

CH107 Home Assignment Week-2

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This week we started with Hydrogen Atom after finishing Particle in a Box (PIB). Some of the essential topics covered this week are -

- **Wavefunction in a 2D potential well** – We extended our knowledge of 1D PIB, including the property of separability of the Hamiltonian operator
- **Degeneracy is a manifestation of symmetry** – When we calculated energies for different pairs of n_x and n_y , we found that some energy levels overlapped for a square box.
- **Wavefunction in a 3D box** – Similar results unfolded by extending our knowledge to a 3D box.
- **Importance of PIB in Chemistry** – Then we discussed the importance of PIB, out of which I mainly found Quantum Confinement interesting.
- **HYDROGEN ATOM (A Completely Solvable problem)** - We started with the Hydrogen atom, which happens to be a completely solvable problem, which is very rare in QM.
- **Spherical Polar Coordinates** – The TISE that we got presented us with a roadblock in Rectangular coordinates; hence we changed the coordinate system.
- **Periodic Boundary Conditions (A new Quantum number) – Quantization of Angular Momentum** – On providing boundary conditions to our azimuth, a new quantum number popped out.
- **Z component of Orbital angular momentum** – We could relate our new found quantum number with the z component of orbital angular momentum.
- **Angular momentum operators** – We then found QM operators for Angular Momentum, which we used to find the L^2 operator.
- **Rigid Rotor** – It has only an angular momentum component. (A completely solvable problem in QM)
- **Unlike PIB, three Quantum Numbers are inter-related in H-atom** – From the Radial part, we also found the azimuthal quantum number (l). All the quantum numbers found were related to one another.
- **Radial Solutions depend on n and l**
- **Surface plot of Ψ and Ψ^2 is not deterministic of the maximum probability of finding the electron; hence we use the Radial probability distribution function.**
- **Number of radial nodes = $n-l-1$**
- **Number of angular nodes = l**
- **Shapes of orbitals depend on l and m_l**
- **Plot of the Angular Part of the wavefunction** – This week, we concluded after seeing the angular part of the wavefunction and to build it further to generate plots of the wavefunction.