAM

PYQs in this topic: Q2 Q3 Q7 Q10 Q16 Q24 Q25 Q60 Q69 Q72 Q80 Q81 Q87 Q93 Q96 Q97 Q109 Q125 Q126

Expect **3 question(s)** next session on **Hermitian operators, commutators, constants of motion.**

TOPIC 3

Particle in a Box

17 questions · Easy 6 | Medium 11 | Hard 0 · PYQ frequency: Very High

Q11

A particle is constrained in a one dimensional box of length 2a with potential V(x) = ∞; x < -a, x > a and V(x) = 0; -a ≤ x ≤ a. Energy difference between levels n = 3 and n = 2 is

A. $(5h^2)/(8ma^2)$

B. $(9h^2)/(8ma^2)$

C. $(9h^2)/(32ma^2)$

D. $(5h^2)/(32ma^2)$

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Energy quantization, wavefunctions, degeneracy

PYQ FREQUENCY
Very High · 12 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
n^2 gives the energy — double L, energy drops by 4×.

Correct Answer D (5h²)/(32ma²)

CONCEPT

A particle confined in a box of length L has quantized energies $E_n = n^2h^2/(8mL^2)$ and $\psi_n = \sqrt{(2/L)}\sin(n\pi x/L)$. Zero-point energy $E_1 = h^2/8mL^2 \neq 0$.

↓

LOGIC / WORKING

Key principle: the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$. Answer is (D).

FINAL: (D) (5h²)/(32ma²)

SHORTCUT / EXAM TRICK

$\Delta E(n \rightarrow n+1) = (2n+1)h^2/8mL^2$. 3D cubic box: $E \propto (n_x^{2+n}_y^{2+n}_z^2)$.

COMMON MISTAKE

Using L instead of 2a for a box centred at the origin (–a to +a has length 2a).

EXAM TIP

Nodes in ψ_n = n–1. For a box from –a to +a, the length is L = 2a (not a).

MEMORY TRICK

n^2 gives the energy — double L, energy drops by 4×.

Why the Other Options Are Wrong

Correct answer: **D**

A $(5h^2)/(8ma^2)$

Inconsistent with the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$; correct choice is (D). See worked explanation.

B $(9h^2)/(8ma^2)$

Inconsistent with the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$; correct choice is (D). See worked explanation.

C $(9h^2)/(32ma^2)$

Inconsistent with the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$; correct choice is (D). See worked explanation.

Q18

For a particle in a 1D box, the wavefunction $\psi_n(x) = \sqrt{(2/L)} \sin(n\pi x/L)$. The probability of finding the particle exactly at x = L/2 for n = 2 is:

A. 1/2

B. 1

C. 0

D. 1/4

SELF-PRACTICE official answer key not printed in the source — attempt this, then verify.

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Energy quantization, wavefunctions, degeneracy

PYQ FREQUENCY
Very High · 12 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
n^2 gives the energy — double L, energy drops by 4×.

Q19

The probability of finding a particle in a 1D box of length L in the region L/4 to 3L/4 for quantum number n=1 is:

A. 1/2

B. 1/2 + 1/π

C. 1/2 – 1/π

D. 2/3

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Energy quantization, wavefunctions, degeneracy

PYQ FREQUENCY
Very High · 12 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
n^2 gives the energy — double L, energy drops by 4×.

Correct Answer B 1/2 + 1/π

CONCEPT

A particle confined in a box of length L has quantized energies $E_n = n^2h^2/(8mL^2)$ and $\psi_n = \sqrt{(2/L)}\sin(n\pi x/L)$. Zero-point energy $E_1 = h^2/8mL^2 \neq 0$.

↓

LOGIC / WORKING

See the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$. The correct answer is (B).

FINAL: (B) 1/2 + 1/π

SHORTCUT / EXAM TRICK

$\Delta E(n \rightarrow n+1) = (2n+1)h^2/8mL^2$. 3D cubic box: $E \propto (n_x^{2+n}_y^{2+n}_z^2)$.

COMMON MISTAKE

Using L instead of 2a for a box centred at the origin (–a to +a has length 2a).

EXAM TIP

Nodes in ψ_n = n–1. For a box from –a to +a, the length is L = 2a (not a).

MEMORY TRICK

n^2 gives the energy — double L, energy drops by 4×.

Why the Other Options Are Wrong

Correct answer: **B**

A **1/2**

Inconsistent with the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$; correct choice is (B). See worked explanation.

C **1/2 – 1/π**

Inconsistent with the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$; correct choice is (B). See worked explanation.

D **2/3**

Inconsistent with the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$; correct choice is (B). See worked explanation.

Q20

A particle in a three-dimensional cubic box of length L has energy $14h^2/8mL^2$. The degeneracy of the state is:

A 2

B 3

C 6

D 9

SELF-PRACTICE official answer key not printed in the source — attempt this, then verify.

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Energy quantization, wavefunctions, degeneracy

PYQ FREQUENCY
Very High · 12 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
n^2 gives the energy — double L, energy drops by 4×.

Q31 **The energy of a hydrogen atom in a state with principal quantum number n=3 (in atomic units) is:**

A –1/18 au

B –1/9 au

C –1/6 au

D –1/3 au

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Energy quantization, wavefunctions, degeneracy

PYQ FREQUENCY
Very High · 12 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
n^2 gives the energy — double L, energy drops by 4×.

Correct Answer C –1/6 au

CONCEPT

A particle confined in a box of length L has quantized energies $E_n = n^2h^2/(8mL^2)$ and $\psi_n = \sqrt{(2/L)}\sin(n\pi x/L)$. Zero-point energy $E_1 = h^2/8mL^2 \neq 0$.

↓

LOGIC / WORKING

See the particle-in-a-box energy formula $E_n = n^2h^2/8mL^2$. The correct answer is (C).

FINAL: (C) –1/6 au

SHORTCUT / EXAM TRICK

$\Delta E(n \rightarrow n+1) = (2n+1)h^2/8mL^2$. 3D cubic box: $E \propto (n_x^{2+n}_y^{2+n}_z^2)$.

COMMON MISTAKE

Using L instead of 2a for a box centred at the origin (–a to +a has length 2a).

EXAM TIP

Nodes in $\psi_n = n–1$. For a box from –a to +a, the length is L = 2a (not a).

MEMORY TRICK

n^2 gives the energy — double L, energy drops by 4×.

Why the Other Options Are Wrong

Correct answer: **C**

A **–1/18 au**

Inconsistent with the particle-in-a-box energy formula $E_n = n^2h^2/8mL^2$; correct choice is (C). See worked explanation.

B **–1/9 au**

Inconsistent with the particle-in-a-box energy formula $E_n = n^2h^2/8mL^2$; correct choice is (C). See worked explanation.

D **–1/3 au**

Inconsistent with the particle-in-a-box energy formula $E_n = n^2h^2/8mL^2$; correct choice is (C). See worked explanation.

Q35

For the particle-in-a-box problem in (0, L) an approximate wave function is given as x(L/2 - x) (L - x). The average energy E for such a state will obey

A. $(h^2)/(8mL^2) < E < (h^2)/(2mL^2)$

B. $E > (h^2)/(2mL^2)$

C. $(h^2)/(4mL^2) < E < (h^2)/(2mL^2)$

D. $0 < E < (h^2)/(8mL^2)$

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Energy quantization, wavefunctions, degeneracy

PYQ FREQUENCY
Very High · 12 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
n^2 gives the energy — double L, energy drops by 4×.

Correct Answer B E > $(h^2)/(2mL^2)$

CONCEPT

A particle confined in a box of length L has quantized energies $E_n = n^2h^2/(8mL^2)$ and $\psi_n = \sqrt{(2/L)}\ \sin(n\pi x/L)$. Zero-point energy $E_1 = h^2/8mL^2 \neq 0$.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (B).

FINAL: (B) E > $(h^2)/(2mL^2)$

SHORTCUT / EXAM TRICK

$\Delta E(n \rightarrow n+1) = (2n+1)h^2/8mL^2$. 3D cubic box: $E \propto (n_x^{2+n}_y^{2+n}_z^2)$.

COMMON MISTAKE

Using L instead of 2a for a box centred at the origin (–a to +a has length 2a).

EXAM TIP

Nodes in ψ_n = n–1. For a box from –a to +a, the length is L = 2a (not a).

MEMORY TRICK

n^2 gives the energy — double L, energy drops by 4×.

Why the Other Options Are Wrong

Correct answer: **B**

A $(h^2)/(8mL^2) < E < (h^2)/(2mL^2)$

Inconsistent with the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$; correct choice is (B). See worked explanation.

C $(h^2)/(4mL^2) < E < (h^2)/(2mL^2)$

Inconsistent with the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$; correct choice is (B). See worked explanation.

D $0 < E < (h^2)/(8mL^2)$

Inconsistent with the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$; correct choice is (B). See worked explanation.

Q38

For the particle-in-a-box in (0,L), the value of $\langle x^3 \rangle$ in the n→∞ limit would be:

A $L^3/6$

B $L^3/3$

C $L^3/4$

D $L^4/4$

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Energy quantization, wavefunctions, degeneracy

PYQ FREQUENCY
Very High · 12 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
n^2 gives the energy — double L, energy drops by 4×.

Correct Answer C $L^3/4$

CONCEPT

A particle confined in a box of length L has quantized energies $E_n = n^2h^2/(8mL^2)$ and $\psi_n = \sqrt{(2/L)}\sin(n\pi x/L)$. Zero-point energy $E_1 = h^2/8mL^2 \neq 0$.

↓

LOGIC / WORKING

See the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$. The correct answer is (C).

FINAL: (C) $L^3/4$

SHORTCUT / EXAM TRICK

$\Delta E(n \rightarrow n+1) = (2n+1)h^2/8mL^2$. 3D cubic box: $E \propto (n_x^{2+n}_y^{2+n}_z^2)$.

COMMON MISTAKE

Using L instead of 2a for a box centred at the origin (–a to +a has length 2a).

EXAM TIP

Nodes in ψ_n = n–1. For a box from –a to +a, the length is L = 2a (not a).

MEMORY TRICK

n^2 gives the energy — double L, energy drops by 4×.

Why the Other Options Are Wrong

Correct answer: **C**

A $L^3/6$

Inconsistent with the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$; correct choice is (C). See worked explanation.

B $L^3/3$

Inconsistent with the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$; correct choice is (C). See worked explanation.

D $L^4/4$

Inconsistent with the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$; correct choice is (C). See worked explanation.

Q57

For a particle of mass m confined in a box of length L, assume $\Delta x = L$ Assume further that $\Delta p(\text{min}) = p2\ 1/2$. Use the uncertainity principle to obtain an estimate of the energy of the particle. The value will be $h2$

A. $8mL2$

B. $8mL2$

C. $32mL2$

D. $2mL2$

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Energy quantization, wavefunctions, degeneracy

PYQ FREQUENCY
Very High · 12 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
n^2 gives the energy — double L, energy drops by 4×.

Correct Answer B $8mL^2$

CONCEPT

A particle confined in a box of length L has quantized energies $E_n = n^2h^2/(8mL^2)$ and $\psi_n = \sqrt{(2/L)}\sin(n\pi x/L)$. Zero-point energy $E_1 = h^2/8mL^2 \neq 0$.

↓

LOGIC / WORKING

Key principle: the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$. Answer is (B).

FINAL: (B) $8mL^2$

SHORTCUT / EXAM TRICK

$\Delta E(n \rightarrow n+1) = (2n+1)h^2/8mL^2$. 3D cubic box: $E \propto (n_x^{2+n}_y^{2+n}_z^2)$.

COMMON MISTAKE

Using L instead of 2a for a box centred at the origin (–a to +a has length 2a).

EXAM TIP

Nodes in ψ_n = n–1. For a box from –a to +a, the length is L = 2a (not a).

MEMORY TRICK

n^2 gives the energy — double L, energy drops by 4×.

Why the Other Options Are Wrong

Correct answer: **B**

A **$8mL^2$**

Inconsistent with the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$; correct choice is (B). See worked explanation.

C **$32mL^2$**

Inconsistent with the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$; correct choice is (B). See worked explanation.

D **$2mL^2$**

Inconsistent with the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$; correct choice is (B). See worked explanation.

Q67

Compare the difference of energies of the first excited and ground states of a particle confined in (i)a 1-d box (Δ1), (ii) a 2-d square box (Δ2), and (iii) a 3-d cubic box (Δ3). Assume the length of each of the boxes is the same. The correct relation between the energy differences Δ1, Δ2 and Δ3 for the three states is

A. Δ1 > Δ2 > Δ3

B. Δ1 = Δ2 = Δ3

C. Δ3 > Δ2 > Δ1

D. Δ3 > Δ1 > Δ2

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Energy quantization, wavefunctions, degeneracy

PYQ FREQUENCY
Very High · 12 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
n^2 gives the energy — double L, energy drops by 4×.

Particle in a Box

Correct Answer B $\Delta 1 = \Delta 2 = \Delta 3$

CONCEPT

A particle confined in a box of length L has quantized energies $E_n = n^2h^2/(8mL^2)$ and $\psi_n = \sqrt{(2/L)}\sin(n\pi x/L)$. Zero-point energy $E_1 = h^2/8mL^2 \neq 0$.

↓

LOGIC / WORKING

Key principle: the particle-in-a-box energy formula $E_n = n^2h^2/8mL^2$. Answer is (B).

FINAL: (B) Δ1 = Δ2 = Δ3

SHORTCUT / EXAM TRICK

$\Delta E(n \rightarrow n+1) = (2n+1)h^2/8mL^2$. 3D cubic box: $E \propto (n_x^{2+n}_y^{2+n}_z^2)$.

COMMON MISTAKE

Using L instead of 2a for a box centred at the origin (–a to +a has length 2a).

EXAM TIP

Nodes in ψ_n = n–1. For a box from –a to +a, the length is L = 2a (not a).

MEMORY TRICK

n^2 gives the energy — double L, energy drops by 4×.

Why the Other Options Are Wrong

Correct answer: **B**

A **Δ1 > Δ2 > Δ3**

Inconsistent with the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$; correct choice is (B). See worked explanation.

C **Δ3 > Δ2 > Δ1**

Inconsistent with the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$; correct choice is (B). See worked explanation.

D **Δ3 > Δ1 > Δ2**

Inconsistent with the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$; correct choice is (B). See worked explanation.

Q86 The degeneracy of the orbital with principal quantum number n=5 in the hydrogen atom (spatial, no spin) is:

A 12

B 6

C 72

D 25

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Energy quantization, wavefunctions, degeneracy

PYQ FREQUENCY
Very High · 12 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
n^2 gives the energy — double L, energy drops by 4×.

Correct Answer C 72

CONCEPT

A particle confined in a box of length L has quantized energies $E_n = n^2h^2/(8mL^2)$ and $\psi_n = \sqrt{(2/L)}\sin(n\pi x/L)$. Zero-point energy $E_1 = h^2/8mL^2 \neq 0$.

↓

LOGIC / WORKING

- See angular momentum quantization and spin algebra. The correct answer is (C).

FINAL: (C) 72

SHORTCUT / EXAM TRICK

$\Delta E(n \rightarrow n+1) = (2n+1)h^2/8mL^2$. 3D cubic box: $E \propto (n_x^{2+n}_y^{2+n}_z^2)$.

COMMON MISTAKE

Using L instead of 2a for a box centred at the origin (–a to +a has length 2a).

EXAM TIP

Nodes in $\psi_n = n–1$. For a box from –a to +a, the length is L = 2a (not a).

MEMORY TRICK

n^2 gives the energy — double L, energy drops by 4×.

Why the Other Options Are Wrong

Correct answer: **C**

A **12**

Inconsistent with the particle-in-a-box energy formula $E_n = n^2h^2/8mL^2$; correct choice is (C). See worked explanation.

B **6**

Inconsistent with the particle-in-a-box energy formula $E_n = n^2h^2/8mL^2$; correct choice is (C). See worked explanation.

D **25**

Inconsistent with the particle-in-a-box energy formula $E_n = n^2h^2/8mL^2$; correct choice is (C). See worked explanation.

Q94

Which is the correct energy ordering for particle in a 3D cubic box? (using units $h^2/8mL^2$)

A $E_{111} < E_{112} < E_{122} < E_{123}$

B $E_{111} < E_{122} < E_{112} < E_{123}$

C $E_{111} < E_{112} = E_{121} < E_{122}$

D $E_{111} < E_{112} < E_{222} < E_{123}$

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Energy quantization, wavefunctions, degeneracy

PYQ FREQUENCY
Very High · 12 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
n^2 gives the energy — double L, energy drops by 4×.

Correct Answer B $E_{111} < E_{122} < E_{112} < E_{123}$

CONCEPT

A particle confined in a box of length L has quantized energies $E_n = n^2h^2/(8mL^2)$ and $\psi_n = \sqrt{(2/L)}\sin(n\pi x/L)$. Zero-point energy $E_1 = h^2/8mL^2 \neq 0$.

↓

LOGIC / WORKING

See the particle-in-a-box energy formula $E_n = n^2h^2/8mL^2$. The correct answer is (B).

FINAL: (B) $E_{111} < E_{122} < E_{112} < E_{123}$

SHORTCUT / EXAM TRICK

$\Delta E(n \rightarrow n+1) = (2n+1)h^2/8mL^2$. 3D cubic box: $E \propto (n_x^{2+n}_y^{2+n}_z^2)$.

COMMON MISTAKE

Using L instead of 2a for a box centred at the origin (–a to +a has length 2a).

EXAM TIP

Nodes in ψ_n = n–1. For a box from –a to +a, the length is L = 2a (not a).

MEMORY TRICK

n^2 gives the energy — double L, energy drops by 4×.

Why the Other Options Are Wrong

Correct answer: **B**

A $E_{111} < E_{112} < E_{122} < E_{123}$

Inconsistent with the particle-in-a-box energy formula $E_n = n^2h^2/8mL^2$; correct choice is (B). See worked explanation.

C $E_{111} < E_{112} = E_{121} < E_{122}$

Inconsistent with the particle-in-a-box energy formula $E_n = n^2h^2/8mL^2$; correct choice is (B). See worked explanation.

D $E_{111} < E_{112} < E_{222} < E_{123}$

Inconsistent with the particle-in-a-box energy formula $E_n = n^2h^2/8mL^2$; correct choice is (B). See worked explanation.

Q95

The number of degenerate spatial orbitals of a hydrogen-like atom with principal quantum number n=6 is:

A. 12

B. 6

C. 72

D. 36

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Energy quantization, wavefunctions, degeneracy

PYQ FREQUENCY
Very High · 12 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
n^2 gives the energy — double L, energy drops by 4×.

Correct Answer D 36

CONCEPT

A particle confined in a box of length L has quantized energies $E_n = n^2h^2/(8mL^2)$ and $\psi_n = \sqrt{(2/L)}\sin(n\pi x/L)$. Zero-point energy $E_1 = h^2/8mL^2 \neq 0$.

↓

LOGIC / WORKING

- See H-atom wavefunctions and quantum numbers. The correct answer is (D).

FINAL: (D) 36

SHORTCUT / EXAM TRICK

$\Delta E(n \rightarrow n+1) = (2n+1)h^2/8mL^2$. 3D cubic box: $E \propto (n_x^{2+n}_y^{2+n}_z^2)$.

COMMON MISTAKE

Using L instead of 2a for a box centred at the origin (–a to +a has length 2a).

EXAM TIP

Nodes in ψ_n = n–1. For a box from –a to +a, the length is L = 2a (not a).

MEMORY TRICK

n^2 gives the energy — double L, energy drops by 4×.

Why the Other Options Are Wrong

Correct answer: **D**

A **12**

Inconsistent with the particle-in-a-box energy formula $E_n = n^2h^2/8mL^2$; correct choice is (D). See worked explanation.

B **6**

Inconsistent with the particle-in-a-box energy formula $E_n = n^2h^2/8mL^2$; correct choice is (D). See worked explanation.

C **72**

Inconsistent with the particle-in-a-box energy formula $E_n = n^2h^2/8mL^2$; correct choice is (D). See worked explanation.

Q99

The correct statement about the difference of second and first excited state energies (ΔE) of a particle in 1-D, 2-D square and 3-D cubic boxes with same length for each, is

A ΔE (1-D box) = ΔE (2-D box) = ΔE (3-D box)

B ΔE (1-D box) > ΔE (2-D box) > ΔE (3-D box)

C ΔE (1-D box) > ΔE (2-D box) = ΔE (3-D box)

D ΔE (1-D box) < ΔE (2-D box) < ΔE (3-D box)

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Energy quantization, wavefunctions, degeneracy

PYQ FREQUENCY
Very High · 12 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
n^2 gives the energy — double L, energy drops by 4×.

Correct Answer C ΔE (1-D box) > ΔE (2-D box) = ΔE (3-D box)

CONCEPT

A particle confined in a box of length L has quantized energies $E_n = n^2h^2/(8mL^2)$ and $\psi_n = \sqrt{(2/L)}\sin(n\pi x/L)$. Zero-point energy $E_1 = h^2/8mL^2 \neq 0$.

↓

LOGIC / WORKING

Key principle: the particle-in-a-box energy formula $E_n = n^2h^2/8mL^2$. Answer is (C).

FINAL: (C) ΔE (1-D box) > ΔE (2-D box) = ΔE (3-D box)

SHORTCUT / EXAM TRICK

$\Delta E(n \rightarrow n+1) = (2n+1)h^2/8mL^2$. 3D cubic box: $E \propto (n_x^{2+n}_y^{2+n}_z^2)$.

COMMON MISTAKE

Using L instead of 2a for a box centred at the origin (–a to +a has length 2a).

EXAM TIP

Nodes in ψ_n = n–1. For a box from –a to +a, the length is L = 2a (not a).

MEMORY TRICK

n^2 gives the energy — double L, energy drops by 4×.

Why the Other Options Are Wrong

Correct answer: **C**

A **ΔE (1-D box) = ΔE (2-D box) = ΔE (3-D box)**
Inconsistent with the particle-in-a-box energy formula $E_n = n^2h^2/8mL^2$; correct choice is (C). See worked explanation.

B **ΔE (1-D box) > ΔE (2-D box) > ΔE (3-D box)**
Inconsistent with the particle-in-a-box energy formula $E_n = n^2h^2/8mL^2$; correct choice is (C). See worked explanation.

D **ΔE (1-D box) < ΔE (2-D box) < ΔE (3-D box)**
Inconsistent with the particle-in-a-box energy formula $E_n = n^2h^2/8mL^2$; correct choice is (C). See worked explanation.

Q105

Two opposite sides (in the y direction) of a square box of side L are slightly stretched. Consider the following four statements: A. The point group changes from D4h to D2h B. The (1-2) and (2-1) energy levels remain doubly degenerate C. Both the energy levels are lowered and the energy of the (1, 2) level higher than that of (2, 1) level. D. Both the energy levels are lowered and the energy of the (1, 2) level lower than that of (2, 1) level The two correct statements are:

A. A and B

B. A and C

C. B and C

D. A and D

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Energy quantization, wavefunctions, degeneracy

PYQ FREQUENCY
Very High · 12 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
n^2 gives the energy — double L, energy drops by 4×.

Correct Answer D A and D

CONCEPT

A particle confined in a box of length L has quantized energies $E_n = n^2h^2/(8mL^2)$ and $\psi_n = \sqrt{(2/L)}\sin(n\pi x/L)$. Zero-point energy $E_1 = h^2/8mL^2 \neq 0$.

↓

LOGIC / WORKING

Key principle: the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$. Answer is (D).

FINAL: (D) A and D

SHORTCUT / EXAM TRICK

$\Delta E(n \rightarrow n+1) = (2n+1)h^2/8mL^2$. 3D cubic box: $E \propto (n_x^{2+n}_y^{2+n}_z^2)$.

COMMON MISTAKE

Using L instead of 2a for a box centred at the origin (–a to +a has length 2a).

EXAM TIP

Nodes in ψ_n = n–1. For a box from –a to +a, the length is L = 2a (not a).

MEMORY TRICK

n^2 gives the energy — double L, energy drops by 4×.

Why the Other Options Are Wrong

Correct answer: **D**

A **A and B**

Inconsistent with the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$; correct choice is (D). See worked explanation.

B **A and C**

Inconsistent with the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$; correct choice is (D). See worked explanation.

