CML101: Tutorial 3 - Quantum Chemistry
UG Semester - I (2023-24)

Q1: Consider a particle of mass 100 g can be located within a distance range 10^{-8} cm. What is the uncertainty in its velocity measurement? Do the same exercise for an electron with mass $\sim 10^{-27}$ g. Compare and rationalize the uncertainty values.

Q2: Photochemical studies with a sodium surface resulted the following data,

Wavelength (Å):	3125	3650	4047	4339	5461
Retarding potential (Volts):	- 0.382	-0.915	-1.295	-1.485	-2.043

Calculate the work function and the Planck's constant. You can take the help of a graphical method.

Q3: The work function (ϕ) for Cesium is 3.43×10^{-19} J. What is the kinetic energy of an electron released by radiation of 550 nm? What is the stopping voltage (V)? How many photons are absorbed if the total energy supplied to the surface at the same wavelength is 1.00×10^{-19} J?
[V = $\frac{KE_{max}}{e}$, Charge of an electron (e) is 1.602×10^{-19}C]

Q4: Calculate the wavelength of (i) a 65 g tennis ball served at a velocity of 100 mph, and (ii) an electron ejected from an atom with kinetic energy 2.5 eV. What inference you draw from the calculated wavelengths of the two objects?
[100 mph $\approx$ 45 m s^{-1} and 1 eV = 1.6×10^{-19} J]

Q5: Assume a wave function has the following form,
$\psi(x) = N(a^2 - x^2)$ Find out it's normalization constant N if the function is bound between -a to +a.

Q6: Which of the functions (i) sinkx, (ii) $5x^2$, (iii) 1/x, and (iv) $5e^{-5x}$ are eigenfunctions of $\frac{d^2}{dx^2}$? Find out the eignevalues.

Q7: Evaluate the commutators

$$\left[x, \frac{d}{dx}\right], \left[\frac{d}{dx}, \frac{d^2}{dx^2}\right], \left[3x^2, \frac{d}{dx}\right], \left[\frac{d}{dx} - x, \frac{d}{dx} + x\right]$$

Q8: Show that, $\left[\hat{x}, \hat{p}_x\right] = ih/2\pi$
What is the significance of this outcome?

Q9: Consider a function ψ = Nx(l-x) confined in a box of length (0,l), where N is the normalization constant. Find the average kinetic energy of the particle.

Q10: A wavefunction of a particle in a 1D box is given as,

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

(i) Find $< x >$ and $< x^2 >$ for a particle of mass m in the ground state of a box of length L.

(ii) The technical definition of uncertainty is

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$

What is Δx for the ground state in a box?

Q11: For an electron in a 1-D box of length 2.0 Å
(i) Calculate the energy difference between n=2 and n=3 levels.
(ii) Calculate the wavelength of the photon corresponding to a transition between these two energy levels.
(iii) In what part of the electromagnetic spectrum will this wavelength be?

Q12: The generalized wavefunction of a particle in a 1D box is given as,

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

Show that the wavefunctions $\psi_{n=1}$ and $\psi_{n=2}$ are orthogonal to each other.

Q13: Consider a particle in its ground state confined to a 1-D box in the interval (0,8). What is the probability of finding the particle in between [4 - d/2 to 4 + d/2] where d is very small so that function can be taken as constant?

Q14: What is the degeneracy of the energy level which has three times energy than that of the lowest energy level in 3-D box?