Rajiv Gandhi Institute of Petroleum Technology

An Instituiton of National Importance

Jais, Amethi, Uttar Pradesh

Tutorial/Assignment – IV

1. (a) Explain the limiting cases of Planck's formula in Black Body Radiation. (b) The sun's surface temperature is 5000K. How much power is radiated by one square meter of the sun's surface?

2. A retarding potential of 1.18 volts just suffices to stop photoelectrons emitted from Sodium by light of frequency 1.13×10^{15} s^{-1}. What is the work function, W, of potassium?

3. (a) The lifetime of an excited state of a molecule is 1×10^{-9} s.

What is the uncertainty in its energy in cm^{-1}?

(b) How would this manifest itself experimentally?

4. (a) Write down the Hamiltonian Operator for He atom.

(b) Find out the normalization constant for a function $\psi = x$ between 0 to L.

5. (a) Show that Time-independent Schrödinger Equation is an eigen-value equation. (b) Write down the Time-independent Schrödinger Equation for "n" particle system.

6. (a) For the particle in a 1-D box, what is the probability of finding the electron between x = 0.48 and 0.52 for both n=1 and n=2. (b) Rationalize your answer.

7. For a particle in a 3-D box with $L_x=L_y=L_z$ How many distinct transitions can be possible in the system. Consider n_i=1,2,3 (for i=x,y,z)?

8. (a) Use the Planck distribution to deduce the Wien's displacement law, that maximum radiant energy density of black body radiation is inversely proportional to wavelength.

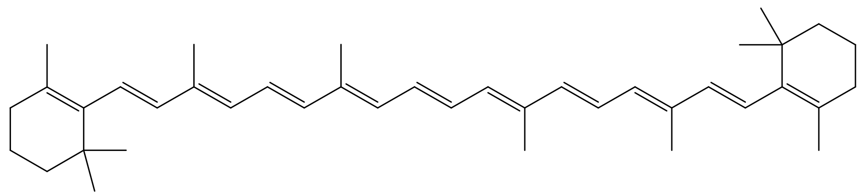
(b) Calculate the wavelength of a tennis ball of mass 60 gm in motion. The fastest serve in tennis is about 140miles/hour or 62 m/s. Rationalize your answer.

(c) Evaluate the kinetic energy of the particle with wavefunction,

$$\psi = (\cos\chi)e^{ikx} + (\sin\chi)e^{-ikx}$$

where χ is a parameter.

(d) Estimate the electronic absorption wavelength in nm for β-Carotene using Particle in 1-D box solutions. (Assume each C-C bond length = 140 pm)



9. (a) Assume that water absorbs light of wavelength 4.20×10^{-6} m with 100% efficiency. How many photons are required to heat 5.75 g of water by 1.00 K at this wavelength? The heat capacity of water is 75.3 J mol^{-1} K^{-1}.

10. (a) Calculate the de Broglie wavelength (in m) of a mass of 1.0 g travelling at 95% of the speed of light (ignore relativistic effects). (b) Is $\psi(x,t)$ an eigenfunction of the p_x^2 operator for the 1-dimensional particle in a box? Given, $\psi(x,t) = \exp(iEt/h) \times \sin(n\pi x/L)$.

11. For the particle in a 1-D box, what is the probability of finding the electron between x = 0.49 and x = 0.51 for both n=2 and n=4. Rationalize the answer.

12. The terms states and levels are **NOT** synonymous in quantum mechanics. For the particle in a three dimensional box (L_x=L_y=L_y) consider the energy range $E < 13h^2/8mL^2$. Find out number of energy levels and states using appropriate quantum numbers.

13. (a) What are the differences between orbit and orbital ?

(b) The operator for the angular momentum of a particle travelling in a circle in the xy plane is $\hat{l}_z = (\hbar/i)d/d\varphi$, where φ is its angular position, what is the angular momentum of a particle described by the wavefunction, $e^{-2i\varphi+\theta}$?

14 Find the probability of finding the particle in the first tenth (from x=0 to x= L/10) of the box for n=2 and n=1000 states.

Compare the quantum mechanical predictions with the classical prediction and rationalize the observation.

15. (a) The function $\psi(x) = \left(\frac{105}{L}\right)^{1/2}\left(\frac{x}{L}\right)^{2}\left[1-\left(\frac{x}{L}\right)\right]$ is an acceptable wave function for the particle in a 1-D box of length L. Calculate the average values of x and x^2 .

(b) Using the average values of x and x^2 calculate the standard deviation (σ_x) in position (x), where $\sigma_x = \sqrt{\langle x^2\rangle - \langle x\rangle^2}$. Based on the Heisenberg uncertainty principle, what then is the minimum standard deviation in the momentum σ_p

16. Draw the energy level diagram (π-molecular orbital) showing the HOMO and the LUMO one for 1,3,5-hexatriene, C_6H_8. Calculate the wavelength of light required to induce a transition from its ground state to the first excited state.

Assume that the molecule is linear and use the values 135 and 154 pm for the C=C and C–C bonds, respectively.

17. **(a)** Summarize the evidence that led to the introduction of quantum mechanics

(b) The work function for metallic rubidium is 2.09 eV. Calculate the kinetic energy and the speed of the electrons ejected by light of wavelength, 650 nm.

18. **(a)** Show that the kinetic energy of the free particle is consistent with the classical result.

(b) Discuss the physical origin of quantization energy for a particle confined to moving inside a one-dimensional box

19. **(a)** Estimate the minimum uncertainty in the speed of an electron in a one-dimensional region of length $2a_0$.

(b) Find out the wave function $\psi(x)$ is normalized or not. And calculate the average value $\langle x \rangle$.

$$\psi(x) = x\left(1 - \frac{x}{a}\right)$$

20. **(a)** Evaluate the arbitrary constants (A & B) of the wave function, $\Psi = A\exp(3x) + B\exp(-2x)$

for the boundary conditions: y = 0 at x = 0 and $\frac{dy}{dx} = 1$ at x = 0.

(b) An electron in a stationary state of a one-dimensional box of length 0.300 nm emits a photon of frequency 5.05×10^{15} s^{-1}. Find the initial and final quantum numbers for this transition.

(c) Sketch the graphs of ψ and of $|\psi|^2$ for the n=4 and n=5 particle-in-a-box states.

21. **(a)** A particle is in the n-th energy state $\psi_n(x)$ of an infinite square well potential with width L. Determine the average/expectation value for kinetic energy of the particle.

(b) Determine the probability P_n for the confinement of the particle to the first 1/a of the width of the well. Comment on the n-dependence of P_n

22. **(a)** What is Ultra-violet Catastrophe? How does quantization (Plank's Theory) solve this problem?

$$\boldsymbol{\rho_\nu (T) d\nu = \frac{8\pi h}{c^3} \frac{\nu^3 d\nu}{\left(e^{\frac{h\nu}{k_B T}} - 1\right)}}$$

(b) When a particle of mass 9.1×10^{-28} g in a certain one-dimensional box goes from the n = 5 level to the n = 2 level, it emits a photon of frequency 6.0×10^{14} s^{-1}. Find the length of the box.

(c) A certain one-particle, one-dimensional system has wave function, ψ (x,t). Find the potential-energy function V for this system. $\boldsymbol{\Psi(x, t) = ae^{-ibt}e^{-bmx^2/\hbar}}$, where a and b are constants and m is the particle's mass.