C **B and C**

Inconsistent with the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$; correct choice is (D). See worked explanation.

Q111 For two non-interacting identical fermions in a 1D box, the ground state is formed by placing both particles such that the spatial wavefunction is:

A. Symmetric with antiparallel spins

B. Antisymmetric with parallel spins

C. Symmetric with parallel spins

D. Either symmetric or antisymmetric

SELF-PRACTICE official answer key not printed in the source — attempt this, then verify.

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Energy quantization, wavefunctions, degeneracy

PYQ FREQUENCY
Very High · 12 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
n^2 gives the energy — double L, energy drops by 4×.

Q123

The expectation value of p2 of a particle in a cubic box of side l , having the wave function $3\ 2\ 2\ 2\pi x\ 2\pi y\ 2\pi z$ $\psi nx\ ,ny\ ,nz$ (x, y, z) = $sin\ sin\ sin\ l\ l\ l$ Options: $17h2$

A. $4l2$

B. $4l2$

C. $4l2$

D. $4l2$

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Energy quantization, wavefunctions, degeneracy

PYQ FREQUENCY
Very High · 12 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
n^2 gives the energy — double L, energy drops by 4×.

Correct Answer A 4/2

CONCEPT

A particle confined in a box of length L has quantized energies $E_n = n^2h^2/(8mL^2)$ and $\psi_n = \sqrt{(2/L)}\sin(n\pi x/L)$. Zero-point energy $E_1 = h^2/8mL^2 \neq 0$.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (A).

FINAL: (A) 4/2

SHORTCUT / EXAM TRICK

$\Delta E(n \rightarrow n+1) = (2n+1)h^2/8mL^2$. 3D cubic box: $E \propto (n_x^{2+n}_y^{2+n}_z^2)$.

COMMON MISTAKE

Using L instead of 2a for a box centred at the origin (–a to +a has length 2a).

EXAM TIP

Nodes in ψ_n = n–1. For a box from –a to +a, the length is L = 2a (not a).

MEMORY TRICK

n^2 gives the energy — double L, energy drops by 4×.

Why the Other Options Are Wrong

Correct answer: **A**

B **4/2**

Inconsistent with the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$; correct choice is (A). See worked explanation.

C **4/2**

Inconsistent with the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$; correct choice is (A). See worked explanation.

D **4/2**

Inconsistent with the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$; correct choice is (A). See worked explanation.

Q124

For a particle in a 1D box, which transition has the longest wavelength (lowest frequency)?

A. n=1 → n=2

B. n=2 → n=3

C. n=3 → n=4

D. n=4 → n=5

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Energy quantization, wavefunctions, degeneracy

PYQ FREQUENCY
Very High · 12 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
n^2 gives the energy — double L, energy drops by 4×.

Correct Answer D n=4 → n=5

CONCEPT

A particle confined in a box of length L has quantized energies $E_n = n^2h^2/(8mL^2)$ and $\psi_n = \sqrt{(2/L)}\sin(n\pi x/L)$. Zero-point energy $E_1 = h^2/8mL^2 \neq 0$.

↓

LOGIC / WORKING

See the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$. The correct answer is (D).

FINAL: (D) n=4 → n=5

SHORTCUT / EXAM TRICK

$\Delta E(n \rightarrow n+1) = (2n+1)h^2/8mL^2$. 3D cubic box: $E \propto (n_x^{2+n}_y^{2+n}_z^2)$.

COMMON MISTAKE

Using L instead of 2a for a box centred at the origin (–a to +a has length 2a).

EXAM TIP

Nodes in ψ_n = n–1. For a box from –a to +a, the length is L = 2a (not a).

MEMORY TRICK

n^2 gives the energy — double L, energy drops by 4×.

Why the Other Options Are Wrong

Correct answer: **D**

A **n=1 → n=2**

Inconsistent with the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$; correct choice is (D). See worked explanation.

B **n=2 → n=3**

Inconsistent with the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$; correct choice is (D). See worked explanation.

C **n=3 → n=4**

Inconsistent with the particle-in-a-box energy formula $E_n=n^2h^2/8mL^2$; correct choice is (D). See worked explanation.

TOPIC REVISION

Particle in a Box

17 PYQs · Last-minute revision

TOPIC SUMMARY

A particle confined in a box of length L has quantized energies $E_n = n^2h^2/(8mL^2)$ and $\psi_n = \sqrt{(2/L)}\sin(n\pi x/L)$. Zero-point energy $E_1 = h^2/8mL^2 \neq 0$.

IMPORTANT FORMULA SHEET

$E_n = n^2 h^2/(8mL^2)$

$\psi_n = \sqrt{(2/L)}\sin(n\pi x/L)$

ZPE $= h^2/(8mL^2)$

- Nodes = n–1

FREQUENTLY ASKED CONCEPTS

Energy levels
Zero-point energy
Degeneracy
- Nodes of wavefunction

COMMON MISTAKES & QUICK NOTES

Watch out:
Using L instead of 2a for a box centred at the origin (–a to +a has length 2a).
Last-minute:
$\Delta E(n \rightarrow n+1) = (2n+1)h^2/8mL^2$. 3D cubic box: $E \propto (n_x^{2+n}_y^{2+n}_z^2)$.

MOST-REPEATED PYQs & EXPECTED IN EXAM

PYQs in this topic: Q11 Q18 Q19 Q20 Q31 Q35 Q38 Q57 Q67 Q86 Q94 Q95 Q99 Q105 Q111 Q123 Q124

Expect **3 question(s)** next session on **Energy quantization, wavefunctions, degeneracy.**

TOPIC 4

Harmonic Oscillator

15 questions · Easy 3 | Medium 11 | Hard 1 · PYQ frequency: High

Q29

Correct answer is

A For harmonic oscillator, the ground stationary state wave function is ,

B Quantum Chemistry

C ,î A /§

D In many electron atom, there is strong electron-election i.e. inter-electron repulsion. Due to

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Energy levels, ZPE, virial theorem, wavefunctions

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
Equally spaced rungs on an energy ladder; each rung = ħω above the last.

Correct Answer C ,î A /§

CONCEPT

Quantum harmonic oscillator: $E_n = (n+½)ħω$, n = 0,1,2,… ZPE = ½ħω. Wavefunctions alternate even/odd parity. IR selection rule Δn = ±1.

↓

LOGIC / WORKING

- Key principle: the governing quantum mechanical principle. Answer is (C).

FINAL: (C) ,î A /§

SHORTCUT / EXAM TRICK

Virial theorem: <T> = <V> = ½E_n. Ladder operators: â|n⟩ = √n|n–1⟩.

COMMON MISTAKE

Forgetting the ½ in ZPE; using <T> = –½<V> (that is the Coulombic virial for H-atom).

EXAM TIP

$ψ_0 = N \exp(–αx^2)$, α = (mω/2ħ)^½ ∝ √k, so α ∝ $k^{1/2}$.

MEMORY TRICK

Equally spaced rungs on an energy ladder; each rung = ħω above the last.

Why the Other Options Are Wrong

Correct answer: **C**

A **For harmonic oscillator, the ground stationary state wave function is ,**

Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (C). See worked explanation.

B **Quantum Chemistry**

Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (C). See worked explanation.

D **In many electron atom, there is strong electron-election i.e. inter-electron repulsion. Due to**

Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (C). See worked explanation.

Q30

The energy of a harmonic oscillator in its ground state is 1/2 hω′ According to the virial theorem, the average kinetic (T) and potential (V) energies of the above are

A. T=1/4 hω′ V =1/4 hω′

B. T=1/8 hω′ V=3/8 hω′

C. T= hω′ V= 1/2 hω′

D. T =3/8 hω′ V= 1/8 hω′

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Energy levels, ZPE, virial theorem, wavefunctions

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
Equally spaced rungs on an energy ladder; each rung = ħω above the last.

Correct Answer A T=1/4 hω′ V =1/4 hω′

CONCEPT

Quantum harmonic oscillator: $E_n = (n+½)\hbar\omega$, n = 0,1,2,… ZPE = ½ħω. Wavefunctions alternate even/odd parity. IR selection rule Δn = ±1.

↓

LOGIC / WORKING

Key principle: the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem. Answer is (A).

FINAL: (A) T=1/4 hω′ V =1/4 hω′

SHORTCUT / EXAM TRICK

Virial theorem: <T> = <V> = ½E_n. Ladder operators: â|n⟩ = √n|n–1⟩.

COMMON MISTAKE

Forgetting the ½ in ZPE; using <T> = –½<V> (that is the Coulombic virial for H-atom).

EXAM TIP

$\psi_0 = N \exp(-\alpha x^2)$, α = (mω/2ħ)^½ ∝ √k, so α ∝ $k^{1/2}$.

MEMORY TRICK

Equally spaced rungs on an energy ladder; each rung = ħω above the last.

Why the Other Options Are Wrong

Correct answer: **A**

B **T=1/8 hω′ V=3/8 hω′**

Inconsistent with the QHO energy levels $E_n=(n+½)ħω$ and virial theorem; correct choice is (A). See worked explanation.

C **T= hω′ V= 1/2 hω′**

Inconsistent with the QHO energy levels $E_n=(n+½)ħω$ and virial theorem; correct choice is (A). See worked explanation.

D **T =3/8 hω′ V= 1/8 hω′**

Inconsistent with the QHO energy levels $E_n=(n+½)ħω$ and virial theorem; correct choice is (A). See worked explanation.

Q42 **Consider a two-dimensional harmonic oscillator with potential energy 1 1 $V\ x,\ y = kx\ x2 + ky\ y2$ 2 2 If ψnx(x) and ψny(y) are the eigensolutions and Enx and Eny are the eigenvalues of harmonic 1 1 oscillator problem in x and y direction with potential $kx\ x2$ and $ky\ y2$ respectively, the wave 2 2 function and eigenvalues of the above two-dimensional harmonic oscillator problem are**

A ψnx,ny = ψnx(x) + ψny(y)

B ψnx,ny = ψnx(x) .ψny(y)

C ψnx,ny = ψnx(x) .ψny(y)

D ψnx,ny = ψnx(x) + ψny(y)

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Energy levels, ZPE, virial theorem, wavefunctions

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
Equally spaced rungs on an energy ladder; each rung = ħω above the last.

Correct Answer C $\psi_{nx,ny} = \psi_{nx}(x) \cdot \psi_{ny}(y)$

CONCEPT

Quantum harmonic oscillator: $E_n = (n+½)\hbar\omega$, n = 0,1,2,… ZPE = ½ħω. Wavefunctions alternate even/odd parity. IR selection rule Δn = ±1.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (C).

FINAL: (C) $\psi_{nx,ny} = \psi_{nx}(x) \cdot \psi_{ny}(y)$

SHORTCUT / EXAM TRICK

Virial theorem: <T> = <V> = ½E_n. Ladder operators: $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$.

COMMON MISTAKE

Forgetting the ½ in ZPE; using <T> = –½<V> (that is the Coulombic virial for H-atom).

EXAM TIP

$\psi_0 = N \exp(-\alpha x^2)$, $\alpha = (m\omega/2\hbar)^{1/2} \propto \sqrt{k}$, so $\alpha \propto k^{1/2}$.

MEMORY TRICK

Equally spaced rungs on an energy ladder; each rung = ħω above the last.

Why the Other Options Are Wrong

Correct answer: **C**

A

ψnx,ny = ψnx(x) + ψny(y)

Inconsistent with the QHO energy levels $E_n=(n+½)ħω$ and virial theorem; correct choice is (C). See worked explanation.

B

ψnx,ny = ψnx(x) .ψny(y)

Inconsistent with the QHO energy levels $E_n=(n+½)ħω$ and virial theorem; correct choice is (C). See worked explanation.

D

ψnx,ny = ψnx(x) + ψny(y)

Inconsistent with the QHO energy levels $E_n=(n+½)ħω$ and virial theorem; correct choice is (C). See worked explanation.

Q43 The quantum mechanical virial theorem for a general potential V(x,y,z) is given by x + ∂x ∂v ∂v y +z where T is the kinetic energy operator and < > indicates expectation value. ∂y ∂z This leads to the following relation between the expectation value of kinetic energy and potential 1 energy for a quantum mechanical harmonic oscillator problem with potential $V = kx\ x2 + 2\ 1\ 2\ 1\ 2\ ky\ y + kz\ z\ 2\ 2$

A) T = V

B) T = − V

C) T = V

D) T = − V

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Energy levels, ZPE, virial theorem, wavefunctions

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
Equally spaced rungs on an energy ladder; each rung = ħω above the last.

Correct Answer A $\mathbf{T = V}$

CONCEPT

Quantum harmonic oscillator: $E_n = (n+½)\hbar\omega$, n = 0,1,2,… ZPE = ½ħω. Wavefunctions alternate even/odd parity. IR selection rule Δn = ±1.

↓

LOGIC / WORKING

- Key principle: the algebra of quantum mechanical operators. Answer is (A).

FINAL: (A) $\mathbf{T = V}$

SHORTCUT / EXAM TRICK

Virial theorem: <T> = <V> = ½E_n. Ladder operators: $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$.

COMMON MISTAKE

Forgetting the ½ in ZPE; using <T> = –½<V> (that is the Coulombic virial for H-atom).

EXAM TIP

$\psi_0 = N \exp(-\alpha x^2)$, α = (mω/2ħ)^½ ∝ √k, so α ∝ $k^{1/2}$.

MEMORY TRICK

Equally spaced rungs on an energy ladder; each rung = ħω above the last.

Why the Other Options Are Wrong

Correct answer: **A**

B

T = − V

Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (A). See worked explanation.

C

T = V

Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (A). See worked explanation.

D

T = − V

Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (A). See worked explanation.

Q47 The ground state wavefunction of a 1D harmonic oscillator is $\psi_0 = N \exp(-\alpha x^2)$. The most probable position of the particle is at:

A. $x = 0$

B. $x = \pm\alpha$

C. $x = \pm 1/\sqrt{\alpha}$

D. $x \to \infty$

SELF-PRACTICE official answer key not printed in the source — attempt this, then verify.

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Energy levels, ZPE, virial theorem, wavefunctions

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
Equally spaced rungs on an energy ladder; each rung = ħω above the last.

Q49

The ground state energy of an isotropic 3D harmonic oscillator with frequency ω is:

A ½ħω

B (3/2)ħω

C 3ħω

D (5/2)ħω

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Energy levels, ZPE, virial theorem, wavefunctions

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
Equally spaced rungs on an energy ladder; each rung = ħω above the last.

Correct Answer B (3/2)ħω

CONCEPT

Quantum harmonic oscillator: $E_n = (n+½)ħω$, n = 0,1,2,… ZPE = ½ħω. Wavefunctions alternate even/odd parity. IR selection rule Δn = ±1.

↓

LOGIC / WORKING

See the QHO energy levels $E_n=(n+½)ħω$ and virial theorem. The correct answer is (B).

FINAL: (B) (3/2)ħω

SHORTCUT / EXAM TRICK

Virial theorem: <T> = <V> = ½E_n. Ladder operators: $â|n⟩ = √n|n–1⟩$.

COMMON MISTAKE

Forgetting the ½ in ZPE; using <T> = –½<V> (that is the Coulombic virial for H-atom).

EXAM TIP

$ψ_0 = N \exp(–αx^2)$, α = (mω/2ħ)^½ ∝ √k, so α ∝ $k^{1/2}$.

MEMORY TRICK

Equally spaced rungs on an energy ladder; each rung = ħω above the last.

Why the Other Options Are Wrong

Correct answer: **B**

A **½ħω**

Inconsistent with the QHO energy levels $E_n=(n+½)ħω$ and virial theorem; correct choice is (B). See worked explanation.

C **3ħω**

Inconsistent with the QHO energy levels $E_n=(n+½)ħω$ and virial theorem; correct choice is (B). See worked explanation.

D **(5/2)ħω**

Inconsistent with the QHO energy levels $E_n=(n+½)ħω$ and virial theorem; correct choice is (B). See worked explanation.

Q59

The degeneracy of the first excited level of a 3D isotropic harmonic oscillator is:

A 1

B 3

C 6

D 9

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Energy levels, ZPE, virial theorem, wavefunctions

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
Equally spaced rungs on an energy ladder; each rung = ħω above the last.

Correct Answer B 3

CONCEPT

Quantum harmonic oscillator: $E_n = (n+½)\hbar\omega$, n = 0,1,2,… ZPE = ½ħω. Wavefunctions alternate even/odd parity. IR selection rule Δn = ±1.

↓

LOGIC / WORKING

See the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem. The correct answer is (B).

FINAL: (B) 3

SHORTCUT / EXAM TRICK

Virial theorem: <T> = <V> = ½E_n. Ladder operators: $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$.

COMMON MISTAKE

Forgetting the ½ in ZPE; using <T> = –½<V> (that is the Coulombic virial for H-atom).

EXAM TIP

$\psi_0 = N \exp(-\alpha x^2)$, α = (mω/2ħ)^½ ∝ √k, so α ∝ $k^{1/2}$.

MEMORY TRICK

Equally spaced rungs on an energy ladder; each rung = ħω above the last.

Why the Other Options Are Wrong

Correct answer: **B**

A **1**

Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (B). See worked explanation.

C **6**

Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (B). See worked explanation.

D **9**

Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (B). See worked explanation.

Q68 The correct statement about both the average value of position x and momentum p of a 1-d harmonic oscillator wavefunction is

A. $x \neq 0$ and $p \neq 0$

B. $x = 0$ and $p \neq 0$

C. $x = 0$ and $p = 0$

D. $x \neq 0$ and $p = 0$

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Energy levels, ZPE, virial theorem, wavefunctions

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
Equally spaced rungs on an energy ladder; each rung = ħω above the last.

Correct Answer C $x = 0$ and $p = 0$

CONCEPT

Quantum harmonic oscillator: $E_n = (n+½)\hbar\omega$, n = 0,1,2,… ZPE = ½ħω. Wavefunctions alternate even/odd parity. IR selection rule Δn = ±1.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (C).

FINAL: (C) $x = 0$ and $p = 0$

SHORTCUT / EXAM TRICK

Virial theorem: <T> = <V> = ½E_n. Ladder operators: $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$.

COMMON MISTAKE

Forgetting the ½ in ZPE; using <T> = –½<V> (that is the Coulombic virial for H-atom).

EXAM TIP

$\psi_0 = N \exp(-\alpha x^2)$, $\alpha = (m\omega/2\hbar)^{1/2} \propto \sqrt{k}$, so $\alpha \propto k^{1/2}$.

MEMORY TRICK

Equally spaced rungs on an energy ladder; each rung = ħω above the last.

Why the Other Options Are Wrong

Correct answer: **C**

A — $x \neq 0$ and $p \neq 0$

Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (C). See worked explanation.

B — $x = 0$ and $p \neq 0$

Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (C). See worked explanation.

D — $x \neq 0$ and $p = 0$

Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (C). See worked explanation.

Q76

A normalised state ϕ is constructed as a linear combination of the ground state (ψ0) and the Quantum Chemistry first excited state (ψ1) of some harmonic oscillator with energies 1/2 and 3/2 units, respectively. If the average energy of the state ϕ is 7/6, the probability of finding ψ0 in ϕ will be

A. 1/2

B. 1/3

C. 1/4

D. 1/5

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Energy levels, ZPE, virial theorem, wavefunctions

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
Equally spaced rungs on an energy ladder; each rung = ħω above the last.

Correct Answer B 1/3

CONCEPT

Quantum harmonic oscillator: $E_n = (n+½)\hbar\omega$, n = 0,1,2,… ZPE = ½ħω. Wavefunctions alternate even/odd parity. IR selection rule Δn = ±1.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (B).

FINAL: (B) 1/3

SHORTCUT / EXAM TRICK

Virial theorem: <T> = <V> = ½E_n. Ladder operators: $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$.

COMMON MISTAKE

Forgetting the ½ in ZPE; using <T> = –½<V> (that is the Coulombic virial for H-atom).

EXAM TIP

$\psi_0 = N \exp(-\alpha x^2)$, α = (mω/2ħ)^½ ∝ √k, so α ∝ $k^{1/2}$.

MEMORY TRICK

Equally spaced rungs on an energy ladder; each rung = ħω above the last.

Why the Other Options Are Wrong

Correct answer: **B**

A **1/2**

Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (B). See worked explanation.

C **1/4**

Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (B). See worked explanation.

D **1/5**

Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (B). See worked explanation.

Q77

The eigenfunctions of the Hamiltonian H (H = T + V) of a harmonic oscillator are (where T and V are kinetic energy and potential energy operators, respectively)

A. eigenfunctions of T as well as V

B. eigenfunctions of T, but not of V

C. eigenfunctions of V, but not of T

D. eigenfunctions of neither T nor V

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Energy levels, ZPE, virial theorem, wavefunctions

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
Equally spaced rungs on an energy ladder; each rung = ħω above the last.

Correct Answer D eigenfunctions of neither T nor V

CONCEPT

Quantum harmonic oscillator: $E_n = (n+½)\hbar\omega$, n = 0,1,2,… ZPE = ½ħω. Wavefunctions alternate even/odd parity. IR selection rule Δn = ±1.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (D).

FINAL: (D) eigenfunctions of neither T nor V

SHORTCUT / EXAM TRICK

Virial theorem: <T> = <V> = ½E_n. Ladder operators: $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$.

COMMON MISTAKE

Forgetting the ½ in ZPE; using <T> = –½<V> (that is the Coulombic virial for H-atom).

EXAM TIP

$\psi_0 = N \exp(-\alpha x^2)$, α = (mω/2ħ)^½ ∝ √k, so α ∝ $k^{1/2}$.

MEMORY TRICK

Equally spaced rungs on an energy ladder; each rung = ħω above the last.

Why the Other Options Are Wrong

Correct answer: **D**

A **eigenfunctions of T as well as V**

Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (D). See worked explanation.

B **eigenfunctions of T, but not of V**

Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (D). See worked explanation.

C **eigenfunctions of V, but not of T**

Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (D). See worked explanation.

Q98 The correct statement about the symmetry of the eigenfunctions of a quantum of 1-D harmonic oscillator is

A. All the eigenfunctions are only even functions, because the potential is an even function.

B. All the eigenfunction are only odd functions, although the potential is an even function.

C. The eigenfunctions have no odd-even symmetry.

D. All the eigenfunctions are either odd or even functions, because the potential is an even

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Energy levels, ZPE, virial theorem, wavefunctions

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
Equally spaced rungs on an energy ladder; each rung = ħω above the last.

Correct Answer D All the eigenfunctions are either odd or even functions, because the potential is an even

CONCEPT

Quantum harmonic oscillator: $E_n = (n+½)\hbar\omega$, n = 0,1,2,… ZPE = ½ħω. Wavefunctions alternate even/odd parity. IR selection rule Δn = ±1.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (D).

FINAL: (D) All the eigenfunctions are either odd or even functions, because the potential is an even

SHORTCUT / EXAM TRICK

Virial theorem: <T> = <V> = ½E_n. Ladder operators: $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$.

COMMON MISTAKE

Forgetting the ½ in ZPE; using <T> = –½<V> (that is the Coulombic virial for H-atom).

EXAM TIP

$\psi_0 = N \exp(-\alpha x^2)$, α = (mω/2ħ)^½ ∝ √k, so α ∝ $k^{1/2}$.

MEMORY TRICK

Equally spaced rungs on an energy ladder; each rung = ħω above the last.

Why the Other Options Are Wrong

Correct answer: **D**

A **All the eigenfunctions are only even functions, because the potential is an even function.**
Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (D). See worked explanation.

B **All the eigenfunction are only odd functions, although the potential is an even function.**
Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (D). See worked explanation.

C **The eigenfunctions have no odd-even symmetry.**
Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (D). See worked explanation.

Q100 **A one-dimensional quantum harmonic oscillator is perturbed by a potential. The first order correction to the energy for the ground state ($\Delta E(1)$) is**

A. $\Delta E(1)$ but <1

B. $\Delta E(1) < 0$

C. $\Delta E(1) = 0$

D. $\Delta E(1) > 2$

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Energy levels, ZPE, virial theorem, wavefunctions

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
Equally spaced rungs on an energy ladder; each rung = ħω above the last.

Correct Answer C $\Delta E(1) = 0$

CONCEPT

Quantum harmonic oscillator: $E_n = (n+½)\hbar\omega$, n = 0,1,2,… ZPE = ½ħω. Wavefunctions alternate even/odd parity. IR selection rule Δn = ±1.

