CH 107 Week 3 Summary

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In this week, we finished solving the Schrödinger Equation for the Hydrogen Atom and found that

$$\Psi_{nlm} = R_{nl}(r)\Theta_{lm}(\theta)\Phi_m(\phi) = R_{nl}(r)Y_l^m(\theta,\phi) \tag{1}$$

Here, Y_l^m represent the Spherical Harmonics. Unfortunately, for $m \neq 0$, Ψ_{nlm} is complex. This is because $\Phi_m(\phi) = e^{im\phi}$. Therefore, to construct the real orbitals, we took the Real and Imaginary Parts of the Complex Orbitals. This amounted to taking Linear combinations of the Complex Orbitals with of magnetic quantum number $+m$ and $-m$.

$$\Psi_+ = \frac{\Psi_{nlm} + \Psi_{nl-m}}{\sqrt{2}} \tag{2}$$

$$\Psi_- = \frac{\Psi_{nlm} - \Psi_{nl-m}}{i\sqrt{2}} \tag{3}$$

Since the real orbitals with $m \neq 0$ are made of Linear Combinations of Complex Orbitals with the same n and l, but different m. They remain eigenstates of $\hat{H}$ and $\hat{L}^2$ but they are no longer eigenstates of $\hat{L}_z$. That is, they have definite Principal and Azimuthal Quantum Numbers, but no fixed Magnetic Quantum Number.

It turns out, that all the real orbitals (except the s orbitals, which have $l = 0$) can be written in the form $\Psi = f(r)F(x,y,z)$. Hence these orbitals are denoted by $\boxed{nA_{F(x,y,z)}}$ (for the s orbitals, we omit the subscript). Here n is their Principal Quantum Number and A is a symbol denoting their value of l, the Azimuthal Quantum Number. For $l = 0$, we call the orbitals s orbitals, for $l = 1$, we call them p orbitals, for $l = 2$, we call them d orbitals and so on. For example,

$$\Psi_{1s} = \frac{1}{\sqrt{\pi a^3}} e^{-\frac{r}{a}} \tag{4}$$

$$\Psi_{2p_x} = \frac{1}{4\sqrt{2\pi}}(\frac{1}{a})^{\frac{5}{2}} e^{-\frac{r}{2a}} x \tag{5}$$

$$\Psi_{3d_{2z^2-x^2-y^2}} = \frac{1}{48\sqrt{\pi}}(\frac{2}{3a})^{\frac{7}{2}} e^{-\frac{r}{3a}} (2z^2 - x^2 - y^2) \tag{6}$$

Note that above orbital is often called the d_{z^2} orbital.

We then discussed the Radial Probability Distribution Curves $r^2 R_{nl}^2$, and noticed that while the height of the maxima of R_{nl} decreased with increasing r, the height of the maxima of $r^2 R_{nl}^2$ increased with increasing r and therefore the electron was more likely to be found in the outer lobes of the orbital and had negligible probability of being inside the nucleus.

We then discussed the Graphs of various Orbitals and Radial Probability Distribution Curves and saw many methods to graph them.