

CH-107 Tutorial-1

Solve these problems before coming to the tutorials. TA is going to guide you solve the questions.

1. If an electron in a hydrogen atom is confined to a region of size 53 picometer (pm) from the nucleus, what is the indeterminacy in its momentum and velocity?

2. Consider the eigenvalue equation $C^2\Psi = \Psi$ where C is a quantum mechanical operator, and Ψ is an eigenfunction. What are the possible eigenvalues of the operator C ?

3. The eigenvalue equation is given as $\hat{H}\Psi = a\Psi$. Suggest eigenfunctions for the following operators

(i) $\frac{d}{dx}$ (ii) $\frac{d^2}{dx^2}$ (iii) $\int dx$ (iv) $-i\hbar \frac{\partial}{\partial q}$ (v) $\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

4. Under what conditions will a linear combination of two or more eigenfunctions also be an eigenfunction of an operator \hat{H} ?

5. Following the postulates of Quantum Mechanics, how would one calculate the expectation value of a physically observable quantity? How would one calculate the most probable value? What is the need to calculate average or most-probable values for quantum-mechanical particles?

6. Distinguish between expectation value and eigenvalue.

7. Which of the following CAN NOT be a valid wavefunction? Use graphical arguments.

(i) $\frac{1}{x} \sin x$ (ii) $x \sin x$ (iii) $Ae^{-\alpha x^2}$

CH-107 Tutorial -2

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1. Calculate the wavelength of light absorbed to bring out the transition from $n = 1$ and $n = 2$ for an electron in a one dimensional box of length of 1.0 nm.
2. For the particle in a box given in the above question, what is the probability of finding the electron between (i) $x = 0.49$ and 0.51 , (ii) $x = 0$ and 0.020 and (iii) $x = 0.24$ and 0.26 (x in nm) for both $n=1$ and $n=2$. Rationalize your answers.
3. Consider a particle in a 3-D box with $L_x=L_y=L_z$. How many *distinct* transitions can be possible (*i.e. may be observed*) in the system if you only consider $n_i=1,2,3$ (for $i=x,y,z$)?
4. The wavefunctions of a particle in a 1D box are orthonormal to each other, i.e. $\langle \psi_i | \psi_j \rangle = \delta_{ij}$ (Kronecker delta) Verify this for $i = 2, j = 1, 2$. Given $\sin \theta \sin \varphi = \frac{\cos(\theta - \varphi) - \cos(\theta + \varphi)}{2}$
5. The Schrodinger equation for a particle of mass m constrained to move on a circle of radius a is given by $-\frac{\hbar^2}{2I} \frac{d^2\psi(\theta)}{d^2\theta} = E_n \psi(\theta)$, where $I=ma^2$ is the moment of inertia and θ is the angle that describes the position of the particle on the circular ring. Suggest acceptable solution, permissible values of the quantum number n and obtain the expression for the eigenvalue E_n using appropriate boundary condition.
6. Under what conditions for the Hamiltonian is it possible to express $\Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3, \dots, \vec{r}_N)$ in the form $\prod_{i=1}^N \Psi(\vec{r}_i)$? Under such situations, what will be the expression for the total energy?
7. Why do we need spherical coordinates for the hydrogen atom problem and not for a particle in a box problem?
8. Obtain the formula for the volume element in spherical polar coordinates?
9. Separate out the motions of the center of mass (M) and reduced mass (μ) for two particle system.
10. Assuming the ground state wave function for hydrogen atom to be $\Psi(r, \theta, \phi) = N \exp\left(\frac{-r}{a_0}\right)$ find the normalization constant N . Use $\int x^n \cdot e^{-ax} dx = \frac{n!}{a^{n+1}}$