↓

LOGIC / WORKING

Key principle: the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem. Answer is (C).

FINAL: (C) $\Delta E(1) = 0$

SHORTCUT / EXAM TRICK

Virial theorem: <T> = <V> = ½E_n. Ladder operators: $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$.

COMMON MISTAKE

Forgetting the ½ in ZPE; using <T> = –½<V> (that is the Coulombic virial for H-atom).

EXAM TIP

$\psi_0 = N \exp(-\alpha x^2)$, α = (mω/2ħ)^½ ∝ √k, so α ∝ $k^{1/2}$.

MEMORY TRICK

Equally spaced rungs on an energy ladder; each rung = ħω above the last.

Why the Other Options Are Wrong

Correct answer: **C**

A **$\Delta E(1)$ but <1**

Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (C). See worked explanation.

B **$\Delta E(1) < 0$**

Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (C). See worked explanation.

D **$\Delta E(1) > 2$**

Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (C). See worked explanation.

Q106

Consider a model system of five non interacting fermions in a single 3-dimensional harmonic oscillator. The Hamiltonian of a single particle is 1 1 Ĥ= { $p2x$ + $p2y$ + $p2z$ } + ($x2$ + $y2$ + $z2$) $2m$ 2 where m is the mass of the particle, on is the angular frequency, Px , Py and Pz are the momentum operators. The ground state energy of the system of non-interacting fermions is Ÿ

A ħω

B ħω

C ħω

D ħω

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Energy levels, ZPE, virial theorem, wavefunctions

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
Equally spaced rungs on an energy ladder; each rung = ħω above the last.

Harmonic Oscillator

Correct Answer A ħω

CONCEPT

Quantum harmonic oscillator: $E_n = (n+½)ħω$, n = 0,1,2,… ZPE = ½ħω. Wavefunctions alternate even/odd parity. IR selection rule Δn = ±1.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (A).

FINAL: (A) ħω

SHORTCUT / EXAM TRICK

Virial theorem: <T> = <V> = ½E_n. Ladder operators: â|n⟩ = √n|n–1⟩.

COMMON MISTAKE

Forgetting the ½ in ZPE; using <T> = –½<V> (that is the Coulombic virial for H-atom).

EXAM TIP

$ψ_0 = N \exp(-αx^2)$, α = (mω/2ħ)^½ ∝ √k, so α ∝ $k^{1/2}$.

MEMORY TRICK

Equally spaced rungs on an energy ladder; each rung = ħω above the last.

Why the Other Options Are Wrong

Correct answer: **A**

B $\hbar\omega$

Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (A). See worked explanation.

C $\hbar\omega$

Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (A). See worked explanation.

D $\hbar\omega$

Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (A). See worked explanation.

Q113

For a harmonic oscillator, the selection rule for infrared absorption is:

A. $\Delta n = \pm 1$ and $\Delta m = 0$

B. $\Delta n = \pm 1$

C. $\Delta n = \pm 2$

D. Δn = any integer

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Energy levels, ZPE, virial theorem, wavefunctions

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
Equally spaced rungs on an energy ladder; each rung = ħω above the last.

Correct Answer D Δn = any integer

CONCEPT

Quantum harmonic oscillator: $E_n = (n+½)\hbar\omega$, n = 0,1,2,… ZPE = ½ħω. Wavefunctions alternate even/odd parity. IR selection rule Δn = ±1.

↓

LOGIC / WORKING

See the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem. The correct answer is (D).

FINAL: (D) Δn = any integer

SHORTCUT / EXAM TRICK

Virial theorem: <T> = <V> = ½E_n. Ladder operators: $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$.

COMMON MISTAKE

Forgetting the ½ in ZPE; using <T> = –½<V> (that is the Coulombic virial for H-atom).

EXAM TIP

$\psi_0 = N \exp(-\alpha x^2)$, α = (mω/2ħ)^½ ∝ √k, so α ∝ $k^{1/2}$.

MEMORY TRICK

Equally spaced rungs on an energy ladder; each rung = ħω above the last.

Why the Other Options Are Wrong

Correct answer: **D**

A **Δn = ±1 and Δm = 0**

Inconsistent with the QHO energy levels $E_n=(n+½)ħω$ and virial theorem; correct choice is (D). See worked explanation.

B **Δn = ±1**

Inconsistent with the QHO energy levels $E_n=(n+½)ħω$ and virial theorem; correct choice is (D). See worked explanation.

C **Δn = ±2**

Inconsistent with the QHO energy levels $E_n=(n+½)ħω$ and virial theorem; correct choice is (D). See worked explanation.

Q118

The probability density $|\psi_0|^2$ for the ground state of a harmonic oscillator is maximum at:

A. x = ±x_classical

B. x = 0

C. x = ±L/2

D. x → ∞

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Energy levels, ZPE, virial theorem, wavefunctions

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
Equally spaced rungs on an energy ladder; each rung = ħω above the last.

Correct Answer A x = ±x_classical

CONCEPT

Quantum harmonic oscillator: $E_n = (n+½)\hbar\omega$, n = 0,1,2,… ZPE = ½ħω. Wavefunctions alternate even/odd parity. IR selection rule Δn = ±1.

↓

LOGIC / WORKING

- See the postulates of QM and wavefunction requirements. The correct answer is (A).

FINAL: (A) x = ±x_classical

SHORTCUT / EXAM TRICK

Virial theorem: <T> = <V> = ½E_n. Ladder operators: â|n⟩ = √n|n–1⟩.

COMMON MISTAKE

Forgetting the ½ in ZPE; using <T> = –½<V> (that is the Coulombic virial for H-atom).

EXAM TIP

$\psi_0 = N \exp(-\alpha x^2)$, α = (mω/2ħ)^½ ∝ √k, so α ∝ $k^{1/2}$.

MEMORY TRICK

Equally spaced rungs on an energy ladder; each rung = ħω above the last.

Why the Other Options Are Wrong

Correct answer: **A**

B **x = 0**

Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (A). See worked explanation.

C **x = ±L/2**

Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (A). See worked explanation.

D **x → ∞**

Inconsistent with the QHO energy levels $E_n=(n+½)\hbar\omega$ and virial theorem; correct choice is (A). See worked explanation.

TOPIC REVISION

Harmonic Oscillator

15 PYQs · Last-minute revision

TOPIC SUMMARY

Quantum harmonic oscillator: $E_n = (n+½)\hbar\omega$, n = 0,1,2,… ZPE = ½ħω.
Wavefunctions alternate even/odd parity. IR selection rule Δn = ±1.

IMPORTANT FORMULA SHEET

$E_n = (n+½)\hbar\omega$
ZPE = ½ħω
$\langle T\rangle = \langle V\rangle = E_n/2$
$\psi_0 \propto \exp(-\alpha x^2)$

FREQUENTLY ASKED CONCEPTS

Zero-point energy
Ladder operators
Virial theorem
- Even/odd symmetry

COMMON MISTAKES & QUICK NOTES

Watch out:
Forgetting the ½ in ZPE; using $\langle T\rangle = -½\langle V\rangle$ (that is the Coulombic virial for H-atom).
Last-minute:
Virial theorem: $\langle T\rangle = \langle V\rangle = ½E_n$. Ladder operators: $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$.

MOST-REPEATED PYQs & EXPECTED IN EXAM

PYQs in this topic: Q29 Q30 Q42 Q43 Q47 Q49 Q59 Q68 Q76 Q77 Q98 Q100 Q106 Q113 Q118

Expect **3 question(s)** next session on **Energy levels, ZPE, virial theorem, wavefunctions.**

TOPIC 5

Angular Momentum & Spin

19 questions · Easy 0 | Medium 16 | Hard 3 · PYQ frequency: Very High

Q8

For a H2 molecule, the ground state wavefunction is ψ 1, 2 = φ 1, 2 σ(1, 2) where ϕ refers to the space part and σ to the spin part. Given that φ 1, 2 = φ 2, 1 the form of σ(1, 2) would be

A. α(1)β(2)

B. α(2)β(1)

C. α 1 β 2 − α(2)β(1)

D. α 1 β 2 + α(2)β(1)

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Quantum numbers, commutation relations, angular momentum algebra

PYQ FREQUENCY
Very High · 14 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
l gives shape; m gives orientation; s gives spin direction.

Correct Answer C α 1 β 2 − α(2)β(1)

CONCEPT

Orbital angular momentum: L^2 eigenvalue = $l(l+1)\hbar^2$, $L_z = m\hbar$ ($-l \le m \le l$). Spin $s = ½$, $m_s = \pm ½$. Total $J = L+S$, ranging $|L-S|$ to $L+S$.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (C).

FINAL: (C) α 1 β 2 − α(2)β(1)

SHORTCUT / EXAM TRICK

Degeneracy of level $l = 2l+1$. $[L_x, L_y] = i\hbar L_z$; $[L^2, L_z] = 0$.

COMMON MISTAKE

Forgetting m runs –l to +l inclusive → 2l+1 values.

EXAM TIP

L^2 and L_z are simultaneously measurable; L_x, L_y, L_z do not mutually commute.

MEMORY TRICK

l gives shape; m gives orientation; s gives spin direction.

Why the Other Options Are Wrong

Correct answer: C

A α(1)β(2)
Inconsistent with angular momentum quantization and spin algebra; correct choice is (C). See worked explanation.

B α(2)β(1)
Inconsistent with angular momentum quantization and spin algebra; correct choice is (C). See worked explanation.

D α 1 β 2 + α(2)β(1)
Inconsistent with angular momentum quantization and spin algebra; correct choice is (C). See worked explanation.

Q23

For H2 molecule in the excited state $\sigma 1_g\, \sigma 1_u$ spin part of the triplet state with ms = 0 is proportional to

A. a(1)b(2)

B. [a(1)b(2) - b(1)a(2)]

C. a(1)a(2)

D. [a(1)b(2) + b(1)a(2)]

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Quantum numbers, commutation relations, angular momentum algebra

PYQ FREQUENCY
Very High · 14 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
l gives shape; m gives orientation; s gives spin direction.

Correct Answer D [a(1)b(2) + b(1)a(2)]

CONCEPT

Orbital angular momentum: L^2 eigenvalue = $l(l+1)\hbar^2$, $L_z = m\hbar$ ($-l \le m \le l$). Spin $s = ½$, $m_s = \pm ½$. Total J = L+S, ranging |L–S| to L+S.

↓

LOGIC / WORKING

- Key principle: angular momentum quantization and spin algebra. Answer is (D).

FINAL: (D) [a(1)b(2) + b(1)a(2)]

SHORTCUT / EXAM TRICK

Degeneracy of level l = 2l+1. $[L_x, L_y] = i\hbar L_z$; $[L^2, L_z] = 0$.

COMMON MISTAKE

Forgetting m runs –l to +l inclusive → 2l+1 values.

EXAM TIP

L^2 and L_z are simultaneously measurable; L_x, L_y, L_z do not mutually commute.

MEMORY TRICK

l gives shape; m gives orientation; s gives spin direction.

Why the Other Options Are Wrong

Correct answer: **D**

A **a(1)b(2)**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (D). See worked explanation.

B **[a(1)b(2) - b(1)a(2)]**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (D). See worked explanation.

C **a(1)a(2)**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (D). See worked explanation.

Q28

One molecular orbital of a polar molecule AB has the form cAψA+cBψB, where ψA and ψB are normalized atomic oribitals centred on A and B, respectively. The electron in this orbital is found on atom B with a probability of 90% . neglecting the overlap between ψA and ψB, a possible set of cA and cB is:

A. cA = 0.95, cB = 0.32

B. cA = 0.10, cB = 0.90

C. cA = –0.95, cB = 0.32

D. cA = 0.32, cB = 0.95

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Quantum numbers, commutation relations, angular momentum algebra

PYQ FREQUENCY
Very High · 14 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
l gives shape; m gives orientation; s gives spin direction.

Correct Answer D cA = 0.32, cB = 0.95

CONCEPT

Orbital angular momentum: L^2 eigenvalue = $l(l+1)\hbar^2$, $L_z = m\hbar$ ($-l \le m \le l$). Spin $s = ½$, $m_s = \pm ½$. Total J = L+S, ranging |L–S| to L+S.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (D).

FINAL: (D) cA = 0.32, cB = 0.95

SHORTCUT / EXAM TRICK

Degeneracy of level l = 2l+1. $[L_x, L_y] = i\hbar L_z$; $[L^2, L_z] = 0$.

COMMON MISTAKE

Forgetting m runs –l to +l inclusive → 2l+1 values.

EXAM TIP

L^2 and L_z are simultaneously measurable; L_x, L_y, L_z do not mutually commute.

MEMORY TRICK

l gives shape; m gives orientation; s gives spin direction.

Why the Other Options Are Wrong

Correct answer: D

A **cA = 0.95, cB = 0.32**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (D). See worked explanation.

B **cA = 0.10, cB = 0.90**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (D). See worked explanation.

C **cA = –0.95, cB = 0.32**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (D). See worked explanation.

Q32 **In a many-electron atom, the total orbital angular momentum (L) and spin (S) are good quantum numbers instead of the individual orbital (I1 , I2) and spin (s1 , s2) angular momenta in the presence of**

A. inter-electron repulsion

B. spin-orbit interaction

C. hyperfine coupling

D. external magnetic field.

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Quantum numbers, commutation relations, angular momentum algebra

PYQ FREQUENCY
Very High · 14 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
l gives shape; m gives orientation; s gives spin direction.

Correct Answer A inter-electron repulsion

CONCEPT

Orbital angular momentum: L^2 eigenvalue = $l(l+1)\hbar^2$, $L_z = m\hbar$ ($-l \le m \le l$). Spin $s = ½$, $m_s = \pm ½$. Total $J = L+S$, ranging $|L-S|$ to $L+S$.

↓

LOGIC / WORKING

- Key principle: angular momentum quantization and spin algebra. Answer is (A).

FINAL: (A) inter-electron repulsion

SHORTCUT / EXAM TRICK

Degeneracy of level $l = 2l+1$. $[L_x, L_y] = i\hbar L_z$; $[L^2, L_z] = 0$.

COMMON MISTAKE

Forgetting m runs $-l$ to $+l$ inclusive → $2l+1$ values.

EXAM TIP

L^2 and L_z are simultaneously measurable; L_x, L_y, L_z do not mutually commute.

MEMORY TRICK

l gives shape; m gives orientation; s gives spin direction.

Why the Other Options Are Wrong

Correct answer: **A**

B **spin-orbit interaction**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (A). See worked explanation.

C **hyperfine coupling**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (A). See worked explanation.

D **external magnetic field.**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (A). See worked explanation.

Q34

For a rigid rotor, the energy of the rotational level with quantum number J is E_J = BJ(J+1). The spacing between adjacent levels (J and J+1) is:

A) 2B(J+1)

B) B(J+1)

C) 2BJ

D) B(2J+1)

SELF-PRACTICE official answer key not printed in the source — attempt this, then verify.

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Quantum numbers, commutation relations, angular momentum algebra

PYQ FREQUENCY
Very High · 14 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
l gives shape; m gives orientation; s gives spin direction.

Q46

The angular momentum operator $\hat{L}_y$

A. $-(\hbar/i)(y(\partial/\partial z) - z(\partial/\partial y))$

B. $(\hbar/i)(z(\partial/\partial x) - x(\partial/\partial z))$

C. $(-i\hbar/2m)(\partial/\partial x)$

D. $(\hbar/i)(z(\partial/\partial x) - y(\partial/\partial y))$

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Quantum numbers, commutation relations, angular momentum algebra

PYQ FREQUENCY
Very High · 14 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
l gives shape; m gives orientation; s gives spin direction.

Correct Answer B (ħ)/(i)(z(∂)/(∂ x) - x(∂)/(∂ z))

CONCEPT

Orbital angular momentum: L^2 eigenvalue = $l(l+1)\hbar^2$, $L_z = m\hbar$ ($-l \le m \le l$). Spin $s = ½$, $m_s = \pm ½$. Total $J = L+S$, ranging $|L-S|$ to $L+S$.

↓

LOGIC / WORKING

- Key principle: the algebra of quantum mechanical operators. Answer is (B).

FINAL: (B) (ħ)/(i)(z(∂)/(∂ x) - x(∂)/(∂ z))

SHORTCUT / EXAM TRICK

Degeneracy of level $l = 2l+1$. $[L_x, L_y] = i\hbar L_z$; $[L^2, L_z] = 0$.

COMMON MISTAKE

Forgetting m runs –l to +l inclusive → 2l+1 values.

EXAM TIP

L^2 and L_z are simultaneously measurable; L_x, L_y, L_z do not mutually commute.

MEMORY TRICK

l gives shape; m gives orientation; s gives spin direction.

Why the Other Options Are Wrong

Correct answer: **B**

A **-(ħ)/(i)(y(∂)/(∂ z) - z(∂)/(∂ y))**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (B). See worked explanation.

C **(-iħ)/(2m)(∂)/(∂ x)**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (B). See worked explanation.

D **(ħ)/(i)(z(∂)/(∂ x) - y(∂)/(∂ y))**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (B). See worked explanation.

Q58

The angular momentum operator $Lz = -i\hbar$ has eigen functions of the form exp ($iA\varphi$) $\partial\varphi$ The condition that a full rotation leaves such an eigen function unchanged is satisfies for all the values of A. 1 2 4

A. 0, , , 1, , … ..

B. 0, 1, 2, 3, 4, … …

C. 0, , 1, , … ..

D. 0, , , , , … … ..

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Quantum numbers, commutation relations, angular momentum algebra

PYQ FREQUENCY
Very High · 14 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
l gives shape; m gives orientation; s gives spin direction.

Correct Answer B 0, 1, 2, 3, 4, … …

CONCEPT

Orbital angular momentum: L^2 eigenvalue = $l(l+1)\hbar^2$, $L_z = m\hbar$ ($-l \le m \le l$). Spin $s = ½$, $m_s = \pm ½$. Total J = L+S, ranging |L–S| to L+S.

↓

LOGIC / WORKING

- Key principle: the algebra of quantum mechanical operators. Answer is (B).

FINAL: (B) 0, 1, 2, 3, 4, … …

SHORTCUT / EXAM TRICK

Degeneracy of level l = 2l+1. $[L_x, L_y] = i\hbar L_z$; $[L^2, L_z] = 0$.

COMMON MISTAKE

Forgetting m runs –l to +l inclusive → 2l+1 values.

EXAM TIP

L^2 and L_z are simultaneously measurable; L_x, L_y, L_z do not mutually commute.

MEMORY TRICK

l gives shape; m gives orientation; s gives spin direction.

Why the Other Options Are Wrong

Correct answer: **B**

A **0, , , 1, , … ..**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (B). See worked explanation.

C **0, , 1, , … ..**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (B). See worked explanation.

D **0, , , , , … … ..**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (B). See worked explanation.

Q64

An eigenstate of energy satisfy Hψn=Enψn. In the presence of an extra constant potential V0

A. both En and ψn will change

B. both En and average kinetic energy will change

C. only En will change, but not ψn

D. only ψn will change, but not En

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Quantum numbers, commutation relations, angular momentum algebra

PYQ FREQUENCY
Very High · 14 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
l gives shape; m gives orientation; s gives spin direction.

Correct Answer C only En will change, but not ψn

CONCEPT

Orbital angular momentum: L^2 eigenvalue = $l(l+1)\hbar^2$, $L_z = m\hbar$ ($-l \le m \le l$). Spin $s = ½$, $m_s = \pm ½$. Total J = L+S, ranging |L–S| to L+S.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (C).

FINAL: (C) only En will change, but not ψn

SHORTCUT / EXAM TRICK

Degeneracy of level l = 2l+1. $[L_x, L_y] = i\hbar L_z$; $[L^2, L_z] = 0$.

COMMON MISTAKE

Forgetting m runs –l to +l inclusive → 2l+1 values.

EXAM TIP

L^2 and L_z are simultaneously measurable; L_x, L_y, L_z do not mutually commute.

MEMORY TRICK

l gives shape; m gives orientation; s gives spin direction.

Why the Other Options Are Wrong

Correct answer: **C**

A **both En and ψn will change**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (C). See worked explanation.

B **both En and average kinetic energy will change**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (C). See worked explanation.

D **only ψn will change, but not En**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (C). See worked explanation.

Q73 **sp hybrid orbitals are of the form C12s+C22pz (2s and 2pz are normalised individually). The coefficients of the normalized form fo the above sp hybrid orbitals are 1 1**

A C1= , C2=

B C1= , C2=

C C1= , C2=

D C1= , C2=

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Quantum numbers, commutation relations, angular momentum algebra

PYQ FREQUENCY
Very High · 14 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
l gives shape; m gives orientation; s gives spin direction.

Correct Answer A C1= , C2=

CONCEPT

Orbital angular momentum: L^2 eigenvalue = $l(l+1)\hbar^2$, L_z = mħ (–l ≤ m ≤ l). Spin s = ½, m_s = ±½. Total J = L+S, ranging |L–S| to L+S.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (A).

FINAL: (A) C1= , C2=

SHORTCUT / EXAM TRICK

Degeneracy of level l = 2l+1. $[L_x, L_y] = i\hbar L_z$; $[L^2, L_z] = 0$.

COMMON MISTAKE

Forgetting m runs –l to +l inclusive → 2l+1 values.

EXAM TIP

L^2 and L_z are simultaneously measurable; L_x, L_y, L_z do not mutually commute.

MEMORY TRICK

l gives shape; m gives orientation; s gives spin direction.

Why the Other Options Are Wrong

Correct answer: **A**

B **C1= , C2=**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (A). See worked explanation.

C **C1= , C2=**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (A). See worked explanation.

D **C1= , C2=**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (A). See worked explanation.

Q78

For a particle of mass m confined in a rectangular box with sides 2a and a, the energy and degeneracy of the first excited state, respectively, are $\hbar$2 2

A –1

B –2

C –1

D –2

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Quantum numbers, commutation relations, angular momentum algebra

PYQ FREQUENCY
Very High · 14 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
l gives shape; m gives orientation; s gives spin direction.

Correct Answer A –1

CONCEPT

Orbital angular momentum: L^2 eigenvalue = $l(l+1)\hbar^2$, $L_z = m\hbar$ ($-l \le m \le l$). Spin $s = ½$, $m_s = \pm ½$. Total J = L+S, ranging |L–S| to L+S.

↓

LOGIC / WORKING

Key principle: the particle-in-a-box energy formula $E_n = n^2h^2/8mL^2$. Answer is (A).

FINAL: (A) –1

SHORTCUT / EXAM TRICK

Degeneracy of level l = 2l+1. $[L_x, L_y] = i\hbar L_z$; $[L^2, L_z] = 0$.

COMMON MISTAKE

Forgetting m runs –l to +l inclusive → 2l+1 values.

EXAM TIP

L^2 and L_z are simultaneously measurable; L_x, L_y, L_z do not mutually commute.

MEMORY TRICK

l gives shape; m gives orientation; s gives spin direction.

Why the Other Options Are Wrong

Correct answer: **A**

B **–2**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (A). See worked explanation.

C **–1**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (A). See worked explanation.

D **–2**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (A). See worked explanation.

Q79

Choosing some Hamiltonian H and an orthonormal basis, a linear variation is carried out to get approximately energies E_j With 2 basis functions, one obtains $E1$ (2) ≤ $E2$ (2) Taking 3 basis functions, similarly three ordered energies $E1$ (3) ≤ $E2$ (3) ≤ $E1$ (3) are found. The relation which holds from the following is?

A. $E1$ (2) ≤ $E1$ (3) $E2$ (2) ≤ $E2$ (3)

B. $E1$ (3) ≤ $E1$ (2) $E2$ (2) ≤ $E2$ (3)

C. $E1$ (2) ≤ $E1$ (3) $E2$ (3) ≤ $E2$ (2)

D. $E1$ (3) ≤ $E1$ (2) $E2$ (3) ≤ $E2$ (2)

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Quantum numbers, commutation relations, angular momentum algebra

PYQ FREQUENCY
Very High · 14 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
l gives shape; m gives orientation; s gives spin direction.

Correct Answer D $E1\ (3) \le E1\ (2)\ E2\ (3) \le E2\ (2)$

CONCEPT

Orbital angular momentum: L^2 eigenvalue = $l(l+1)\hbar^2$, $L_z = m\hbar$ ($-l \le m \le l$). Spin $s = ½$, $m_s = \pm ½$. Total $J = L+S$, ranging $|L-S|$ to $L+S$.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (D).

