CH 107 Week 2 Summary

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In the second Week, we learnt about the Rigid Rotor, and how we reduced it from a two body problem to a one body problem by taking our coordinates about the Centre of Mass. We reduced it into a one body problem of a body of mass μ (reduced mass) given by

$$\mu = \frac{m_1 m_2}{m_1 + m_2} \tag{1}$$

We then learned about Spherical Coordinates, and derived the expression for the Laplacian Operator in Spherical Coordinates

$$\nabla^2\Psi = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial\Psi}{\partial r}) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial\Psi}{\partial\theta}) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\Psi}{\partial\phi^2} \tag{2}$$

It was noticed that the angular part of the Laplacian was similar to the form of the operator $\hat{L}^2 = -\hbar^2(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2})$. In fact, for a rigid rotor:

$$\hat{KE} = -\frac{\hbar^2}{2m}\nabla^2 = \frac{\hat{L}^2}{2mr^2} = \frac{\hat{L}^2}{2I} \tag{3}$$

We then found the eigenfunctions of $\hat{L}^2$ (which were also the eigenfunctions of $\hat{H}$ for the rigid rotor). These turned out to be the Spherical Harmonics.

$$Y_l^m(\theta,\phi) = (-1)^m\sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}P_l^m(\cos\theta)e^{im\phi} \tag{4}$$

Where, $P_l^m(x)$ are the Associated Legendre Polynomials. Using this, we solved the Schrödinger Equation for the rigid rotor, and found the allowed Energies to be:

$$E_l = \frac{\hbar^2 l(l+1)}{2\mu r_0^2} \tag{5}$$

We then solved the Schrödinger Equation for the Hydrogen Atom. We first separated the Coordinates into Centre of Mass and Internal Coordinates. We represented the Internal Coordinates with a Spherical Coordinate System, in order to use Separation of Variables on the Internal Coordinates. We wrote the Internal Wave Equation in the form of $R(r)\Theta(\theta)\Phi(\phi)$.
Now to solve the Schrödinger Equation, we had to introduce three separation constants, which were called Quantum Numbers. The Principal Quantum Number (n), the Azimuthal Quantum Number (l) and the Magnetic Quantum Number (m). We then proved that n must be a positive integer, and that $l = 0, ...n-1$ and $m = -l, ...0, ...l$. We associated the values of n, l, m to different Orbitals. $l = 0$ represents s orbitals, $l = 1$ represents the p orbitals, $l = 2$ represents the d orbitals, and so on. The values of m give different orbitals of the same type. For example $l = 1$ means that $m = -1, 0, 1$. Therefore there are three p orbitals, (p_x, p_y, p_z), whereas there is only one s orbital. On solving the Schrödinger equation, we find that:

$$E_n = -\frac{me^4}{32\pi^2\epsilon_0^2\hbar^2}\frac{1}{n^2} = -\frac{13.6\,\mathrm{eV}}{n^2} \tag{6}$$

$$L^2 = \hbar^2 l(l+1) \tag{7}$$

$$L_z = m\hbar \tag{8}$$

The expressions for $R(r)$, $\Theta(\theta)$ and $\Phi(\phi)$ were found to be such that:

$$\Theta_l^m(\theta)\Phi_m(\phi) = Y_l^m(\theta,\phi) \tag{9}$$

$$R(r) = \sqrt{(\frac{2}{na_0})^3\frac{(n-l-1)!}{2n(n+l)!}}(\frac{2r}{na_0})^l L_{n-l-1}^{2l+1}(\frac{2r}{na_0})e^{-\frac{r}{na}} \tag{10}$$

Here $a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2}$ represents the Bohr radius, and $L_p^q(x)$ represent the associated Laguerre Polynomials.