QUANTUM CHEMISTRY(QB)

1. State Heisenberg's position-momentum uncertainty principle. How is position uncertainty is defined here?
2. 2.14 eV is required to remove an electron from Cs. (i) What is the cut off λ for photo electric emission from Cs (ii) Will a light of 6000Å liberate an electron from Cs?
3. Find the zero point energy of particle of mass 1×10^{-28} kg confined in a rectangular box of sides $L_x = L$ and $L_y = 2L$, where L is 10 nm.
4. Evaluate the commutators [x, y] and [$\frac{1}{x}$, p_x] .
5. Calculate the probability of finding a particle of mass m confined in a 1-D box of Length L within the length X= $\frac{L}{4}$ to X= $\frac{3L}{4}$.
6. Justify or contradict the following statement.
   "The energy values of a particle of mass m, which is confined in a 1-D box of length L is given as, $E_n = \frac{n2h2}{8mL2}$, = , where $n = \pm1, \pm 2, \pm 3,$........"
7. Draw the Ψ^2 versus x curve for a harmonic oscillator at its zero point energy level. How does the profile satisfy Bohr correspondence principle at high quantum numbers? — Explain.
8. Show that if $\hat{A}$ and $\hat{B}$ are Hermitian then $\hat{A}\hat{B}$ is also Hermitian only if $\hat{A}$ and $\hat{B}$ commute.

9. $\Psi = \Psi_1 + \sqrt{3}\,\Psi_2$ where Ψ_1 and Ψ_2 are normalized and mutually orthogonal functions. Normalize Ψ.
10. If $\hat{A} = \frac{d^2}{dx^2}$ and $\hat{B} = \hat{x}$ Find out whether (i) $A\hat{}$, $B\hat{}$ commute (ii) (e_x + sin x) is an eigen function of ($A\hat{} + B\hat{}$) .
11. The stopping potential for photo electrons emitted from a surface irradiated with light of wavelength 3000 Å is 1.91 V. When the incident wavelength is changed the potential is found to be 0.9 V. What is the new wavelength ?
12. Show that adding a constant 'c' to the potential energy leaves the stationary state wave functions unchanged and simply adds 'c' to the energy eigenvalues.
13. Justify or criticize the following statements:
    (i) The state function Ψ must be a real function.
    (ii) The term *state* and *energy level* are synonymous in quantum mechanics.
14. Show that product of two linear operators is a linear operator.
15. Without evaluating any integral, justify the following:
    (i) For n = 2 state, the probabilities of finding the particle in the *left half* and the *right half* of a one dimensional box are same.
    (ii) The relation of average values <A + B> = <A> + <B> holds true.
16. Show that if f is an eigenfunction of A with eigenvalue a then f will the eigenvalue a^2 for operator A^2 What property of A you have assumed in your answer?
17. What is meant by Hermitian operator? Verify whether the operator d/dx Hermitian operator or not.
18. Explain why $d\Psi/dx$ should be continuous for $\Psi(x)$ to be a well-behaved eigenfunction of the Hamiltonian operator. Why is normalization of Ψ necessary?

19. Test whether the function $f(x) = \sin x \cos x$ is eigenfunction of the operator d^2/dx^2 or not.
20. Determine whether the following functions are well behaved or not in the indicated intervals.
    (i) $1/x$ $(0,\infty)$
    (ii) $\tan x$ $(0, \pi)$