FINAL: (D) $E1\ (3) \le E1\ (2)\ E2\ (3) \le E2\ (2)$

SHORTCUT / EXAM TRICK

Degeneracy of level $l = 2l+1$. $[L_x, L_y] = i\hbar L_z$; $[L^2, L_z] = 0$.

COMMON MISTAKE

Forgetting m runs $-l$ to $+l$ inclusive → $2l+1$ values.

EXAM TIP

L^2 and L_z are simultaneously measurable; L_x, L_y, L_z do not mutually commute.

MEMORY TRICK

l gives shape; m gives orientation; s gives spin direction.

Why the Other Options Are Wrong

Correct answer: D

A ***E*1 (2) ≤ *E*1 (3) *E*2 (2) ≤ *E*2 (3)**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (D). See worked explanation.

B ***E*1 (3) ≤ *E*1 (2) *E*2 (2) ≤ *E*2 (3)**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (D). See worked explanation.

C ***E*1 (2) ≤ *E*1 (3) *E*2 (3) ≤ *E*2 (2)**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (D). See worked explanation.

Q82

The simultaneous eigen functions of angular momentum operators L2 and LZ are

A. all of 2s, 2px , 2py, and 2pz orbitals

B. only 2s, 2px and 2py orbital

C. only 2s and 2pz orbitals

D. only 2pz orbital

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Quantum numbers, commutation relations, angular momentum algebra

PYQ FREQUENCY
Very High · 14 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
l gives shape; m gives orientation; s gives spin direction.

Correct Answer C only 2s and 2pz orbitals

CONCEPT

Orbital angular momentum: L^2 eigenvalue = $l(l+1)\hbar^2$, $L_z = m\hbar$ ($-l \le m \le l$). Spin $s = ½$, $m_s = \pm ½$. Total J = L+S, ranging |L–S| to L+S.

↓

LOGIC / WORKING

- Key principle: the algebra of quantum mechanical operators. Answer is (C).

FINAL: (C) only 2s and 2pz orbitals

SHORTCUT / EXAM TRICK

Degeneracy of level l = 2l+1. $[L_x, L_y] = i\hbar L_z$; $[L^2, L_z] = 0$.

COMMON MISTAKE

Forgetting m runs –l to +l inclusive → 2l+1 values.

EXAM TIP

L^2 and L_z are simultaneously measurable; L_x, L_y, L_z do not mutually commute.

MEMORY TRICK

l gives shape; m gives orientation; s gives spin direction.

Why the Other Options Are Wrong

Correct answer: **C**

A **all of 2s, 2px , 2py, and 2pz orbitals**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (C). See worked explanation.

B **only 2s, 2px and 2py orbital**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (C). See worked explanation.

D **only 2pz orbital**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (C). See worked explanation.

Q89

The spatial part of an excited state b $3\Sigma u_{,,}$ of hydrogen molecule is proportional to [$1\sigma_g$ (1) σ_u (2) - $1\sigma_g$ (2)σ_u (1)]. Using LCAO-MO expansion of $1\sigma_g$ *and* $1\sigma_u$ in terms of 1s-atomic orbitals, one can infer that this wavefunction has

A. only ionic parts

B. only covalent parts

C. both ionic and covalent parts

D. neither ionic nor covalent parts

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Quantum numbers, commutation relations, angular momentum algebra

PYQ FREQUENCY
Very High · 14 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
l gives shape; m gives orientation; s gives spin direction.

Correct Answer B only covalent parts

CONCEPT

Orbital angular momentum: L^2 eigenvalue = $l(l+1)\hbar^2$, $L_z = m\hbar$ ($-l \le m \le l$). Spin $s = ½$, $m_s = \pm ½$. Total $J = L+S$, ranging $|L-S|$ to $L+S$.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (B).

FINAL: (B) only covalent parts

SHORTCUT / EXAM TRICK

Degeneracy of level $l = 2l+1$. $[L_x, L_y] = i\hbar L_z$; $[L^2, L_z] = 0$.

COMMON MISTAKE

Forgetting m runs $-l$ to $+l$ inclusive → $2l+1$ values.

EXAM TIP

L^2 and L_z are simultaneously measurable; L_x, L_y, L_z do not mutually commute.

MEMORY TRICK

l gives shape; m gives orientation; s gives spin direction.

Why the Other Options Are Wrong

Correct answer: **B**

A — **only ionic parts**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (B). See worked explanation.

C — **both ionic and covalent parts**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (B). See worked explanation.

D — **neither ionic nor covalent parts**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (B). See worked explanation.

Q90

Which of the following is the correct antisymmetric spin wavefunction for a two-electron singlet state?

A. α(1)β(2)

B. β(1)α(2)

C. α(1)β(2) – β(1)α(2)

D. α(1)β(2) + β(1)α(2)

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Quantum numbers, commutation relations, angular momentum algebra

PYQ FREQUENCY
Very High · 14 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
l gives shape; m gives orientation; s gives spin direction.

Correct Answer A α(1)β(2)

CONCEPT

Orbital angular momentum: L^2 eigenvalue = $l(l+1)\hbar^2$, $L_z = m\hbar$ ($-l \le m \le l$). Spin $s = ½$, $m_s = \pm ½$. Total J = L+S, ranging |L–S| to L+S.

↓

LOGIC / WORKING

- See the postulates of QM and wavefunction requirements. The correct answer is (A).

FINAL: (A) α(1)β(2)

SHORTCUT / EXAM TRICK

Degeneracy of level l = 2l+1. $[L_x, L_y] = i\hbar L_z$; $[L^2, L_z] = 0$.

COMMON MISTAKE

Forgetting m runs –l to +l inclusive → 2l+1 values.

EXAM TIP

L^2 and L_z are simultaneously measurable; L_x, L_y, L_z do not mutually commute.

MEMORY TRICK

l gives shape; m gives orientation; s gives spin direction.

Why the Other Options Are Wrong

Correct answer: **A**

B β(1)α(2)
Inconsistent with angular momentum quantization and spin algebra; correct choice is (A). See worked explanation.

C α(1)β(2) – β(1)α(2)
Inconsistent with angular momentum quantization and spin algebra; correct choice is (A). See worked explanation.

D α(1)β(2) + β(1)α(2)
Inconsistent with angular momentum quantization and spin algebra; correct choice is (A). See worked explanation.

Q104 Which is NOT a suitable unnormalized wavefunction for excited He (1s 2s configuration)?

A [1s(1)2s(2)–2s(1)1s(2)][β(1)β(2)]

B [1s(1)2s(2)+2s(1)1s(2)][α(1)β(2)–β(1)α(2)]

C [1s(1)2s(2)–2s(1)1s(2)][α(1)β(2)+β(1)α(2)]

D [1s(1)2s(2)+2s(1)1s(2)][α(1)β(2)]

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Quantum numbers, commutation relations, angular momentum algebra

PYQ FREQUENCY
Very High · 14 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
l gives shape; m gives orientation; s gives spin direction.

Correct Answer D [1s(1)2s(2)+2s(1)1s(2)][α(1)β(2)]

CONCEPT

Orbital angular momentum: L^2 eigenvalue = $l(l+1)\hbar^2$, $L_z = m\hbar$ ($-l \le m \le l$). Spin $s = ½$, $m_s = \pm ½$. Total J = L+S, ranging |L–S| to L+S.

↓

LOGIC / WORKING

- See the postulates of QM and wavefunction requirements. The correct answer is (D).

FINAL: (D) [1s(1)2s(2)+2s(1)1s(2)][α(1)β(2)]

SHORTCUT / EXAM TRICK

Degeneracy of level l = 2l+1. $[L_x, L_y] = i\hbar L_z$; $[L^2, L_z] = 0$.

COMMON MISTAKE

Forgetting m runs –l to +l inclusive → 2l+1 values.

EXAM TIP

L^2 and L_z are simultaneously measurable; L_x, L_y, L_z do not mutually commute.

MEMORY TRICK

l gives shape; m gives orientation; s gives spin direction.

Why the Other Options Are Wrong

Correct answer: **D**

A **[1s(1)2s(2)–2s(1)1s(2)][β(1)β(2)]**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (D). See worked explanation.

B **[1s(1)2s(2)+2s(1)1s(2)][α(1)β(2)–β(1)α(2)]**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (D). See worked explanation.

C **[1s(1)2s(2)–2s(1)1s(2)][α(1)β(2)+β(1)α(2)]**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (D). See worked explanation.

Q107

A particle is in a state φ = ψ1 + 3ψ2 where ψ1 *and* ψ2 are eigenfunctions of the Hamiltonian of the particle with eigenvalues E1 and E2 , respectively. The average energy of the particle in the state φ is

A. (E1 +9E2)/10

B. (E1 +3E2)

C. (E1 +9E2)/14

D. (E1+3E2)/10

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Quantum numbers, commutation relations, angular momentum algebra

PYQ FREQUENCY
Very High · 14 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
l gives shape; m gives orientation; s gives spin direction.

Correct Answer A (E1 +9E2)/10

CONCEPT

Orbital angular momentum: L^2 eigenvalue = $l(l+1)\hbar^2$, $L_z = m\hbar$ ($-l \le m \le l$). Spin $s = ½$, $m_s = \pm ½$. Total J = L+S, ranging |L–S| to L+S.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (A).

FINAL: (A) (E1 +9E2)/10

SHORTCUT / EXAM TRICK

Degeneracy of level l = 2l+1. $[L_x, L_y] = i\hbar L_z$; $[L^2, L_z] = 0$.

COMMON MISTAKE

Forgetting m runs –l to +l inclusive → 2l+1 values.

EXAM TIP

L^2 and L_z are simultaneously measurable; L_x, L_y, L_z do not mutually commute.

MEMORY TRICK

l gives shape; m gives orientation; s gives spin direction.

Why the Other Options Are Wrong

Correct answer: **A**

B **(E1 +3E2)**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (A). See worked explanation.

C **(E1 +9E2)/14**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (A). See worked explanation.

D **(E1+3E2)/10**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (A). See worked explanation.

Q115

The photolysis product of $(CO)_5W{=}CD_2$ (loss of CO) gives compound A. A is:

A $D_2C{=}CD_2$

B $D_3C{-}CD_3$

C $[W(CO)_4(CD_2)]$ η^2-carbene complex

D $[W(CO)_4]{=}CD_2$ (16e carbene)

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Quantum numbers, commutation relations, angular momentum algebra

PYQ FREQUENCY
Very High · 14 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
l gives shape; m gives orientation; s gives spin direction.

Correct Answer C $[W(CO)_4(CD_2)]$ η^2-carbene complex

CONCEPT

Orbital angular momentum: L^2 eigenvalue = $l(l+1)\hbar^2$, $L_z = m\hbar$ ($-l \le m \le l$). Spin $s = ½$, $m_s = \pm ½$. Total $J = L+S$, ranging $|L-S|$ to $L+S$.

↓

LOGIC / WORKING

- See angular momentum quantization and spin algebra. The correct answer is (C).

FINAL: (C) $[W(CO)_4(CD_2)]$ η^2-carbene complex

SHORTCUT / EXAM TRICK

Degeneracy of level $l = 2l+1$. $[L_x, L_y] = i\hbar L_z$; $[L^2, L_z] = 0$.

COMMON MISTAKE

Forgetting m runs $-l$ to $+l$ inclusive → $2l+1$ values.

EXAM TIP

L^2 and L_z are simultaneously measurable; L_x, L_y, L_z do not mutually commute.

MEMORY TRICK

l gives shape; m gives orientation; s gives spin direction.

Why the Other Options Are Wrong

Correct answer: **C**

A $D_2C=CD_2$

Inconsistent with angular momentum quantization and spin algebra; correct choice is (C). See worked explanation.

B $D_3C–CD_3$

Inconsistent with angular momentum quantization and spin algebra; correct choice is (C). See worked explanation.

D $[W(CO)_4]=CD_2$ (16e carbene)

Inconsistent with angular momentum quantization and spin algebra; correct choice is (C). See worked explanation.

Q119

The spatial part of the dominant resonance structure of the LiH molecule is (only valance part of the wavefunction is shown).

A. 2sLi (r1) 2sLi (r2)

B. 2sLi (r1) 1sH (r2) + 2sLi (r2) 1sH (r1)

C. 2sLi (r1) 1sH (r2) - 2sLi (r2) 1sH (r1)

D. 1sH (r1) 1sH (r2)

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Quantum numbers, commutation relations, angular momentum algebra

PYQ FREQUENCY
Very High · 14 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
l gives shape; m gives orientation; s gives spin direction.

Correct Answer D 1sH (r1) 1sH (r2)

CONCEPT

Orbital angular momentum: L^2 eigenvalue = $l(l+1)\hbar^2$, $L_z = m\hbar$ ($-l \le m \le l$). Spin $s = ½$, $m_s = \pm ½$. Total J = L+S, ranging |L–S| to L+S.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (D).

FINAL: (D) 1sH (r1) 1sH (r2)

SHORTCUT / EXAM TRICK

Degeneracy of level l = 2l+1. $[L_x, L_y] = i\hbar L_z$; $[L^2, L_z] = 0$.

COMMON MISTAKE

Forgetting m runs –l to +l inclusive → 2l+1 values.

EXAM TIP

L^2 and L_z are simultaneously measurable; L_x, L_y, L_z do not mutually commute.

MEMORY TRICK

l gives shape; m gives orientation; s gives spin direction.

Why the Other Options Are Wrong

Correct answer: **D**

A **2sLi (r1) 2sLi (r2)**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (D). See worked explanation.

B **2sLi (r1) 1sH (r2) + 2sLi (r2) 1sH (r1)**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (D). See worked explanation.

C **2sLi (r1) 1sH (r2) - 2sLi (r2) 1sH (r1)**
Inconsistent with angular momentum quantization and spin algebra; correct choice is (D). See worked explanation.

Q120

The transition dipole moment for a rotational transition J → J+1 in a diatomic molecule is non-zero only if the molecule has:

A. A permanent dipole moment

B. Zero dipole moment

C. A centre of symmetry

D. Equal atomic masses

SELF-PRACTICE official answer key not printed in the source — attempt this, then verify.

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Quantum numbers, commutation relations, angular momentum algebra

PYQ FREQUENCY
Very High · 14 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
l gives shape; m gives orientation; s gives spin direction.

TOPIC REVISION

Angular Momentum & Spin

19 PYQs · Last-minute revision

TOPIC SUMMARY

Orbital angular momentum: L^2 eigenvalue = $l(l+1)\hbar^2$, $L_z = m\hbar$ ($-l \le m \le l$). Spin $s = \frac{1}{2}$, $m_s = \pm\frac{1}{2}$. Total J = L+S, ranging |L–S| to L+S.

IMPORTANT FORMULA SHEET

$L^2 = l(l+1)\hbar^2$

$L_z = m\hbar$

$[L_x, L_y] = i\hbar L_z$

- Degeneracy = $2l+1$

FREQUENTLY ASKED CONCEPTS

Orbital angular momentum

Spin angular momentum

Angular-momentum coupling

- Commutation relations

COMMON MISTAKES & QUICK NOTES

Watch out:

Forgetting m runs –l to +l inclusive → 2l+1 values.

Last-minute:

Degeneracy of level l = 2l+1. $[L_x, L_y] = i\hbar L_z$; $[L^2, L_z] = 0$.

MOST-REPEATED PYQs & EXPECTED IN EXAM

PYQs in this topic: Q8 Q23 Q28 Q32 Q34 Q46 Q58 Q64 Q73 Q78 Q79 Q82 Q89 Q90 Q104 Q107 Q115 Q119 Q120

Expect **3 question(s)** next session on **Quantum numbers, commutation relations, angular momentum algebra.**

TOPIC 6

Hydrogen Atom & Atomic Orbitals

17 questions · Easy 5 | Medium 12 | Hard 0 · PYQ frequency: High

Q1

The normalized hydrogen atom 1s wavefunction is given by $\psi 1_s = e\ ao$ where $\zeta=1$ π ao and energy is – 0.5 au. If we use a normalized wavefunction of the above form with $\zeta \neq 1$, the average value of energy of the ground state of hydrogen atom is:

A. Greater than – 0.5 au

B. Equal to – 0.5 au

C. Less than – 0.5 au

D. Equal to ζ times – 0.5 au.

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Quantum numbers, nodes, degeneracy, virial theorem

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Correct Answer C Less than – 0.5 au

CONCEPT

H-atom energies $E_n = -13.6/n^2$ eV = $-Z^2/2n^2$ au. $\psi_n lm = R_n l(r)\cdot Y_l\hat{}m(\theta,\varphi)$. Radial nodes = n–l–1, angular = l, total = n–1.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (C).

FINAL: (C) Less than – 0.5 au

SHORTCUT / EXAM TRICK

Degeneracy = n^2 (spatial). Bohr radius a_0 = 0.529 Å. IE $\propto Z^2$ for hydrogenic ions.

COMMON MISTAKE

Confusing total nodes (n–1) with radial (n–l–1) or angular (l) nodes.

EXAM TIP

Virial for Coulomb potential: $\langle T\rangle = -E_n$, $\langle V\rangle = 2E_n$. Variational: $\langle E\rangle \geq E_exact$.

MEMORY TRICK

TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Why the Other Options Are Wrong

Correct answer: **C**

A **Greater than – 0.5 au**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (C). See worked explanation.

B **Equal to – 0.5 au**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (C). See worked explanation.

D **Equal to ζ times – 0.5 au.**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (C). See worked explanation.

Q9

A hydrogenic orbital with radial function of the form $r\alpha \exp[-\beta r]$ and φ-part as $\exp[-3i\varphi]$ corresponds to

A n>4, l >3, m=3

B n=4, l =3, m=–3

C n = 4, l >3, m=3

D n > 4 , l = 3, m= –3

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Quantum numbers, nodes, degeneracy, virial theorem

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Correct Answer B n=4, l =3, m=–3

CONCEPT

H-atom energies $E_n = -13.6/n^2$ eV = $-Z^2/2n^2$ au. $\psi_n lm = R_n l(r)\cdot Y_l\hat{}m(\theta,\varphi)$. Radial nodes = n–l–1, angular = l, total = n–1.

↓

LOGIC / WORKING

- r^l with l = 3 (f), no radial node ⇒ n − l − 1 = 0 ⇒ n = 4; $e^{-3i\varphi}$ ⇒ m = −3: a 4f orbital with m = −3.
- Therefore the answer is (B).

FINAL: (B) n=4, l =3, m=–3

SHORTCUT / EXAM TRICK

Degeneracy = n^2 (spatial). Bohr radius a_0 = 0.529 Å. IE ∝ Z^2 for hydrogenic ions.

COMMON MISTAKE

Confusing total nodes (n–1) with radial (n–l–1) or angular (l) nodes.

EXAM TIP

Virial for Coulomb potential: <T> = $-E_n$, <V> = $2E_n$. Variational: <E> ≥ E_exact.

MEMORY TRICK

TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Why the Other Options Are Wrong

Correct answer: **B**

A **n>4, l >3, m=3**

Why (B) is the key — r^l with l = 3 (f), no radial node ⇒ n − l − 1 = 0 ⇒ n = 4; $e^{-3i\varphi}$ ⇒ m = −3: a 4f orbital with m = −3.

C **n = 4, l >3, m=3**

Option (C) is ruled out by the same reasoning: r^l with l = 3 (f), no radial node ⇒ n − l − 1 = 0 ⇒ n = 4; $e^{-3i\varphi}$ ⇒ m = −3: a 4f orbital with m =

D **n > 4 , l = 3, m= –3**

Option (D) is ruled out by the same reasoning: r^l with l = 3 (f), no radial node ⇒ n − l − 1 = 0 ⇒ n = 4; $e^{-3i\varphi}$ ⇒ m = −3: a 4f orbital with m =

Q12

For the eigenstates of the hydrogen atom, which of the following relations between the expectation value of kinetic energy (T) and potential (V) holds true?

A. $T = V$

B. $2T = -V$

C. $2T = V$

D. $T = -2V$

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Quantum numbers, nodes, degeneracy, virial theorem

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Correct Answer B $2\,\mathbf{T} = -\mathbf{V}$

CONCEPT

H-atom energies $E_n = -13.6/n^2$ eV $= -Z^2/2n^2$ au. $\psi_n lm = R_n l(r)\cdot Y_l\hat{}m(\theta,\varphi)$. Radial nodes = n–l–1, angular = l, total = n–1.

↓

LOGIC / WORKING

- Key principle: H-atom wavefunctions and quantum numbers. Answer is (B).

FINAL: (B) $2\,\mathbf{T} = -\mathbf{V}$

SHORTCUT / EXAM TRICK

Degeneracy = n^2 (spatial). Bohr radius $a_0 = 0.529$ Å. IE $\propto Z^2$ for hydrogenic ions.

COMMON MISTAKE

Confusing total nodes (n–1) with radial (n–l–1) or angular (l) nodes.

EXAM TIP

Virial for Coulomb potential: $\langle T\rangle = -E_n$, $\langle V\rangle = 2E_n$. Variational: $\langle E\rangle \geq E_exact$.

MEMORY TRICK

TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Why the Other Options Are Wrong

Correct answer: **B**

A **T = V**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (B). See worked explanation.

C **2 T = V**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (B). See worked explanation.

D **T = −2 V**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (B). See worked explanation.

Q13

Which of the following is true for the radial part of the hydrogen atom wavefunctions Rnl(r) (n principal quantum number) and the nodes associated with them?

A. The radial part of only s function is non-zero at the origin and has (n – 1) nodes.

B. The radial part of s function is zero at the origin and has n number of nodes.

C. All radial functions have values of zero at the origin and have (n –1) nodes.

D. The radial parts of all s functions are zero at the origin and have no nodes.

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Quantum numbers, nodes, degeneracy, virial theorem

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Correct Answer A The radial part of only s function is non-zero at the origin and has (n – 1) nodes.

CONCEPT

H-atom energies $E_n = -13.6/n^2$ eV = $-Z^2/2n^2$ au. $\psi_n lm = R_n l(r)\cdot Y_l\hat{}m(\theta,\varphi)$. Radial nodes = n–l–1, angular = l, total = n–1.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (A).

FINAL: (A) The radial part of only s function is non-zero at the origin and has (n – 1) nodes.

SHORTCUT / EXAM TRICK

Degeneracy = n^2 (spatial). Bohr radius a_0 = 0.529 Å. IE ∝ Z^2 for hydrogenic ions.

COMMON MISTAKE

Confusing total nodes (n–1) with radial (n–l–1) or angular (l) nodes.

EXAM TIP

Virial for Coulomb potential: $\langle T\rangle = -E_n$, $\langle V\rangle = 2E_n$. Variational: $\langle E\rangle \geq E_exact$.

MEMORY TRICK

TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Why the Other Options Are Wrong

Correct answer: **A**

B **The radial part of s function is zero at the origin and has n number of nodes.**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (A). See worked explanation.

C **All radial functions have values of zero at the origin and have (n –1) nodes.**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (A). See worked explanation.

D **The radial parts of all s functions are zero at the origin and have no nodes.**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (A). See worked explanation.

Q36

The hydrogenic orbital with the form of the radial function r 2 (α1 − r)(α2 − r)exp [−βr] where a1, a2 and b are constants, may be identified as a

A. 3d orbital

B. 4f orbital

C. 5d orbital

D. 5f orbital

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Quantum numbers, nodes, degeneracy, virial theorem

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Correct Answer C 5d orbital

CONCEPT

H-atom energies $E_n = -13.6/n^2$ eV $= -Z^2/2n^2$ au. $\psi_n lm = R_n l(r)\cdot Y_l\hat{}m(\theta,\varphi)$. Radial nodes = n–l–1, angular = l, total = n–1.

↓

LOGIC / WORKING

- Key principle: H-atom wavefunctions and quantum numbers. Answer is (C).

FINAL: (C) 5d orbital

SHORTCUT / EXAM TRICK

Degeneracy = n^2 (spatial). Bohr radius a_0 = 0.529 Å. IE $\propto Z^2$ for hydrogenic ions.

COMMON MISTAKE

Confusing total nodes (n–1) with radial (n–l–1) or angular (l) nodes.

EXAM TIP

Virial for Coulomb potential: $\langle T\rangle = -E_n$, $\langle V\rangle = 2E_n$. Variational: $\langle E\rangle \geq E_exact$.

MEMORY TRICK

TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Why the Other Options Are Wrong

Correct answer: **C**

A **3d orbital**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (C). See worked explanation.

B **4f orbital**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (C). See worked explanation.

D **5f orbital**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (C). See worked explanation.

Q41

The orbital with two radial and two angular nodes is

A. 3p

B. 5d

C. 5f

D. 8d

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Quantum numbers, nodes, degeneracy, virial theorem

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Correct Answer B 5d

CONCEPT

H-atom energies $E_n = -13.6/n^2$ eV $= -Z^2/2n^2$ au. $\psi_n lm = R_n l(r)\cdot Y_l\hat{}m(\theta,\varphi)$. Radial nodes = n–l–1, angular = l, total = n–1.

↓

LOGIC / WORKING

- Key principle: H-atom wavefunctions and quantum numbers. Answer is (B).

FINAL: (B) 5d

SHORTCUT / EXAM TRICK

Degeneracy = n^2 (spatial). Bohr radius a_0 = 0.529 Å. IE $\propto Z^2$ for hydrogenic ions.

COMMON MISTAKE

Confusing total nodes (n–1) with radial (n–l–1) or angular (l) nodes.

EXAM TIP

Virial for Coulomb potential: $\langle T\rangle = -E_n$, $\langle V\rangle = 2E_n$.
Variational: $\langle E\rangle \geq E_exact$.

MEMORY TRICK

TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Why the Other Options Are Wrong

Correct answer: **B**

A — **3p**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (B). See worked explanation.

C — **5f**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (B). See worked explanation.

D — **8d**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (B). See worked explanation.

Q45

The most probable value of ‘r’ for an electron in 1s orbital of hydrogen atom is

A. a0 / 2

B. a0

C. 2a0

D. 3a0 / 2

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Quantum numbers, nodes, degeneracy, virial theorem

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Correct Answer B a0

CONCEPT

H-atom energies $E_n = -13.6/n^2$ eV $= -Z^2/2n^2$ au. $\psi_n lm = R_n l(r)\cdot Y_l\hat{}m(\theta,\varphi)$. Radial nodes = n–l–1, angular = l, total = n–1.

↓

LOGIC / WORKING

- Key principle: H-atom wavefunctions and quantum numbers. Answer is (B).

FINAL: (B) a0

SHORTCUT / EXAM TRICK

Degeneracy = n^2 (spatial). Bohr radius a_0 = 0.529 Å. IE $\propto Z^2$ for hydrogenic ions.

COMMON MISTAKE

Confusing total nodes (n–1) with radial (n–l–1) or angular (l) nodes.

EXAM TIP

Virial for Coulomb potential: $\langle T\rangle = -E_n$, $\langle V\rangle = 2E_n$. Variational: $\langle E\rangle \geq E_exact$.

MEMORY TRICK

TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Why the Other Options Are Wrong

Correct answer: **B**

A — **a0 / 2**

Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (B). See worked explanation.

C — **2a0**

Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (B). See worked explanation.

D — **3a0 / 2**

Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (B). See worked explanation.

Q48 The number of radial nodes for a 3d orbital of hydrogen atom is:

A 0

B 1

C 2

D 3

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Quantum numbers, nodes, degeneracy, virial theorem

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Correct Answer A 0

CONCEPT

H-atom energies $E_n = -13.6/n^2$ eV $= -Z^2/2n^2$ au. $\psi_n lm = R_n l(r)\cdot Y_l\hat{}m(\theta,\varphi)$. Radial nodes = n–l–1, angular = l, total = n–1.

↓

LOGIC / WORKING

- See H-atom wavefunctions and quantum numbers. The correct answer is (A).

FINAL: (A) 0

SHORTCUT / EXAM TRICK

Degeneracy = n^2 (spatial). Bohr radius $a_0 = 0.529$ Å. IE $\propto Z^2$ for hydrogenic ions.

COMMON MISTAKE

Confusing total nodes (n–1) with radial (n–l–1) or angular (l) nodes.

EXAM TIP

Virial for Coulomb potential: $\langle T\rangle = -E_n$, $\langle V\rangle = 2E_n$. Variational: $\langle E\rangle \geq E_exact$.

MEMORY TRICK

TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Why the Other Options Are Wrong

Correct answer: **A**

B **1**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (A). See worked explanation.

C **2**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (A). See worked explanation.

D **3**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (A). See worked explanation.

Q51

The ground state energy of hydrogen atom is –13.598 eV. The expectation values of kinetic energy, T and potential energy, V , in units of eV, are

A. T =13.598, V = −27.196

B. T = −27.196, V = 13.598

C. T = −6.799, V = −6.799

D. T =6.799, V = −20.397

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Quantum numbers, nodes, degeneracy, virial theorem

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Correct Answer A T =13.598, V = −27.196

CONCEPT

H-atom energies $E_n = -13.6/n^2$ eV = $-Z^2/2n^2$ au. $\psi_n lm = R_n l(r)\cdot Y_l\hat{}m(\theta,\varphi)$. Radial nodes = n–l–1, angular = l, total = n–1.

↓

LOGIC / WORKING

- Key principle: H-atom wavefunctions and quantum numbers. Answer is (A).

FINAL: (A) T **=13.598,** V **= −27.196**

SHORTCUT / EXAM TRICK

Degeneracy = n^2 (spatial). Bohr radius a_0 = 0.529 Å. IE ∝ Z^2 for hydrogenic ions.

COMMON MISTAKE

Confusing total nodes (n–1) with radial (n–l–1) or angular (l) nodes.

EXAM TIP

Virial for Coulomb potential: <T> = $-E_n$, <V> = $2E_n$. Variational: <E> ≥ E_exact.

MEMORY TRICK

TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Why the Other Options Are Wrong

Correct answer: **A**

B — ***T*** **= −27.196,** ***V*** **= 13.598**

Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (A). See worked explanation.

C — ***T*** **= −6.799,** ***V*** **= −6.799**

Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (A). See worked explanation.

D — ***T*** **=6.799,** ***V*** **= −20.397**

Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (A). See worked explanation.

Q61

For the normalized hydrogen 1s wavefunction $\psi = (1/\sqrt{\pi})(1/a_0)^{(3/2)} e^{(-r/a_0)}$, the expectation value $\langle r \rangle$ is:

A. a_0

B. $(3/2)a_0$

C. $2a_0$

D. $3a_0$

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Quantum numbers, nodes, degeneracy, virial theorem

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Correct Answer B $(3/2)a_0$

CONCEPT

H-atom energies $E_n = -13.6/n^2$ eV $= -Z^2/2n^2$ au. $\psi_n lm = R_n l(r)\cdot Y_l\hat{}m(\theta,\varphi)$. Radial nodes = n–l–1, angular = l, total = n–1.

↓

LOGIC / WORKING

- See the postulates of QM and wavefunction requirements. The correct answer is (B).

FINAL: (B) $(3/2)a_0$

SHORTCUT / EXAM TRICK

Degeneracy = n^2 (spatial). Bohr radius a_0 = 0.529 Å. IE $\propto Z^2$ for hydrogenic ions.

COMMON MISTAKE

Confusing total nodes (n–1) with radial (n–l–1) or angular (l) nodes.

EXAM TIP

Virial for Coulomb potential: $\langle T\rangle = -E_n$, $\langle V\rangle = 2E_n$. Variational: $\langle E\rangle \geq E_exact$.

MEMORY TRICK

TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Why the Other Options Are Wrong

Correct answer: **B**

A a_0

Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (B). See worked explanation.

C $2a_0$

Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (B). See worked explanation.

D $3a_0$

Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (B). See worked explanation.

Q63

A Slater determinant corresponding to the ionic part of the ground state valence bond wave function of H2 molecule is (1saα, 1saβ!, 1sbα, 1sbβ!!are atomic spin-orbitals of hydrogen atoms a and b of the hydrogen molecule) $1s_a$ α(1) $1s_a$ β(1)

A. 1***sa*** α(2) 1***sa*** β(2)

B. 1***sa*** α(2) 1***sb*** β(2)

C. 1***sa*** α(2) 1***sb*** α(2)

D. 1***sa*** α(1) 1***sb*** β(2)

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Quantum numbers, nodes, degeneracy, virial theorem

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Correct Answer A $1sa\ \alpha(2)\ 1sa\ \beta(2)$

CONCEPT

H-atom energies $E_n = -13.6/n^2$ eV $= -Z^2/2n^2$ au. $\psi_n lm = R_n l(r)\cdot Y_l\hat{}m(\theta,\varphi)$. Radial nodes = n–l–1, angular = l, total = n–1.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (A).

FINAL: (A) $1sa\ \alpha(2)\ 1sa\ \beta(2)$

SHORTCUT / EXAM TRICK

Degeneracy = n^2 (spatial). Bohr radius a_0 = 0.529 Å. IE $\propto Z^2$ for hydrogenic ions.

COMMON MISTAKE

Confusing total nodes (n–1) with radial (n–l–1) or angular (l) nodes.

EXAM TIP

Virial for Coulomb potential: $\langle T\rangle = -E_n$, $\langle V\rangle = 2E_n$. Variational: $\langle E\rangle \geq E_exact$.

MEMORY TRICK

TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Why the Other Options Are Wrong

Correct answer: **A**

B **1*sa* α(2) 1*sb* β(2)**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (A). See worked explanation.

C **1*sa* α(2) 1*sb* α(2)**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (A). See worked explanation.

D **1*sa* α(1) 1*sb* β(2)**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (A). See worked explanation.

Q66

For the hydrogen atom, the radial distribution function $4\pi r^2 R^2(r)$ for the 1s orbital is maximum at:

A. $r = 0$

B. $r = a_0$ (Bohr radius)

C. $r = 2a_0$

D. $r \to \infty$

SELF-PRACTICE official answer key not printed in the source — attempt this, then verify.

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Quantum numbers, nodes, degeneracy, virial theorem

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Q75

The number of nodes (radial + angular) in a 3p orbital of hydrogen is:

A. 1

B. 2

C. 3

D. 0

SELF-PRACTICE official answer key not printed in the source — attempt this, then verify.

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Quantum numbers, nodes, degeneracy, virial theorem

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Q83

The number of angular nodes in a 4f orbital of hydrogen is:

A. 0

B. 1

C. 2

D. 3

QUESTION INSIGHTS

ESTIMATED TIME
1–1.5 min

DIFFICULTY
Easy

CONCEPT TESTED
Quantum numbers, nodes, degeneracy, virial theorem

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★☆☆

EXPECTED LEVEL
Part B

MEMORY HOOK
TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Correct Answer D 3

CONCEPT

H-atom energies $E_n = -13.6/n^2$ eV $= -Z^2/2n^2$ au. $\psi_n lm = R_n l(r)\cdot Y_l\hat{}m(\theta,\varphi)$. Radial nodes = n–l–1, angular = l, total = n–1.

↓

LOGIC / WORKING

- See H-atom wavefunctions and quantum numbers. The correct answer is (D).

FINAL: (D) 3

SHORTCUT / EXAM TRICK

Degeneracy = n^2 (spatial). Bohr radius $a_0 = 0.529$ Å. IE $\propto Z^2$ for hydrogenic ions.

COMMON MISTAKE

Confusing total nodes (n–1) with radial (n–l–1) or angular (l) nodes.

EXAM TIP

Virial for Coulomb potential: $\langle T\rangle = -E_n$, $\langle V\rangle = 2E_n$. Variational: $\langle E\rangle \geq E_exact$.

MEMORY TRICK

TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Why the Other Options Are Wrong

Correct answer: **D**

A **0**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (D). See worked explanation.

B **1**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (D). See worked explanation.

C **2**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (D). See worked explanation.

Q84

In simple molecular orbital theory of hydrogen molecule, bonding σg and anti-bonding σu molecular orbitals are constructed as linear combinations of atomic orbitals of two hydrogen atoms. The spatial part of a purely covalent singlet wave function is obtained by

A. σg2 + σu2

B. σg2

C. σg2 - σu2

D. σg2 + σu2

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Quantum numbers, nodes, degeneracy, virial theorem

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Correct Answer C σg2 - σu2

CONCEPT

H-atom energies $E_n = -13.6/n^2$ eV = $-Z^2/2n^2$ au. $\psi_n lm = R_n l(r)\cdot Y_l\hat{}m(\theta,\varphi)$. Radial nodes = n–l–1, angular = l, total = n–1.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (C).

FINAL: (C) σg2 - σu2

SHORTCUT / EXAM TRICK

Degeneracy = n^2 (spatial). Bohr radius a_0 = 0.529 Å. IE ∝ Z^2 for hydrogenic ions.

COMMON MISTAKE

Confusing total nodes (n–1) with radial (n–l–1) or angular (l) nodes.

EXAM TIP

Virial for Coulomb potential: $\langle T\rangle = -E_n$, $\langle V\rangle = 2E_n$. Variational: $\langle E\rangle \geq E_exact$.

MEMORY TRICK

TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Why the Other Options Are Wrong

Correct answer: **C**

A — **σg2 + σu2**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (C). See worked explanation.

B — **σg2**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (C). See worked explanation.

D — **σg2 + σu2**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (C). See worked explanation.

Q92

The two limiting wave functions of the ground state of H2+ molecular ion, as the internuclear separation R goes to (i) ∞(infinity) and (ii) 0 (zero) are (1sa, 1sb are 1s-orbital wave functions of hydrogen atoms a and b in H2+, and 1sHe is the wave function of the 1s orbital of He+)

A. (i) 1sa(r); (ii) 1sb(r)

B. (i) 1sb (r); (ii) 1sa (r)

C. (i) 1sa (r1) 1sb (r2) ; (ii) 1s He (r1) 1s He (r2)

D. (i) 1sa (r) + 1sb (r): (ii) 1s He (r)

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Quantum numbers, nodes, degeneracy, virial theorem

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Correct Answer B (i) 1sb (r); (ii) 1sa (r)

CONCEPT

H-atom energies $E_n = -13.6/n^2$ eV = $-Z^2/2n^2$ au. $\psi_n lm = R_n l(r)\cdot Y_l\hat{}m(\theta,\varphi)$. Radial nodes = n–l–1, angular = l, total = n–1.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (B).

FINAL: (B) (i) 1sb (r); (ii) 1sa (r)

SHORTCUT / EXAM TRICK

Degeneracy = n^2 (spatial). Bohr radius a_0 = 0.529 Å. IE $\propto Z^2$ for hydrogenic ions.

COMMON MISTAKE

Confusing total nodes (n–1) with radial (n–l–1) or angular (l) nodes.

EXAM TIP

Virial for Coulomb potential: $\langle T\rangle = -E_n$, $\langle V\rangle = 2E_n$.
Variational: $\langle E\rangle \geq E_exact$.

MEMORY TRICK

TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Why the Other Options Are Wrong

Correct answer: **B**

A **(i) 1sa(r); (ii) 1sb(r)**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (B). See worked explanation.

C **(i) 1sa (r1) 1sb (r2) ; (ii) 1s He (r1) 1s He (r2)**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (B). See worked explanation.

D **(i) 1sa (r) + 1sb (r): (ii) 1s He (r)**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (B). See worked explanation.

Q116 An unnormalized wave function of the hydrogen atom is given by $r2\ e3\ (3cos2\ \theta - 1)$. The three quantum numbers, n, l and m, associated with this orbital are, respectively.

A. 2, 2, 0

B. 2, 1, 1

C. 3, 2, 0

D. 3, 1, 1

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Quantum numbers, nodes, degeneracy, virial theorem

PYQ FREQUENCY
High · 10 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Correct Answer C 3, 2, 0

CONCEPT

H-atom energies $E_n = -13.6/n^2$ eV $= -Z^2/2n^2$ au. $\psi_n lm = R_n l(r)\cdot Y_l\hat{}m(\theta,\varphi)$. Radial nodes = n–l–1, angular = l, total = n–1.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (C).

FINAL: (C) 3, 2, 0

SHORTCUT / EXAM TRICK

Degeneracy = n^2 (spatial). Bohr radius a_0 = 0.529 Å. IE $\propto Z^2$ for hydrogenic ions.

COMMON MISTAKE

Confusing total nodes (n–1) with radial (n–l–1) or angular (l) nodes.

EXAM TIP

Virial for Coulomb potential: $\langle T\rangle = -E_n$, $\langle V\rangle = 2E_n$. Variational: $\langle E\rangle \geq E_exact$.

MEMORY TRICK

TAPS: Total nodes = n–1; Angular = l; radial = n–l–1.

Why the Other Options Are Wrong

Correct answer: **C**

A **2, 2, 0**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (C). See worked explanation.

B **2, 1, 1**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (C). See worked explanation.

D **3, 1, 1**
Inconsistent with H-atom wavefunctions and quantum numbers; correct choice is (C). See worked explanation.

TOPIC REVISION

Hydrogen Atom & Atomic Orbitals

17 PYQs · Last-minute revision

TOPIC SUMMARY

H-atom energies $E_n = -13.6/n^2$ eV $= -Z^2/2n^2$ au. $\psi_n lm =$ $R_n l(r)\cdot Y_l\hat{}m(\theta,\varphi)$. Radial nodes = n–l–1, angular = l, total = n–1.

IMPORTANT FORMULA SHEET

$E_n = -Z^2/2n^2$ au
Total nodes = n–1
Radial nodes = n–l–1
Degeneracy = n^2

FREQUENTLY ASKED CONCEPTS

Radial vs angular nodes
Quantum numbers n,l,m
Degeneracy
- Virial theorem

COMMON MISTAKES & QUICK NOTES

Watch out:
Confusing total nodes (n–1) with radial (n–l–1) or angular (l) nodes.
Last-minute:
Degeneracy = n^2 (spatial). Bohr radius $a_0 = 0.529$ Å. IE $\propto Z^2$ for hydrogenic ions.

MOST-REPEATED PYQs & EXPECTED IN EXAM

PYQs in this topic: Q1 Q9 Q12 Q13 Q36 Q41 Q45 Q48 Q51 Q61 Q63 Q66 Q75 Q83 Q84 Q92 Q116

Expect **3 question(s)** next session on **Quantum numbers, nodes, degeneracy, virial theorem.**

TOPIC 7

Tunneling & Barrier Problems

2 questions · Easy 0 | Medium 2 | Hard 0 · PYQ frequency: Rare

Q6

For a certain particle encountering a barrier, the tunneling probability is approximately e–10. If the mass is halved and width of the barrier (rectangular) doubled, approximate value of the tunneling probability will be

A $e^{-}10/\sqrt{(2)}$

B $e^{-10\sqrt{(2)}}$

C $e^{-20\sqrt{(2)}}$

D e^{-10}

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
WKB tunneling probability, barrier parameters

PYQ FREQUENCY
Rare · 2 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
Thin, light, low barrier = more tunneling. Decay is exponential, not linear.

Tunneling & Barrier Problems

Correct Answer B $e^{-1^{0}\sqrt{(2)}}$

CONCEPT

Quantum tunneling probability $T \approx e^{-2\kappa L}$, $\kappa = \sqrt{(2m(V-E))}/\hbar$. Heavier particle or wider/higher barrier → less tunneling. T rises as E → V.

↓

LOGIC / WORKING

- Key principle: angular momentum quantization and spin algebra. Answer is (B).

FINAL: (B) $e^{-1^{0}\sqrt{(2)}}$

SHORTCUT / EXAM TRICK

Exponent ∝ √m × L × √(V–E). Halve m → ÷√2; double L → ×2.

COMMON MISTAKE

Treating tunneling probability as linear in width or mass — it is exponential.

EXAM TIP

Halving mass ($\kappa \to \kappa/\sqrt{2}$) and doubling width ($L \to 2L$): exponent scales by $2/\sqrt{2} = \sqrt{2}$.

MEMORY TRICK

Thin, light, low barrier = more tunneling. Decay is exponential, not linear.

Why the Other Options Are Wrong

Correct answer: **B**

A $e^{-}10/\sqrt{(2)}$

Inconsistent with tunneling probability and WKB approximation; correct choice is (B). See worked explanation.

C $e^{-2^{o}\sqrt{(2)}}$

Inconsistent with tunneling probability and WKB approximation; correct choice is (B). See worked explanation.

D $e^{-1^{o}}$

Inconsistent with tunneling probability and WKB approximation; correct choice is (B). See worked explanation.

Q127 Let the Hamiltonian H, in one-dimension, be $p2$ H = x + V(x). $2m$ The commutator of H with x , [H, x], is Options: $,ih$ 1. px m $,ih$ 2. $p2x$ $2m$ ih 3. px m ih 4. px $2m$ Quantum Chemistry EXPLANATIONS: 1. CORRECT ANSWER (C) The normalized wave function for 1s orbital of H- atom is given by § , Ψµ= e ans E1s=-0.5 atomic units « § .Ÿ¬ § Since, E = − = − = − ∗ 1.5625 = − ∗ 1.6 = −0.8 Ÿ § Ÿ Ÿ Ÿ So, -0.8<-0.5 . 2. CORRECT ANSWER

A. A is a constant of motion (i.e ,does not change with time) ,if

B. Hermitian conjugate or adjoint of an operator A is written as AÊ , and is defined as

C. Second order perturbation for the nth state is given by

D. Given: Tunneling probability, T=e–2kl=e–10

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
WKB tunneling probability, barrier parameters

PYQ FREQUENCY
Rare · 2 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
Thin, light, low barrier = more tunneling. Decay is exponential, not linear.

Correct Answer A A is a constant of motion (i.e ,does not change with time) ,if

CONCEPT

Quantum tunneling probability $T \approx e^{-2\kappa L}$, $\kappa = \sqrt{(2m(V-E))}/\hbar$. Heavier particle or wider/higher barrier → less tunneling. T rises as E → V.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (A).

FINAL: (A) A is a constant of motion (i.e ,does not change with time) ,if

SHORTCUT / EXAM TRICK

Exponent ∝ √m × L × √(V–E). Halve m → ÷√2; double L → ×2.

COMMON MISTAKE

Treating tunneling probability as linear in width or mass — it is exponential.

EXAM TIP

Halving mass (κ → κ/√2) and doubling width (L → 2L): exponent scales by 2/√2 = √2.

MEMORY TRICK

Thin, light, low barrier = more tunneling. Decay is exponential, not linear.

Why the Other Options Are Wrong

Correct answer: **A**

B **Hermitian conjugate or adjoint of an operator A is written as AÊ , and is defined as**

Inconsistent with tunneling probability and WKB approximation; correct choice is (A). See worked explanation.

C **Second order perturbation for the nth state is given by**

Inconsistent with tunneling probability and WKB approximation; correct choice is (A). See worked explanation.

D **Given: Tunneling probability, T=e−2kl=e−10**

Inconsistent with tunneling probability and WKB approximation; correct choice is (A). See worked explanation.

TOPIC REVISION

Tunneling & Barrier Problems

2 PYQs · Last-minute revision

TOPIC SUMMARY

Quantum tunneling probability $T \approx e^{-2\kappa L}$, $\kappa = \sqrt{(2m(V-E))}/\hbar$. Heavier particle or wider/higher barrier → less tunneling. T rises as E → V.

IMPORTANT FORMULA SHEET

$T \approx e^{-2\kappa L}$

$\kappa = \sqrt{(2m(V-E))}/\hbar$

Exponent $\propto \sqrt{m} \cdot L \cdot \sqrt{(V-E)}$

- $T \to 1$ as $E \to V$

FREQUENTLY ASKED CONCEPTS

Tunneling probability
WKB approximation
Mass & width effects
- Barrier-height dependence

COMMON MISTAKES & QUICK NOTES

Watch out:
Treating tunneling probability as linear in width or mass — it is exponential.
Last-minute:
Exponent $\propto \sqrt{m} \times L \times \sqrt{(V-E)}$. Halve m → ÷√2; double L → ×2.

MOST-REPEATED PYQs & EXPECTED IN EXAM

PYQs in this topic: Q6 Q127

Expect **1 question(s)** next session on **WKB tunneling probability, barrier parameters.**

TOPIC 8

Perturbation & Variation Theory

14 questions · Easy 0 | Medium 9 | Hard 5 · PYQ frequency: Very High

Q4 The unperturbed energy levels are $\varepsilon_0=0$, $\varepsilon_1=2$, $\varepsilon_2=4$. With perturbation $V_{10}=2$, $V_{20}=4$, $V_{12}=6$, the second-order correction to ground state energy is:

A. –6

B. 0

C. +6

D. –8

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Perturbation corrections, variational upper bound

PYQ FREQUENCY
Very High · 13 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
First order = diagonal average; second order = mix-in excited states (lowers ground state).

Correct Answer A –6

CONCEPT

First-order: $E_n^{(1)} = \langle n|\hat{H}'|n\rangle$. Second-order: $E_n^{(2)} = \Sigma_{k\neq n} |\langle k|H'|n\rangle|^2/(E_n - E_k)$. Variational: <E>_trial ≥ E_exact.

↓

LOGIC / WORKING

See the particle-in-a-box energy formula $E_n = n^2h^2/8mL^2$. The correct answer is (A).

FINAL: (A) –6

SHORTCUT / EXAM TRICK

$E^{(2)}$ is always negative for the ground state. $E^{(0)}+E^{(1)}$ is a variational upper bound.

COMMON MISTAKE

Thinking $E^{(1)}$ is necessarily negative — only $E^{(2)}$ is, for the ground state.

EXAM TIP

Second-order correction always LOWERS the ground state. Parity can make $E^{(1)}$ vanish.

MEMORY TRICK

First order = diagonal average; second order = mix-in excited states (lowers ground state).

Why the Other Options Are Wrong

Correct answer: **A**

B **0**
Inconsistent with variational principle and perturbation corrections; correct choice is (A). See worked explanation.

C **+6**
Inconsistent with variational principle and perturbation corrections; correct choice is (A). See worked explanation.

D **–8**
Inconsistent with variational principle and perturbation corrections; correct choice is (A). See worked explanation.

Q14

For non-degenerate perturbation theory for ground state, with E0 as zeroth order energy, (1) E0 as the first-order perturbation correction and E0 as the exact energy, which of the following is true? (0) (1)

A. **E**0 + **E**0 is always equal to **E**0

B. **E**0 + **E**0 ≤ **E**0

C. **E**0 + **E**0 ≥ **E**0

D. **E**0 ≤ **E**01 + **E**0

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Perturbation corrections, variational upper bound

PYQ FREQUENCY
Very High · 13 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
First order = diagonal average; second order = mix-in excited states (lowers ground state).

Correct Answer C **E0 + E0 ≥ E0**

CONCEPT

First-order: $E_n^{(1)} = \langle n|\hat{H}'|n\rangle$. Second-order: $E_n^{(2)} = \Sigma_{k\neq n} |\langle k|H'|n\rangle|^2/(E_n - E_k)$. Variational: <E>_trial ≥ E_exact.

↓

LOGIC / WORKING

- Key principle: variational principle and perturbation corrections. Answer is (C).

FINAL: (C) E0 + E0 ≥ E0

SHORTCUT / EXAM TRICK

$E^{(2)}$ is always negative for the ground state. $E^{(0)}+E^{(1)}$ is a variational upper bound.

COMMON MISTAKE

Thinking $E^{(1)}$ is necessarily negative — only $E^{(2)}$ is, for the ground state.

EXAM TIP

Second-order correction always LOWERS the ground state. Parity can make $E^{(1)}$ vanish.

MEMORY TRICK

First order = diagonal average; second order = mix-in excited states (lowers ground state).

Why the Other Options Are Wrong

Correct answer: C

A **E0 + E0 is always equal to E0**
Inconsistent with variational principle and perturbation corrections; correct choice is (C). See worked explanation.

B **E0 + E0 ≤ E0**
Inconsistent with variational principle and perturbation corrections; correct choice is (C). See worked explanation.

D **E0 ≤ E01 + E0**
Inconsistent with variational principle and perturbation corrections; correct choice is (C). See worked explanation.

Q21 The following are the three statements about perturbation theory

A. Second order perturbation correction to the ground state energy is ALWAYS negative.

B. Sum of the zeroth order and the first order corrections to the ground state energy is ALWAYS

C. Sum of the zeroth order and first order corrections to the ground state energy is less than the

D. Only A is true

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Perturbation corrections, variational upper bound

PYQ FREQUENCY
Very High · 13 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
First order = diagonal average; second order = mix-in excited states (lowers ground state).

Correct Answer B Sum of the zeroth order and the first order corrections to the ground state energy is ALWAYS

CONCEPT

First-order: $E_n^{(1)} = \langle n|\hat{H}'|n\rangle$. Second-order: $E_n^{(2)} = \Sigma_{k\neq n} |\langle k|H'|n\rangle|^2/(E_n - E_k)$. Variational: <E>_trial ≥ E_exact.

↓

LOGIC / WORKING

- Key principle: variational principle and perturbation corrections. Answer is (B).

FINAL: (B) Sum of the zeroth order and the first order corrections to the ground state energy is ALWAYS

SHORTCUT / EXAM TRICK

$E^{(2)}$ is always negative for the ground state. $E^{(0)}+E^{(1)}$ is a variational upper bound.

COMMON MISTAKE

Thinking $E^{(1)}$ is necessarily negative — only $E^{(2)}$ is, for the ground state.

EXAM TIP

Second-order correction always LOWERS the ground state. Parity can make $E^{(1)}$ vanish.

MEMORY TRICK

First order = diagonal average; second order = mix-in excited states (lowers ground state).

Why the Other Options Are Wrong

Correct answer: **B**

A **Second order perturbation correction to the ground state energy is ALWAYS negative.**
Inconsistent with variational principle and perturbation corrections; correct choice is (B). See worked explanation.

C **Sum of the zeroth order and first order corrections to the ground state energy is less than the**
Inconsistent with variational principle and perturbation corrections; correct choice is (B). See worked explanation.

D **Only A is true**
Inconsistent with variational principle and perturbation corrections; correct choice is (B). See worked explanation.

Q27

The trial wave function of a system is expanded as $\psi t = c1\ \varphi 1 + c2\ \varphi 2$. The matrix elements of the Hamiltonian are $\varphi 1\ H\ \varphi 1 = 0$; $\varphi 1\ H\ \varphi 2 = 2.\ 0 = \varphi 2\ H\ \varphi 1$ and $\varphi 2\ H\ \varphi 2 = 3.\ 0$. The approximate ground-state energy of the system from the linear variational principle is

A. –1.0

B. –2.0

C. +4.0

D. +5.0

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Perturbation corrections, variational upper bound

PYQ FREQUENCY
Very High · 13 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
First order = diagonal average; second order = mix-in excited states (lowers ground state).

Correct Answer A –1.0

CONCEPT

First-order: $E_n^{(1)} = \langle n|\hat{H}'|n\rangle$. Second-order: $E_n^{(2)} = \Sigma_{k\neq n} |\langle k|H'|n\rangle|^2/(E_n - E_k)$. Variational: <E>_trial ≥ E_exact.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (A).

FINAL: (A) –1.0

SHORTCUT / EXAM TRICK

$E^{(2)}$ is always negative for the ground state. $E^{(0)}+E^{(1)}$ is a variational upper bound.

COMMON MISTAKE

Thinking $E^{(1)}$ is necessarily negative — only $E^{(2)}$ is, for the ground state.

EXAM TIP

Second-order correction always LOWERS the ground state. Parity can make $E^{(1)}$ vanish.

MEMORY TRICK

First order = diagonal average; second order = mix-in excited states (lowers ground state).

Why the Other Options Are Wrong

Correct answer: **A**

B **–2.0**
Inconsistent with variational principle and perturbation corrections; correct choice is (A). See worked explanation.

C **+4.0**
Inconsistent with variational principle and perturbation corrections; correct choice is (A). See worked explanation.

D **+5.0**
Inconsistent with variational principle and perturbation corrections; correct choice is (A). See worked explanation.

Q33 The trial wavefunction of a system is expanded as $\psi_t = c_1\varphi_1 + c_2\varphi_2$. The matrix elements of the Hamiltonian and overlap are used in the variational method to obtain:

(A) The exact ground state energy

(B) An upper bound to the ground state energy

(C) A lower bound to the ground state energy

(D) The first excited state energy only

SELF-PRACTICE official answer key not printed in the source — attempt this, then verify.

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Perturbation corrections, variational upper bound

PYQ FREQUENCY
Very High · 13 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
First order = diagonal average; second order = mix-in excited states (lowers ground state).

Q44

Consider a particle in a one dimensional box of length ‘a’ with the following potential V(x)=∞ x<0 V(x)=∞ x>a V(x)=0 0 ≤ x ≤ a/2 V(x)=V1 a/2 ≤ x ≤ a Starting with the standard particle in a box hamiltonian as the zeroth order Hamiltonian and the Quantum Chemistry potential of V1 from ‘a/2’ to ‘a’ as a perturbation, thefirst-order energy correction to the ground state is

A. V1

B. V1/4

C. –V1

D. V1/2

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Perturbation corrections, variational upper bound

PYQ FREQUENCY
Very High · 13 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
First order = diagonal average; second order = mix-in excited states (lowers ground state).

Correct Answer D V1/2

CONCEPT

First-order: $E_n^{(1)} = \langle n|\hat{H}'|n\rangle$. Second-order: $E_n^{(2)} = \Sigma_{k\neq n} |\langle k|H'|n\rangle|^2/(E_n - E_k)$. Variational: <E>_trial ≥ E_exact.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (D).

FINAL: (D) V1/2

SHORTCUT / EXAM TRICK

$E^{(2)}$ is always negative for the ground state. $E^{(0)}+E^{(1)}$ is a variational upper bound.

COMMON MISTAKE

Thinking $E^{(1)}$ is necessarily negative — only $E^{(2)}$ is, for the ground state.

EXAM TIP

Second-order correction always LOWERS the ground state. Parity can make $E^{(1)}$ vanish.

MEMORY TRICK

First order = diagonal average; second order = mix-in excited states (lowers ground state).

Why the Other Options Are Wrong

Correct answer: **D**

A — **V1**
Inconsistent with variational principle and perturbation corrections; correct choice is (D). See worked explanation.

B — **V1/4**
Inconsistent with variational principle and perturbation corrections; correct choice is (D). See worked explanation.

C — **–V1**
Inconsistent with variational principle and perturbation corrections; correct choice is (D). See worked explanation.

Q50

A particle in a one-dimensional box (potential zero between to a and infinite outside) has the 0.125h2 ground state energy E0= The expectation value of the above Hamiltonian with $\psi(x) = ma2\ x(x - a)$ yields an energy E1. Using a linear combination of two even functions $x\ x - a$ and $x2\ (x - a)2$ we obtain variational mainimum to the ground state energy as E2. Which of the following relations holds for E0, E1 and E2?

A. E0 < E1 < E2

B. E0 < E2 < E1

C. E1 < E0 < E2

D. E2 < E0 < E1

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Perturbation corrections, variational upper bound

PYQ FREQUENCY
Very High · 13 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
First order = diagonal average; second order = mix-in excited states (lowers ground state).

Correct Answer B E0 < E2 < E1

CONCEPT

First-order: $E_n^{(1)} = \langle n|\hat{H}'|n\rangle$. Second-order: $E_n^{(2)} = \Sigma_{k\neq n} |\langle k|H'|n\rangle|^2/(E_n - E_k)$. Variational: <E>_trial ≥ E_exact.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (B).

FINAL: (B) E0 < E2 < E1

SHORTCUT / EXAM TRICK

$E^{(2)}$ is always negative for the ground state. $E^{(0)}+E^{(1)}$ is a variational upper bound.

COMMON MISTAKE

Thinking $E^{(1)}$ is necessarily negative — only $E^{(2)}$ is, for the ground state.

EXAM TIP

Second-order correction always LOWERS the ground state. Parity can make $E^{(1)}$ vanish.

MEMORY TRICK

First order = diagonal average; second order = mix-in excited states (lowers ground state).

Why the Other Options Are Wrong

Correct answer: **B**

A **E0 < E1 < E2**
Inconsistent with variational principle and perturbation corrections; correct choice is (B). See worked explanation.

C **E1 < E0 < E2**
Inconsistent with variational principle and perturbation corrections; correct choice is (B). See worked explanation.

D **E2 < E0 < E1**
Inconsistent with variational principle and perturbation corrections; correct choice is (B). See worked explanation.

Q55

A particle in a one dimensional harmonic oscillator in x-direction is perturbed by a potential λ x (λ is number). The first-order correction to the energy of the ground state

A. is zero

B. is negative

C. is positive

D. may be negative or positive but not zero

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Perturbation corrections, variational upper bound

PYQ FREQUENCY
Very High · 13 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
First order = diagonal average; second order = mix-in excited states (lowers ground state).

Correct Answer A is zero

CONCEPT

First-order: $E_n^{(1)} = \langle n|\hat{H}'|n\rangle$. Second-order: $E_n^{(2)} = \Sigma_{k\neq n} |\langle k|H'|n\rangle|^2/(E_n - E_k)$. Variational: <E>_trial ≥ E_exact.

↓

LOGIC / WORKING

Key principle: the particle-in-a-box energy formula $E_n = n^2h^2/8mL^2$. Answer is (A).

FINAL: (A) is zero

SHORTCUT / EXAM TRICK

$E^{(2)}$ is always negative for the ground state. $E^{(0)}+E^{(1)}$ is a variational upper bound.

COMMON MISTAKE

Thinking $E^{(1)}$ is necessarily negative — only $E^{(2)}$ is, for the ground state.

EXAM TIP

Second-order correction always LOWERS the ground state. Parity can make $E^{(1)}$ vanish.

MEMORY TRICK

First order = diagonal average; second order = mix-in excited states (lowers ground state).

Why the Other Options Are Wrong

Correct answer: **A**

B **is negative**
Inconsistent with variational principle and perturbation corrections; correct choice is (A). See worked explanation.

C **is positive**
Inconsistent with variational principle and perturbation corrections; correct choice is (A). See worked explanation.

D **may be negative or positive but not zero**
Inconsistent with variational principle and perturbation corrections; correct choice is (A). See worked explanation.

Q62

For some one-electron system with l = 0 and m = 0, the functions $No\ e$,σ and $N1\ (2 - σ)e$,σ refer respectively to the ground (Eo) and first excited (E1) energy levels. If a variational wave function $N2\ (3 - σ)e$,σ yields an average energy E, it will satisfy

A. $E \geq 0$

B. $0 \leq E \leq Eo$

C. $E \geq E1$

D. $Eo \leq E \leq E1$

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Perturbation corrections, variational upper bound

PYQ FREQUENCY
Very High · 13 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
First order = diagonal average; second order = mix-in excited states (lowers ground state).

Correct Answer C $E \geq E1$

CONCEPT

First-order: $E_n^{(1)} = \langle n|\hat{H}'|n\rangle$. Second-order: $E_n^{(2)} = \Sigma_{k\neq n} |\langle k|H'|n\rangle|^2/(E_n - E_k)$. Variational: <E>_trial ≥ E_exact.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (C).

FINAL: (C) $E \geq E1$

SHORTCUT / EXAM TRICK

$E^{(2)}$ is always negative for the ground state. $E^{(0)}+E^{(1)}$ is a variational upper bound.

COMMON MISTAKE

Thinking $E^{(1)}$ is necessarily negative — only $E^{(2)}$ is, for the ground state.

EXAM TIP

Second-order correction always LOWERS the ground state. Parity can make $E^{(1)}$ vanish.

MEMORY TRICK

First order = diagonal average; second order = mix-in excited states (lowers ground state).

Why the Other Options Are Wrong

Correct answer: C

A $E \geq 0$

Inconsistent with variational principle and perturbation corrections; correct choice is (C). See worked explanation.

B $0 \leq E \leq Eo$

Inconsistent with variational principle and perturbation corrections; correct choice is (C). See worked explanation.

D $Eo \leq E \leq E1$

Inconsistent with variational principle and perturbation corrections; correct choice is (C). See worked explanation.

Q74

A certain 2-level system has stationary state energies E1 and E2 (E1<E2) with normalized wave functions $\varphi 1$ and $\varphi 2$ respectively. In the presence of a perturbation V, the second-order correction to the energy for the first state ($\varphi 1$) will be $\varphi 1\ V\ \varphi 2$

A. $E1, E2$

B. $E2, E1$

C. $E1, E2$

D. $E1, E2\ 2$

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Perturbation corrections, variational upper bound

PYQ FREQUENCY
Very High · 13 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
First order = diagonal average; second order = mix-in excited states (lowers ground state).

Correct Answer C ***E*1 ,*E*2**

CONCEPT

First-order: $E_n^{(1)} = \langle n|\hat{H}'|n\rangle$. Second-order: $E_n^{(2)} = \Sigma_{k\neq n} |\langle k|H'|n\rangle|^2/(E_n - E_k)$. Variational: <E>_trial ≥ E_exact.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (C).

FINAL: (C) *E*1 ,*E*2

SHORTCUT / EXAM TRICK

$E^{(2)}$ is always negative for the ground state. $E^{(0)}+E^{(1)}$ is a variational upper bound.

COMMON MISTAKE

Thinking $E^{(1)}$ is necessarily negative — only $E^{(2)}$ is, for the ground state.

EXAM TIP

Second-order correction always LOWERS the ground state. Parity can make $E^{(1)}$ vanish.

MEMORY TRICK

First order = diagonal average; second order = mix-in excited states (lowers ground state).

Why the Other Options Are Wrong

Correct answer: **C**

A ***E*1 ,*E*2**
Inconsistent with variational principle and perturbation corrections; correct choice is (C). See worked explanation.

B ***E*2 ,*E*1**
Inconsistent with variational principle and perturbation corrections; correct choice is (C). See worked explanation.

D ***E*1 ,*E*2 2**
Inconsistent with variational principle and perturbation corrections; correct choice is (C). See worked explanation.

Q88 The ground state of a certain system with energy $\in 0$, is subjected to a perturbation V, yielding a first order correction $\in 1$. If E0 is the true ground-state energy of the perturbed system, the inequality that **always** holds is

A $\in 1 \geq 0$

B $\in 1 \geq E0$

C $\in 0 + \in 1 \leq E$”

D $\in 0 + \in 1 \geq E$”

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Perturbation corrections, variational upper bound

PYQ FREQUENCY
Very High · 13 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
First order = diagonal average; second order = mix-in excited states (lowers ground state).

Correct Answer B $\in 1 \geq E0$

CONCEPT

First-order: $E_n^{(1)} = \langle n|\hat{H}'|n\rangle$. Second-order: $E_n^{(2)} = \Sigma_{k\neq n} |\langle k|H'|n\rangle|^2/(E_n - E_k)$. Variational: <E>_trial ≥ E_exact.

↓

LOGIC / WORKING

- Key principle: variational principle and perturbation corrections. Answer is (B).

FINAL: (B) $\in 1 \geq E0$

SHORTCUT / EXAM TRICK

$E^{(2)}$ is always negative for the ground state. $E^{(0)}+E^{(1)}$ is a variational upper bound.

COMMON MISTAKE

Thinking $E^{(1)}$ is necessarily negative — only $E^{(2)}$ is, for the ground state.

EXAM TIP

Second-order correction always LOWERS the ground state. Parity can make $E^{(1)}$ vanish.

MEMORY TRICK

First order = diagonal average; second order = mix-in excited states (lowers ground state).

Why the Other Options Are Wrong

Correct answer: **B**

A $\in 1 \geq 0$

Inconsistent with variational principle and perturbation corrections; correct choice is (B). See worked explanation.

C $\in 0 + \in 1 \leq E$”

Inconsistent with variational principle and perturbation corrections; correct choice is (B). See worked explanation.

D $\in 0 + \in 1 \geq E$”

Inconsistent with variational principle and perturbation corrections; correct choice is (B). See worked explanation.

Q108

Which of the following statements on ground state perturbation theory, involving the zeroth (0) (1) (2) order energy $E0$, first order energy correction $E0$ and second order energy correction $E0$, is false? ( )

A *E*” is the average value of perturbation operator with respect to the ground state of the zeroth order

B *E*” is necessarily negative.

C *E*” is necessarily negative.

D *E*” +*E*” is an upper bound to the exact ground state energy.

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Perturbation corrections, variational upper bound

PYQ FREQUENCY
Very High · 13 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
First order = diagonal average; second order = mix-in excited states (lowers ground state).

Correct Answer B *E*” is necessarily negative.

CONCEPT

First-order: $E_n^{(1)} = \langle n|\hat{H}'|n\rangle$. Second-order: $E_n^{(2)} = \Sigma_{k\neq n} |\langle k|H'|n\rangle|^2/(E_n - E_k)$. Variational: <E>_trial ≥ E_exact.

↓

LOGIC / WORKING

- Key principle: variational principle and perturbation corrections. Answer is (B).

FINAL: (B) *E*” is necessarily negative.

SHORTCUT / EXAM TRICK

$E^{(2)}$ is always negative for the ground state. $E^{(0)}+E^{(1)}$ is a variational upper bound.

COMMON MISTAKE

Thinking $E^{(1)}$ is necessarily negative — only $E^{(2)}$ is, for the ground state.

EXAM TIP

Second-order correction always LOWERS the ground state. Parity can make $E^{(1)}$ vanish.

MEMORY TRICK

First order = diagonal average; second order = mix-in excited states (lowers ground state).

Why the Other Options Are Wrong

Correct answer: **B**

A — ***E*" is the average value of perturbation operator with respect to the ground state of the zeroth order**

Inconsistent with variational principle and perturbation corrections; correct choice is (B). See worked explanation.

C — ***E*" is necessarily negative.**

Inconsistent with variational principle and perturbation corrections; correct choice is (B). See worked explanation.

D — ***E*" +*E*" is an upper bound to the exact ground state energy.**

Inconsistent with variational principle and perturbation corrections; correct choice is (B). See worked explanation.

Q117

In the variation method, if the trial function φ is an eigenfunction of the Hamiltonian, the variational energy W satisfies:

A. W > E_exact

B. W = E_exact

C. W < E_exact

D. W = 0

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Perturbation corrections, variational upper bound

PYQ FREQUENCY
Very High · 13 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
First order = diagonal average; second order = mix-in excited states (lowers ground state).

Correct Answer C W < E_exact

CONCEPT

First-order: $E_n^{(1)} = \langle n|\hat{H}'|n\rangle$. Second-order: $E_n^{(2)} = \Sigma_{k\neq n} |\langle k|H'|n\rangle|^2/(E_n - E_k)$. Variational: <E>_trial ≥ E_exact.

↓

LOGIC / WORKING

- See the postulates of QM and wavefunction requirements. The correct answer is (C).

FINAL: (C) W < E_exact

SHORTCUT / EXAM TRICK

$E^{(2)}$ is always negative for the ground state. $E^{(0)}+E^{(1)}$ is a variational upper bound.

COMMON MISTAKE

Thinking $E^{(1)}$ is necessarily negative — only $E^{(2)}$ is, for the ground state.

EXAM TIP

Second-order correction always LOWERS the ground state. Parity can make $E^{(1)}$ vanish.

MEMORY TRICK

First order = diagonal average; second order = mix-in excited states (lowers ground state).

Why the Other Options Are Wrong

Correct answer: **C**

A **W > E_exact**
Inconsistent with variational principle and perturbation corrections; correct choice is (C). See worked explanation.

B **W = E_exact**
Inconsistent with variational principle and perturbation corrections; correct choice is (C). See worked explanation.

D **W = 0**
Inconsistent with variational principle and perturbation corrections; correct choice is (C). See worked explanation.

Q122

Which statement is FALSE about the second-order perturbation correction $E_n^{(2)}$?

A. $E_n^{(2)}$ is always negative for the ground state

B. $E_n^{(2)}$ involves all excited states of the unperturbed system

C. $E_n^{(2)}$ is necessarily negative for all states

D. $E_n^{(2)}$ lowers the energy of the ground state

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Perturbation corrections, variational upper bound

PYQ FREQUENCY
Very High · 13 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
First order = diagonal average; second order = mix-in excited states (lowers ground state).

Correct Answer D $E_n^{(2)}$ lowers the energy of the ground state

CONCEPT

First-order: $E_n^{(1)} = \langle n|\hat{H}'|n\rangle$. Second-order: $E_n^{(2)} = \Sigma_{k\neq n} |\langle k|H'|n\rangle|^2/(E_n - E_k)$. Variational: $\langle E\rangle_{trial} \geq E_{exact}$.

↓

LOGIC / WORKING

- See variational principle and perturbation corrections. The correct answer is (D).

FINAL: (D) $E_n^{(2)}$ lowers the energy of the ground state

SHORTCUT / EXAM TRICK

$E^{(2)}$ is always negative for the ground state. $E^{(0)}+E^{(1)}$ is a variational upper bound.

COMMON MISTAKE

Thinking $E^{(1)}$ is necessarily negative — only $E^{(2)}$ is, for the ground state.

EXAM TIP

Second-order correction always LOWERS the ground state. Parity can make $E^{(1)}$ vanish.

MEMORY TRICK

First order = diagonal average; second order = mix-in excited states (lowers ground state).

Why the Other Options Are Wrong

Correct answer: D

A $E_n^{(2)}$ is always negative for the ground state

Inconsistent with variational principle and perturbation corrections; correct choice is (D). See worked explanation.

B $E_n^{(2)}$ involves all excited states of the unperturbed system

Inconsistent with variational principle and perturbation corrections; correct choice is (D). See worked explanation.

C $E_n^{(2)}$ is necessarily negative for all states

Inconsistent with variational principle and perturbation corrections; correct choice is (D). See worked explanation.

TOPIC REVISION

Perturbation & Variation Theory

14 PYQs · Last-minute revision

TOPIC SUMMARY

First-order: $E_n^{(1)} = \langle n|\hat{H}'|n\rangle$. Second-order: $E_n^{(2)} = \Sigma_{k\neq n} |\langle k|H'|n\rangle|^2/(E_n - E_k)$. Variational: <E>_trial ≥ E_exact.

IMPORTANT FORMULA SHEET

$E^{(1)} = \langle n|H'|n\rangle$

$E^{(2)} = \Sigma|H'_{kn}|^2/(E_n - E_k) < 0$

<E>_var ≥ E_exact

$E^{(0)}+E^{(1)} \geq$ E_exact

FREQUENTLY ASKED CONCEPTS

First-order correction
Second-order correction
Variational principle
- Upper bound

COMMON MISTAKES & QUICK NOTES

Watch out:
Thinking $E^{(1)}$ is necessarily negative — only $E^{(2)}$ is, for the ground state.
Last-minute:
$E^{(2)}$ is always negative for the ground state. $E^{(0)}+E^{(1)}$ is a variational upper bound.

MOST-REPEATED PYQs & EXPECTED IN EXAM

PYQs in this topic: Q4 Q14 Q21 Q27 Q33 Q44 Q50 Q55 Q62 Q74 Q88 Q108 Q117 Q122

Expect **3 question(s)** next session on **Perturbation corrections, variational upper bound.**

TOPIC 9

Hückel MO Theory

6 questions · Easy 0 | Medium 1 | Hard 5 · PYQ frequency: Moderate

Q5 **The energy levels for cyclobutadiene are α+2β, α, α, and α–2β. The delocalization energy in this molecule is:**

A 0

B –4β

C –8β

D 4α

SELF-PRACTICE official answer key not printed in the source — attempt this, then verify.

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
π-MO energies, delocalization energy, aromaticity

PYQ FREQUENCY
Moderate · 6 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
Bigger |β| → more stabilization (β is negative).

Q22

Using Hückel molecular orbital approximation, the two roots of secular equation of ethene are

A. α + 2β, α − 2β

B. α + β, α

C. α + β, α − β

D. α + 2β, α − 2β

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
π-MO energies, delocalization energy, aromaticity

PYQ FREQUENCY
Moderate · 6 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
Bigger |β| → more stabilization (β is negative).

Correct Answer C α + β, α − β

CONCEPT

Hückel MO: each C gives one p_z electron; α = Coulomb integral, β = resonance integral (negative). π-MO energies are α + xβ. Delocalization energy = E(HMO) – E(localized).

↓

LOGIC / WORKING

- Key principle: variational principle and perturbation corrections. Answer is (C).

FINAL: (C) α + β, α − β

SHORTCUT / EXAM TRICK

Benzene: 6α+8β, DE = 2β. Cyclobutadiene DE = 0. Butadiene DE = 0.47β.

COMMON MISTAKE

Forgetting Hund's rule for degenerate MOs; treating β as positive.

EXAM TIP

Aromatic = 4n+2 π electrons. Cyclobutadiene has degenerate half-filled MOs (antiaromatic).

MEMORY TRICK

Bigger |β| → more stabilization (β is negative).

Why the Other Options Are Wrong

Correct answer: C

A α + 2β, α − 2β
Inconsistent with Hückel MO energies and delocalization; correct choice is (C). See worked explanation.

B α + β, α
Inconsistent with Hückel MO energies and delocalization; correct choice is (C). See worked explanation.

D α + 2β, α − 2β
Inconsistent with Hückel MO energies and delocalization; correct choice is (C). See worked explanation.

Q39

Identify the Huckel determinant for cyclobutadiene

A. α-E & β & 0 & 0 β & α-E & β & 0 0 & β & α-E & β 0 & 0 & β & α-E

B. α-E & β & 0 & β β & α-E & β & 0 0 & β & α-E & β β & β & 0 & α-E

C. α-E & β & 0 & β β & α-E & β & 0 0 & β & α-E & β β & 0 & β & α-E

D. α-E & β & 0 & β β & α-E & β & 0 0 & β & α-E & β 0 & 0 & β & α-E

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
π-MO energies, delocalization energy, aromaticity

PYQ FREQUENCY
Moderate · 6 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
Bigger |β| → more stabilization (β is negative).

Correct Answer C α-E & β & 0 & β β & α-E & β & 0 0 & β & α-E & β β & 0 & β & α-E

CONCEPT

Hückel MO: each C gives one p_z electron; α = Coulomb integral, β = resonance integral (negative). π-MO energies are α + xβ. Delocalization energy = E(HMO) – E(localized).

↓

LOGIC / WORKING

- Key principle: Hückel MO energies and delocalization. Answer is (C).

FINAL: (C) α-E & β & 0 & β β & α-E & β & 0 0 & β & α-E & β β & 0 & β & α-E

SHORTCUT / EXAM TRICK

Benzene: 6α+8β, DE = 2β. Cyclobutadiene DE = 0. Butadiene DE = 0.47β.

COMMON MISTAKE

Forgetting Hund's rule for degenerate MOs; treating β as positive.

EXAM TIP

Aromatic = 4n+2 π electrons. Cyclobutadiene has degenerate half-filled MOs (antiaromatic).

MEMORY TRICK

Bigger |β| → more stabilization (β is negative).

Why the Other Options Are Wrong

Correct answer: **C**

A **α-E & β & 0 & 0 β & α-E & β & 0 0 & β & α-E & β 0 & 0 & β & α-E**

Inconsistent with Hückel MO energies and delocalization; correct choice is (C). See worked explanation.

B **α-E & β & 0 & β β & α-E & β & 0 0 & β & α-E & β β & β & 0 & α-E**

Inconsistent with Hückel MO energies and delocalization; correct choice is (C). See worked explanation.

D **α-E & β & 0 & β β & α-E & β & 0 0 & β & α-E & β 0 & 0 & β & α-E**

Inconsistent with Hückel MO energies and delocalization; correct choice is (C). See worked explanation.

Q54 Simple Hückel molecular orbital theory

A. considers electron-electron repulsion explicitly

B. distinguishes cis-butadiene and trans butadiene

C. distinguishes cyclobutadiene cis-butadiene

D. has different coulomb integrals for non equivalent carbons

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
π-MO energies, delocalization energy, aromaticity

PYQ FREQUENCY
Moderate · 6 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
Bigger |β| → more stabilization (β is negative).

Correct Answer C distinguishes cyclobutadiene cis-butadiene

CONCEPT

Hückel MO: each C gives one p_z electron; α = Coulomb integral, β = resonance integral (negative). π-MO energies are α + xβ. Delocalization energy = E(HMO) – E(localized).

↓

LOGIC / WORKING

- Key principle: Hückel MO energies and delocalization. Answer is (C).

FINAL: (C) distinguishes cyclobutadiene cis-butadiene

SHORTCUT / EXAM TRICK

Benzene: 6α+8β, DE = 2β. Cyclobutadiene DE = 0. Butadiene DE = 0.47β.

COMMON MISTAKE

Forgetting Hund's rule for degenerate MOs; treating β as positive.

EXAM TIP

Aromatic = 4n+2 π electrons. Cyclobutadiene has degenerate half-filled MOs (antiaromatic).

MEMORY TRICK

Bigger |β| → more stabilization (β is negative).

Why the Other Options Are Wrong

Correct answer: C

A **considers electron-electron repulsion explicitly**
Inconsistent with Hückel MO energies and delocalization; correct choice is (C). See worked explanation.

B **distinguishes cis-butadiene and trans butadiene**
Inconsistent with Hückel MO energies and delocalization; correct choice is (C). See worked explanation.

D **has different coulomb integrals for non equivalent carbons**
Inconsistent with Hückel MO energies and delocalization; correct choice is (C). See worked explanation.

Q101

The electronic transition energy from π1→π2 in propenyl radical is 4.8 eV. Within the framework of Huckel theory, the transitions energy from π1 →π3 would be

A. 2.4 eV

B. 4.8 eV

C. 9.6 eV

D. 14.4 eV

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
π-MO energies, delocalization energy, aromaticity

PYQ FREQUENCY
Moderate · 6 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
Bigger |β| → more stabilization (β is negative).

Correct Answer C 9.6 eV

CONCEPT

Hückel MO: each C gives one p_z electron; α = Coulomb integral, β = resonance integral (negative). π-MO energies are α + xβ. Delocalization energy = E(HMO) – E(localized).

↓

LOGIC / WORKING

- Key principle: Hückel MO energies and delocalization. Answer is (C).

FINAL: (C) 9.6 eV

SHORTCUT / EXAM TRICK

Benzene: 6α+8β, DE = 2β. Cyclobutadiene DE = 0. Butadiene DE = 0.47β.

COMMON MISTAKE

Forgetting Hund's rule for degenerate MOs; treating β as positive.

EXAM TIP

Aromatic = 4n+2 π electrons. Cyclobutadiene has degenerate half-filled MOs (antiaromatic).

MEMORY TRICK

Bigger |β| → more stabilization (β is negative).

Why the Other Options Are Wrong

Correct answer: C

A **2.4 eV**
Inconsistent with Hückel MO energies and delocalization; correct choice is (C). See worked explanation.

B **4.8 eV**
Inconsistent with Hückel MO energies and delocalization; correct choice is (C). See worked explanation.

D **14.4 eV**
Inconsistent with Hückel MO energies and delocalization; correct choice is (C). See worked explanation.

Q121 The Hückel molecular orbital of benzene that is degenerate with the molecular orbital ($\chi\ddot{Y} + \chi - \chi¢ - \chi$) $\ddot{Y}$

A (2 χ + $\chi\ddot{Y}$ − χ − $\chi¢$ + χ)

B ($\chi\ddot{Y}$ − χ + $\chi¢$ − χ)

C (2 χ − $\chi\ddot{Y}$ − χ + 2$\chi¬$ − $\chi¢$ − χ)

D (χ − $\chi\ddot{Y}$ + χ − $\chi¬$ + $\chi¢$ − χ)

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
π-MO energies, delocalization energy, aromaticity

PYQ FREQUENCY
Moderate · 6 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
Bigger |β| → more stabilization (β is negative).

Correct Answer A (2 χ + χŸ − χ − χ¢ + χ)

CONCEPT

Hückel MO: each C gives one p_z electron; α = Coulomb integral, β = resonance integral (negative). π-MO energies are α + xβ. Delocalization energy = E(HMO) – E(localized).

↓

LOGIC / WORKING

- Key principle: Hückel MO energies and delocalization. Answer is (A).

FINAL: (A) (2 χ + χŸ − χ − χ¢ + χ)

SHORTCUT / EXAM TRICK

Benzene: 6α+8β, DE = 2β. Cyclobutadiene DE = 0. Butadiene DE = 0.47β.

COMMON MISTAKE

Forgetting Hund's rule for degenerate MOs; treating β as positive.

EXAM TIP

Aromatic = 4n+2 π electrons. Cyclobutadiene has degenerate half-filled MOs (antiaromatic).

MEMORY TRICK

Bigger |β| → more stabilization (β is negative).

Why the Other Options Are Wrong

Correct answer: **A**

B $(\chi\ddot{Y} - \chi + \chi\text{¢} - \chi)$

Inconsistent with Hückel MO energies and delocalization; correct choice is (A). See worked explanation.

C $(2\chi - \chi\ddot{Y} - \chi + 2\chi\neg - \chi\text{¢} - \chi)$

Inconsistent with Hückel MO energies and delocalization; correct choice is (A). See worked explanation.

D $(\chi - \chi\ddot{Y} + \chi - \chi\neg + \chi\text{¢} - \chi)$

Inconsistent with Hückel MO energies and delocalization; correct choice is (A). See worked explanation.

TOPIC REVISION

Hückel MO Theory

6 PYQs · Last-minute revision

TOPIC SUMMARY

Hückel MO: each C gives one p_z electron; α = Coulomb integral, β = resonance integral (negative). π-MO energies are α + xβ. Delocalization energy = E(HMO) – E(localized).

IMPORTANT FORMULA SHEET

E = α + m·β
DE = E(HMO) – E(localized)
Benzene: 6α + 8β

- Cyclobutadiene DE = 0

FREQUENTLY ASKED CONCEPTS

Coulomb integral α
Resonance integral β
Delocalization energy

- 4n+2 aromaticity

COMMON MISTAKES & QUICK NOTES

Watch out:
Forgetting Hund's rule for degenerate MOs; treating β as positive.
Last-minute:
Benzene: 6α+8β, DE = 2β. Cyclobutadiene DE = 0. Butadiene DE = 0.47β.

MOST-REPEATED PYQs & EXPECTED IN EXAM

PYQs in this topic: Q5 Q22 Q39 Q54 Q101 Q121

Expect **1 question(s)** next session on **π-MO energies, delocalization energy, aromaticity.**

TOPIC 10

Many-Electron Systems

6 questions · Easy 0 | Medium 5 | Hard 1 · PYQ frequency: Occasional

Q15 An excited triplet state wave function of hydrogen molecule with the electronic configuration $\sigma 1_g\ \sigma 1_u$ has the following space part

A. σg(1) σu(2)

B. σg(1) σu(2) + σu(1) σg(2)

C. σg(1) σu(2) − σu(1) σg(2)

D. σg(1) σg(2) + σu(1) σu(2)

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Antisymmetry principle, Slater determinants, singlet/triplet states

PYQ FREQUENCY
Occasional · 4 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
PASTA: Para (singlet) = Antisymmetric Spin; Triplet = Antisymmetric Space.

Correct Answer C σg(1) σu(2) − σu(1) σg(2)

CONCEPT

Antisymmetry principle: total wavefunction is antisymmetric under electron exchange → Slater determinants. Singlet spin is antisymmetric; triplet spin is symmetric.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (C).

FINAL: (C) σg(1) σu(2) − σu(1) σg(2)

SHORTCUT / EXAM TRICK

Symmetric space × antisymmetric spin (singlet), or antisymmetric space × symmetric spin (triplet).

COMMON MISTAKE

Using a spin function with no definite symmetry, e.g. α(1)β(2) without symmetrizing.

EXAM TIP

He 1s2s: singlet = symmetric space; triplet = antisymmetric space. α(1)β(2) alone is invalid.

MEMORY TRICK

PASTA: Para (singlet) = Antisymmetric Spin; Triplet = Antisymmetric Space.

Why the Other Options Are Wrong

Correct answer: **C**

A — **σg(1) σu(2)**

Inconsistent with antisymmetry principle and electron correlation; correct choice is (C). See worked explanation.

B — **σg(1) σu(2) + σu(1) σg(2)**

Inconsistent with antisymmetry principle and electron correlation; correct choice is (C). See worked explanation.

D — **σg(1) σg(2) + σu(1) σu(2)**

Inconsistent with antisymmetry principle and electron correlation; correct choice is (C). See worked explanation.

Q40

In the formation of H2 molecules from 2H atoms placed at positions A and B, and separated by a distance rAB , a part of special wavefunction is φ_A 1 φ_A 2 + φ_B (1)φ_B (2)

A. This is a covalent term and is important as rAB → ∞

B. This is a ionic term and is important as rAB → ∞

C. This is a covalent term and is important as rAB → 0

D. This is a ionic term and is important as rAB → 0

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Antisymmetry principle, Slater determinants, singlet/triplet states

PYQ FREQUENCY
Occasional · 4 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
PASTA: Para (singlet) = Antisymmetric Spin; Triplet = Antisymmetric Space.

Correct Answer D This is a ionic term and is important as rAB → 0

CONCEPT

Antisymmetry principle: total wavefunction is antisymmetric under electron exchange → Slater determinants. Singlet spin is antisymmetric; triplet spin is symmetric.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (D).

FINAL: (D) This is a ionic term and is important as rAB → 0

SHORTCUT / EXAM TRICK

Symmetric space × antisymmetric spin (singlet), or antisymmetric space × symmetric spin (triplet).

COMMON MISTAKE

Using a spin function with no definite symmetry, e.g. α(1)β(2) without symmetrizing.

EXAM TIP

He 1s2s: singlet = symmetric space; triplet = antisymmetric space. α(1)β(2) alone is invalid.

MEMORY TRICK

PASTA: Para (singlet) = Antisymmetric Spin; Triplet = Antisymmetric Space.

Why the Other Options Are Wrong

Correct answer: D

A **This is a covalent term and is important as rAB → ∞**
Inconsistent with antisymmetry principle and electron correlation; correct choice is (D). See worked explanation.

B **This is a ionic term and is important as rAB → ∞**
Inconsistent with antisymmetry principle and electron correlation; correct choice is (D). See worked explanation.

C **This is a covalent term and is important as rAB → 0**
Inconsistent with antisymmetry principle and electron correlation; correct choice is (D). See worked explanation.

Q56

The spatial part of the wave function of the atom in its ground state is 1s (1)1s (2). The spin part would be

A. α(1)α(2)

B. β(1) β (2)

C. [α (1) β (2) + β (1)α(2)]

D. [α (1) β (2) - β (1)α(2)]

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Antisymmetry principle, Slater determinants, singlet/triplet states

PYQ FREQUENCY
Occasional · 4 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
PASTA: Para (singlet) = Antisymmetric Spin; Triplet = Antisymmetric Space.

Correct Answer D [α (1) β (2) - β (1)α(2)]

CONCEPT

Antisymmetry principle: total wavefunction is antisymmetric under electron exchange → Slater determinants. Singlet spin is antisymmetric; triplet spin is symmetric.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (D).

FINAL: (D) [α (1) β (2) - β (1)α(2)]

SHORTCUT / EXAM TRICK

Symmetric space × antisymmetric spin (singlet), or antisymmetric space × symmetric spin (triplet).

COMMON MISTAKE

Using a spin function with no definite symmetry, e.g. α(1)β(2) without symmetrizing.

EXAM TIP

He 1s2s: singlet = symmetric space; triplet = antisymmetric space. α(1)β(2) alone is invalid.

MEMORY TRICK

PASTA: Para (singlet) = Antisymmetric Spin; Triplet = Antisymmetric Space.

Why the Other Options Are Wrong

Correct answer: D

A α(1)α(2)
Inconsistent with antisymmetry principle and electron correlation; correct choice is (D). See worked explanation.

B β(1) β (2)
Inconsistent with antisymmetry principle and electron correlation; correct choice is (D). See worked explanation.

C [α (1) β (2) + β (1)α(2)]
Inconsistent with antisymmetry principle and electron correlation; correct choice is (D). See worked explanation.

Q110

The lowest energy unnormalized wavefunction of H_2^+ (r_1 and r_2 = distances to nuclei 1 and 2) is:

A $e^{(-r_1)} + e^{(-r_2)}$ (bonding LCAO)

B $e^{(-r_1)} - e^{(-r_2)}$ (antibonding LCAO)

C $e^{(-(r_1+r_2))}$

D $e^{(-r_1)} \times e^{(-r_2)}$

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Antisymmetry principle, Slater determinants, singlet/triplet states

PYQ FREQUENCY
Occasional · 4 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
PASTA: Para (singlet) = Antisymmetric Spin; Triplet = Antisymmetric Space.

Correct Answer A $e^{(-r_1)} + e^{(-r_2)}$ (bonding LCAO)

CONCEPT

Antisymmetry principle: total wavefunction is antisymmetric under electron exchange → Slater determinants. Singlet spin is antisymmetric; triplet spin is symmetric.

↓

LOGIC / WORKING

- See the postulates of QM and wavefunction requirements. The correct answer is (A).

FINAL: (A) $e^{(-r_1)} + e^{(-r_2)}$ **(bonding LCAO)**

SHORTCUT / EXAM TRICK

Symmetric space × antisymmetric spin (singlet), or antisymmetric space × symmetric spin (triplet).

COMMON MISTAKE

Using a spin function with no definite symmetry, e.g. α(1)β(2) without symmetrizing.

EXAM TIP

He 1s2s: singlet = symmetric space; triplet = antisymmetric space. α(1)β(2) alone is invalid.

MEMORY TRICK

PASTA: Para (singlet) = Antisymmetric Spin; Triplet = Antisymmetric Space.

Why the Other Options Are Wrong

Correct answer: **A**

B $e^{(-r_1)} - e^{(-r_2)}$ (antibonding LCAO)

Inconsistent with antisymmetry principle and electron correlation; correct choice is (A). See worked explanation.

C $e^{(-(r_1+r_2))}$

Inconsistent with antisymmetry principle and electron correlation; correct choice is (A). See worked explanation.

D $e^{(-r_1)} \times e^{(-r_2)}$

Inconsistent with antisymmetry principle and electron correlation; correct choice is (A). See worked explanation.

Q112

The Born-Oppenheimer approximation separates nuclear and electronic motion because:

A. Nuclei are much heavier than electrons so move much slower

B. Electrons have larger charge than nuclei

C. Nuclear wavefunctions are always real

D. Electronic energy is always negative

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Antisymmetry principle, Slater determinants, singlet/triplet states

PYQ FREQUENCY
Occasional · 4 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
PASTA: Para (singlet) = Antisymmetric Spin; Triplet = Antisymmetric Space.

Correct Answer D Electronic energy is always negative

CONCEPT

Antisymmetry principle: total wavefunction is antisymmetric under electron exchange → Slater determinants. Singlet spin is antisymmetric; triplet spin is symmetric.

↓

LOGIC / WORKING

- See antisymmetry principle and electron correlation. The correct answer is (D).

FINAL: (D) Electronic energy is always negative

SHORTCUT / EXAM TRICK

Symmetric space × antisymmetric spin (singlet), or antisymmetric space × symmetric spin (triplet).

COMMON MISTAKE

Using a spin function with no definite symmetry, e.g. α(1)β(2) without symmetrizing.

EXAM TIP

He 1s2s: singlet = symmetric space; triplet = antisymmetric space. α(1)β(2) alone is invalid.

MEMORY TRICK

PASTA: Para (singlet) = Antisymmetric Spin; Triplet = Antisymmetric Space.

Why the Other Options Are Wrong

Correct answer: D

A **Nuclei are much heavier than electrons so move much slower**
Inconsistent with antisymmetry principle and electron correlation; correct choice is (D). See worked explanation.

B **Electrons have larger charge than nuclei**
Inconsistent with antisymmetry principle and electron correlation; correct choice is (D). See worked explanation.

C **Nuclear wavefunctions are always real**
Inconsistent with antisymmetry principle and electron correlation; correct choice is (D). See worked explanation.

Q114

A satisfactory spin wave function for an excited helium atom is 1

A. [α (1) b(2)+ α(2) b(1)]

B. α (1) b(2)

C. [α (1) α (2)+ b(1) b(2)]

D. α (2) b(1)

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Antisymmetry principle, Slater determinants, singlet/triplet states

PYQ FREQUENCY
Occasional · 4 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
PASTA: Para (singlet) = Antisymmetric Spin; Triplet = Antisymmetric Space.

Correct Answer A [α (1) b(2)+ α(2) b(1)]

CONCEPT

Antisymmetry principle: total wavefunction is antisymmetric under electron exchange → Slater determinants. Singlet spin is antisymmetric; triplet spin is symmetric.

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (A).

FINAL: (A) [α (1) b(2)+ α(2) b(1)]

SHORTCUT / EXAM TRICK

Symmetric space × antisymmetric spin (singlet), or antisymmetric space × symmetric spin (triplet).

COMMON MISTAKE

Using a spin function with no definite symmetry, e.g. α(1)β(2) without symmetrizing.

EXAM TIP

He 1s2s: singlet = symmetric space; triplet = antisymmetric space. α(1)β(2) alone is invalid.

MEMORY TRICK

PASTA: Para (singlet) = Antisymmetric Spin; Triplet = Antisymmetric Space.

Why the Other Options Are Wrong

Correct answer: **A**

B **α (1) b(2)**
Inconsistent with antisymmetry principle and electron correlation; correct choice is (A). See worked explanation.

C **[α (1) α (2)+ b(1) b(2)]**
Inconsistent with antisymmetry principle and electron correlation; correct choice is (A). See worked explanation.

D **α (2) b(1)**
Inconsistent with antisymmetry principle and electron correlation; correct choice is (A). See worked explanation.

TOPIC REVISION

Many-Electron Systems

6 PYQs · Last-minute revision

TOPIC SUMMARY

Antisymmetry principle: total wavefunction is antisymmetric under electron exchange → Slater determinants. Singlet spin is antisymmetric; triplet spin is symmetric.

IMPORTANT FORMULA SHEET

$\Psi(1,2) = \varphi(1,2)\sigma(1,2)$
Singlet: $\alpha(1)\beta(2) - \alpha(2)\beta(1)$
Triplet: symmetric spin (3 states)

- Fermi correlation

FREQUENTLY ASKED CONCEPTS

Pauli exclusion
Slater determinants
Singlet vs triplet

- Exchange energy

COMMON MISTAKES & QUICK NOTES

Watch out:
Using a spin function with no definite symmetry, e.g. $\alpha(1)\beta(2)$ without symmetrizing.
Last-minute:
Symmetric space × antisymmetric spin (singlet), or antisymmetric space × symmetric spin (triplet).

MOST-REPEATED PYQs & EXPECTED IN EXAM

PYQs in this topic: Q15 Q40 Q56 Q110 Q112 Q114

Expect **1 question(s)** next session on **Antisymmetry principle, Slater determinants, singlet/triplet states.**

TOPIC 11

Molecular Orbitals & Hybridization

4 questions · Easy 0 | Medium 4 | Hard 0 · PYQ frequency: Occasional

Q52

If $\psi = 0.8\varphi A + 0.4\varphi B$ is a normalized molecular orbital of a diaotmic molecule AB, constructed from φA and φB which are also normalized, the overlap between φA and φB is

A. 0.11

B. 0.31

C. 0.51

D. 0.71

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
LCAO coefficients, normalization, hybridization

PYQ FREQUENCY
Occasional · 3 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
Bigger coefficient on B → more electron density near B.

Correct Answer B 0.31

CONCEPT

LCAO-MO: ψ = c_A χ_A + c_B χ_B. Normalization $c_A^2 + c_B^2 + 2c_Ac_B S = 1$. Electron probability on atom B = c_B^2 (S≈0).

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (B).

FINAL: (B) 0.31

SHORTCUT / EXAM TRICK

sp^2 hybrid has ⅓ s-character ($c_s^2 = 1/3$). $\Sigma c_i^2 = 1$ for a normalized hybrid.

COMMON MISTAKE

Ignoring the overlap integral S in normalization; hybrids that don't satisfy $\Sigma c^2 = 1$.

EXAM TIP

Rotational selection rule ΔJ = ±1; transition moment ∝ permanent dipole.

MEMORY TRICK

Bigger coefficient on B → more electron density near B.

Why the Other Options Are Wrong

Correct answer: **B**

A **0.11**
Inconsistent with LCAO-MO theory and hybridization; correct choice is (B). See worked explanation.

C **0.51**
Inconsistent with LCAO-MO theory and hybridization; correct choice is (B). See worked explanation.

D **0.71**
Inconsistent with LCAO-MO theory and hybridization; correct choice is (B). See worked explanation.

Q85

The correct normalized wave function for one of the sp hybrid orbitals is 1 1 1

A) ψ2***s*** − ψ2***px*** + ψ2***py***

B) ψ2***s*** − ψ2***px*** + ψ2***py***

C) ψ2***s*** − ψψ2***px*** +

D) ψ2***s*** − ψ2***px*** + ψ2***py***

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
LCAO coefficients, normalization, hybridization

PYQ FREQUENCY
Occasional · 3 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
Bigger coefficient on B → more electron density near B.

Correct Answer C $\psi 2s - \psi\psi 2px +$

CONCEPT

LCAO-MO: ψ = c_A χ_A + c_B χ_B. Normalization $c_A^2 + c_B^2 + 2c_Ac_B S = 1$. Electron probability on atom B = c_B^2 (S≈0).

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (C).

FINAL: (C) ψ2s − ψψ2px +

SHORTCUT / EXAM TRICK

sp^2 hybrid has ⅓ s-character ($c_s^2 = 1/3$). $\Sigma c_i^2 = 1$ for a normalized hybrid.

COMMON MISTAKE

Ignoring the overlap integral S in normalization; hybrids that don't satisfy $\Sigma c^2 = 1$.

EXAM TIP

Rotational selection rule ΔJ = ±1; transition moment ∝ permanent dipole.

MEMORY TRICK

Bigger coefficient on B → more electron density near B.

Why the Other Options Are Wrong

Correct answer: **C**

A $\psi 2s - \psi 2px + \psi 2py$

Inconsistent with LCAO-MO theory and hybridization; correct choice is (C). See worked explanation.

B $\psi 2s - \psi 2px + \psi 2py$

Inconsistent with LCAO-MO theory and hybridization; correct choice is (C). See worked explanation.

D $\psi 2s - \psi 2px + \psi 2py$

Inconsistent with LCAO-MO theory and hybridization; correct choice is (C). See worked explanation.

Q102

The transition moment integral for a rotational transition between J= 1; MJ = 0 and J= 2 ; MJ = 0 states for a diatomic molecule along the z axis is proportional to π

A 0 $\cos^2\theta\, 3\cos^2\theta - 1\, d\theta$

B 0 $\cos^2\theta\, 3\cos^2\theta - 1\, \sin\theta d\theta$

C 0 $\cos\theta\, 3\cos^2\theta - 1\, \sin\theta d\theta$

D 0 $\cos^2\theta\, 3\cos^2\theta - 1\, \sin^2 d\theta$

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
LCAO coefficients, normalization, hybridization

PYQ FREQUENCY
Occasional · 3 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
Bigger coefficient on B → more electron density near B.

Correct Answer B 0 $\cos 2\theta$ $3\cos 2\theta - 1$ $\sin\theta d\theta$

CONCEPT

LCAO-MO: ψ = $c_A \chi_A + c_B \chi_B$. Normalization $c_A^2 + c_B^2 + 2c_A c_B S = 1$. Electron probability on atom B = c_B^2 (S≈0).

↓

LOGIC / WORKING

- Key principle: LCAO-MO theory and hybridization. Answer is (B).

FINAL: (B) 0 $\cos 2\theta$ $3\cos 2\theta - 1$ $\sin\theta d\theta$

SHORTCUT / EXAM TRICK

sp^2 hybrid has ⅓ s-character ($c_s^2 = 1/3$). $\Sigma c_i^2 = 1$ for a normalized hybrid.

COMMON MISTAKE

Ignoring the overlap integral S in normalization; hybrids that don't satisfy $\Sigma c^2 = 1$.

EXAM TIP

Rotational selection rule ΔJ = ±1; transition moment ∝ permanent dipole.

MEMORY TRICK

Bigger coefficient on B → more electron density near B.

Why the Other Options Are Wrong

Correct answer: **B**

A $0\ cos2\ \theta\ 3cos2\ \theta - 1\ d\theta$

Inconsistent with LCAO-MO theory and hybridization; correct choice is (B). See worked explanation.

C $0\ cos\theta\ 3cos2\ \theta - 1\ sin\theta d\theta$

Inconsistent with LCAO-MO theory and hybridization; correct choice is (B). See worked explanation.

D $0\ cos2\ \theta\ 3cos2\ \theta - 1\ sin2\ d\theta$

Inconsistent with LCAO-MO theory and hybridization; correct choice is (B). See worked explanation.

Q103 One of the correct normalized sp2 hybridorbitals is 1 1 1

A) φ2***s*** + φ2***px*** + φ2***py***

B) φ2***s*** + φ + φ2***py***

C) φ + φ2***px***

D) φ2***s*** + φ2***p***

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
LCAO coefficients, normalization, hybridization

PYQ FREQUENCY
Occasional · 3 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
Bigger coefficient on B → more electron density near B.

Correct Answer B $\varphi 2s + \varphi + \varphi 2py$

CONCEPT

LCAO-MO: ψ = c_A χ_A + c_B χ_B. Normalization $c_A^2 + c_B^2 + 2c_Ac_B S = 1$. Electron probability on atom B = c_B^2 (S≈0).

↓

LOGIC / WORKING

- Key principle: the postulates of QM and wavefunction requirements. Answer is (B).

FINAL: (B) $\varphi 2s + \varphi + \varphi 2py$

SHORTCUT / EXAM TRICK

sp^2 hybrid has ⅓ s-character ($c_s^2 = 1/3$). $\Sigma c_i^2 = 1$ for a normalized hybrid.

COMMON MISTAKE

Ignoring the overlap integral S in normalization; hybrids that don't satisfy $\Sigma c^2 = 1$.

EXAM TIP

Rotational selection rule ΔJ = ±1; transition moment ∝ permanent dipole.

MEMORY TRICK

Bigger coefficient on B → more electron density near B.

Why the Other Options Are Wrong

Correct answer: **B**

A — **φ2*s* + φ2*px* + φ2*py***
Inconsistent with LCAO-MO theory and hybridization; correct choice is (B). See worked explanation.

C — **φ + φ2*px***
Inconsistent with LCAO-MO theory and hybridization; correct choice is (B). See worked explanation.

D — **φ2*s* + φ2*p***
Inconsistent with LCAO-MO theory and hybridization; correct choice is (B). See worked explanation.

TOPIC REVISION

Molecular Orbitals & Hybridization

4 PYQs · Last-minute revision

TOPIC SUMMARY

LCAO-MO: $\psi = c_A \chi_A + c_B \chi_B$. Normalization $c_A^2 + c_B^2 + 2c_A c_B S = 1$. Electron probability on atom B = c_B^2 ($S \approx 0$).

IMPORTANT FORMULA SHEET

$\psi = c_A \chi_A + c_B \chi_B$
$c_A^2 + c_B^2 = 1$ ($S=0$)
sp^2: $c_s^2 = 1/3$
P(on B) = c_B^2

FREQUENTLY ASKED CONCEPTS

LCAO-MO
Normalization of hybrids
Selection rules
- Polarity from coefficients

COMMON MISTAKES & QUICK NOTES

Watch out:
Ignoring the overlap integral S in normalization; hybrids that don't satisfy $\Sigma c^2 = 1$.
Last-minute:
sp^2 hybrid has ⅓ s-character ($c_s^2 = 1/3$). $\Sigma c_i^2 = 1$ for a normalized hybrid.

MOST-REPEATED PYQs & EXPECTED IN EXAM

PYQs in this topic: Q52 Q85 Q102 Q103

Expect **1 question(s)** next session on **LCAO coefficients, normalization, hybridization.**

TOPIC 12

Quantum Chemistry – General

6 questions · Easy 0 | Medium 4 | Hard 2 · PYQ frequency: Moderate

Q17

For hydrogen-like atom with a nuclear charge Z, the energy of orbital with principal quantum number ‘n’ follows the relation.

A. $E_n \propto n^2Z^2$

B. $E_n \propto -(Z^2)/(n)$

C. $E_n \propto (Z)/(n)$

D. $E_n \propto -(Z^2)/(n^2)$

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Integrated quantum-mechanical reasoning

PYQ FREQUENCY
Moderate · 6 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
Every CSIR quantum question maps onto one of the four standard solved systems.

Correct Answer D $E_n \propto -(Z^2)/(n^2)$

CONCEPT

General quantum-chemistry principles: postulates, operator algebra, boundary conditions and symmetry that connect the model systems (box, oscillator, rotor, H-atom).

↓

LOGIC / WORKING

- Key principle: H-atom wavefunctions and quantum numbers. Answer is (D).

FINAL: (D) $E_n \propto -(Z^2)/(n^2)$

SHORTCUT / EXAM TRICK

Identify the model system first, then apply its energy formula and selection rule.

COMMON MISTAKE

Mixing formulas across models (e.g. oscillator virial vs Coulombic virial).

EXAM TIP

Match the physical setup to the standard model (box / oscillator / rotor / H-atom).

MEMORY TRICK

Every CSIR quantum question maps onto one of the four standard solved systems.

Why the Other Options Are Wrong

Correct answer: **D**

A $E_n \propto n^2Z^2$

Inconsistent with the governing quantum mechanical principle; correct choice is (D). See worked explanation.

B $E_n \propto -(Z^2)/(n)$

Inconsistent with the governing quantum mechanical principle; correct choice is (D). See worked explanation.

C $E_n \propto (Z)/(n)$

Inconsistent with the governing quantum mechanical principle; correct choice is (D). See worked explanation.

Q26

Combining two real wavefunctions φ_1 and φ_2: A = $\varphi_1+\varphi_2$, B = $\varphi_1+i\varphi_2$, C = $\varphi_1-i\varphi_2$, D = $i(\varphi_1+\varphi_2)$. The correct statement is:

A. A and B represent the same state

B. A and C represent the same state

C. A and D represent the same state

D. B and D represent the same state

SELF-PRACTICE official answer key not printed in the source — attempt this, then verify.

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Integrated quantum-mechanical reasoning

PYQ FREQUENCY
Moderate · 6 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
Every CSIR quantum question maps onto one of the four standard solved systems.

Q37 The operator [^x, [^x, ^p²]] is identical with

A [^p^x, [^x, ^p]]

B [^x^p, [^x, ^p]]

C -[^p, [^x², ^p]]

D -[^x, [^x², ^p]]

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Integrated quantum-mechanical reasoning

PYQ FREQUENCY
Moderate · 6 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
Every CSIR quantum question maps onto one of the four standard solved systems.

Correct Answer C -[^p, [^x², ^p]]

CONCEPT

General quantum-chemistry principles: postulates, operator algebra, boundary conditions and symmetry that connect the model systems (box, oscillator, rotor, H-atom).

↓

LOGIC / WORKING

- Key principle: the algebra of quantum mechanical operators. Answer is (C).

FINAL: (C) -[^p, [^x², ^p]]

SHORTCUT / EXAM TRICK

Identify the model system first, then apply its energy formula and selection rule.

COMMON MISTAKE

Mixing formulas across models (e.g. oscillator virial vs Coulombic virial).

EXAM TIP

Match the physical setup to the standard model (box / oscillator / rotor / H-atom).

MEMORY TRICK

Every CSIR quantum question maps onto one of the four standard solved systems.

Why the Other Options Are Wrong

Correct answer: **C**

A **[^p^x, [^x, ^p]]**
Inconsistent with the governing quantum mechanical principle; correct choice is (C). See worked explanation.

B **[^x^p, [^x, ^p]]**
Inconsistent with the governing quantum mechanical principle; correct choice is (C). See worked explanation.

D **-[^x, [^x², ^p]]**
Inconsistent with the governing quantum mechanical principle; correct choice is (C). See worked explanation.

Q53

If the ionization energy of H atom is x, the ionization energy of Li+2 is

A 2x

B 3x

C 9x

D 27x

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Integrated quantum-mechanical reasoning

PYQ FREQUENCY
Moderate · 6 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
Every CSIR quantum question maps onto one of the four standard solved systems.

Correct Answer C 9x

CONCEPT

General quantum-chemistry principles: postulates, operator algebra, boundary conditions and symmetry that connect the model systems (box, oscillator, rotor, H-atom).

↓

LOGIC / WORKING

- Key principle: the governing quantum mechanical principle. Answer is (C).

FINAL: (C) 9x

SHORTCUT / EXAM TRICK

Identify the model system first, then apply its energy formula and selection rule.

COMMON MISTAKE

Mixing formulas across models (e.g. oscillator virial vs Coulombic virial).

EXAM TIP

Match the physical setup to the standard model (box / oscillator / rotor / H-atom).

MEMORY TRICK

Every CSIR quantum question maps onto one of the four standard solved systems.

Why the Other Options Are Wrong

Correct answer: **C**

A — **2x**
Inconsistent with the governing quantum mechanical principle; correct choice is (C). See worked explanation.

B — **3x**
Inconsistent with the governing quantum mechanical principle; correct choice is (C). See worked explanation.

D — **27x**
Inconsistent with the governing quantum mechanical principle; correct choice is (C). See worked explanation.

Q71

Two different non-zero operators A and B ($A \neq B$) satisfy the relation $(A + B)(A - B) = A^2 - B^2$

A. $AB = A^2$ and $BA = B^2$

B. $AB + BA = 0$

C. A and B are arbitrary

D. $AB - BA = 0$

QUESTION INSIGHTS

ESTIMATED TIME
3–5 min

DIFFICULTY
Hard

CONCEPT TESTED
Integrated quantum-mechanical reasoning

PYQ FREQUENCY
Moderate · 6 papers

REVISION PRIORITY
★★★★★

EXPECTED LEVEL
Part C (high merit)

MEMORY HOOK
Every CSIR quantum question maps onto one of the four standard solved systems.

Correct Answer D $AB - BA = 0$

CONCEPT

General quantum-chemistry principles: postulates, operator algebra, boundary conditions and symmetry that connect the model systems (box, oscillator, rotor, H-atom).

↓

LOGIC / WORKING

- Key principle: the algebra of quantum mechanical operators. Answer is (D).

FINAL: (D) $AB - BA = 0$

SHORTCUT / EXAM TRICK

Identify the model system first, then apply its energy formula and selection rule.

COMMON MISTAKE

Mixing formulas across models (e.g. oscillator virial vs Coulombic virial).

EXAM TIP

Match the physical setup to the standard model (box / oscillator / rotor / H-atom).

MEMORY TRICK

Every CSIR quantum question maps onto one of the four standard solved systems.

Why the Other Options Are Wrong

Correct answer: D

A ***AB* = *A* 2 and *BA* = *B*2**

Inconsistent with the governing quantum mechanical principle; correct choice is (D). See worked explanation.

B ***AB* + *BA* = 0**

Inconsistent with the governing quantum mechanical principle; correct choice is (D). See worked explanation.

C ***A* and *B* are arbitrary**

Inconsistent with the governing quantum mechanical principle; correct choice is (D). See worked explanation.

Q91

CORRECT OPTION (C) ¦ eÅ¨ = eÅ¨ , therefore , eigen function ¦¨ $d2$ eix = $i2$ eix , therefore, eigen function. $dx2$ Quantum Chemistry 92. Correct option

A. 2 + 1

B. ***H***11 − ***ES***11 ***H***12 − ***ES***12

C. Orbital degeneracy =n2=62=36

D. ***A***, ***BC*** = ***A***, ***B C*** + ***B A***, ***C*** = 0 { ***since***, ***A***, ***B*** = 0 ***and A***, ***C*** = 0}

QUESTION INSIGHTS

ESTIMATED TIME
2–3 min

DIFFICULTY
Medium

CONCEPT TESTED
Integrated quantum-mechanical reasoning

PYQ FREQUENCY
Moderate · 6 papers

REVISION PRIORITY
★★★★☆

EXPECTED LEVEL
Part B / Part C

MEMORY HOOK
Every CSIR quantum question maps onto one of the four standard solved systems.

Correct Answer C Orbital degeneracy =n2=62=36

CONCEPT

General quantum-chemistry principles: postulates, operator algebra, boundary conditions and symmetry that connect the model systems (box, oscillator, rotor, H-atom).

↓

LOGIC / WORKING

- Key principle: the governing quantum mechanical principle. Answer is (C).

FINAL: (C) Orbital degeneracy =n2=62=36

SHORTCUT / EXAM TRICK

Identify the model system first, then apply its energy formula and selection rule.

COMMON MISTAKE

Mixing formulas across models (e.g. oscillator virial vs Coulombic virial).

EXAM TIP

Match the physical setup to the standard model (box / oscillator / rotor / H-atom).

MEMORY TRICK

Every CSIR quantum question maps onto one of the four standard solved systems.

Why the Other Options Are Wrong

Correct answer: **C**

A **2 + 1**
Inconsistent with the governing quantum mechanical principle; correct choice is (C). See worked explanation.

B $H11 - ES11\ H12 - ES12$
Inconsistent with the governing quantum mechanical principle; correct choice is (C). See worked explanation.

D $A, BC = A, B\,C + B\,A, C = 0$ { *since*, $A, B = 0$ *and* $A, C = 0$}
Inconsistent with the governing quantum mechanical principle; correct choice is (C). See worked explanation.

TOPIC REVISION

Quantum Chemistry – General

6 PYQs · Last-minute revision

TOPIC SUMMARY

General quantum-chemistry principles: postulates, operator algebra, boundary conditions and symmetry that connect the model systems (box, oscillator, rotor, H-atom).

IMPORTANT FORMULA SHEET

Box: $E \propto n^2$
Oscillator: $E = (n+½)\hbar\omega$
Rotor: $E = BJ(J+1)$
H-atom: $E = -Z^2/2n^2$

FREQUENTLY ASKED CONCEPTS

Model systems
Operator postulates
Selection rules
- Symmetry

COMMON MISTAKES & QUICK NOTES

Watch out:
Mixing formulas across models (e.g. oscillator virial vs Coulombic virial).
Last-minute:
Identify the model system first, then apply its energy formula and selection rule.

MOST-REPEATED PYQs & EXPECTED IN EXAM

PYQs in this topic: Q17 Q26 Q37 Q53 Q71 Q91

Expect **1 question(s)** next session on **Integrated quantum-mechanical reasoning.**

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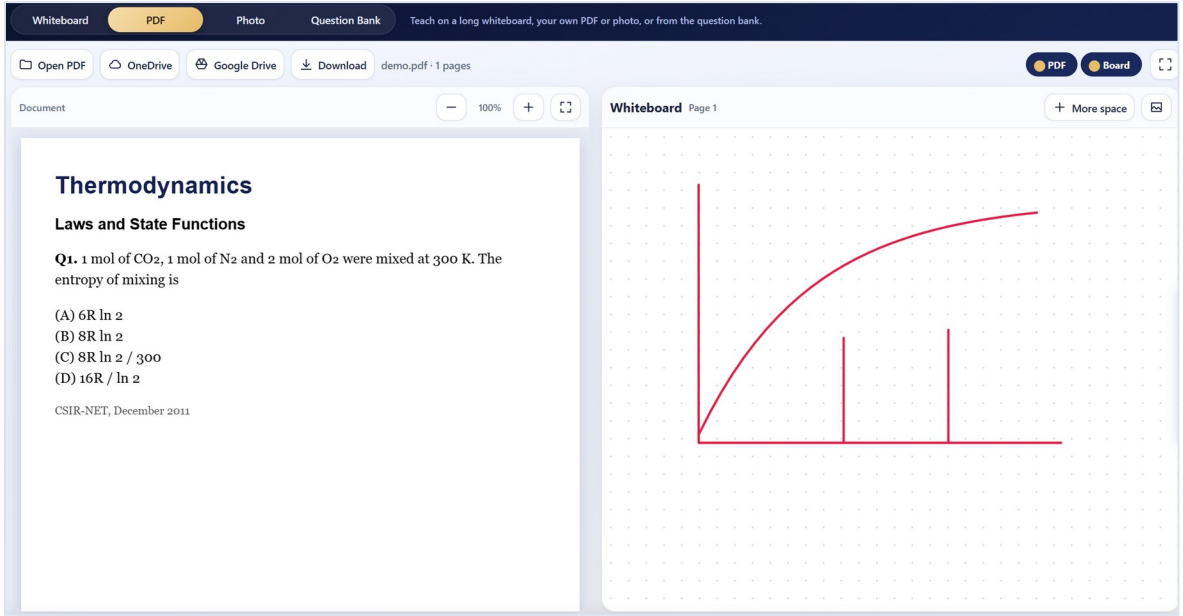
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