

CHEM 3420: Physical Chemistry II — Spring 2009

February 13, 2008

Lecture 11: The Hydrogen Atom: Radial solutions and the big picture

References

1. Engel and Reid, *Physical Chemistry*, Levine 18.1–18.4
2. Hydrogen atom handouts

Key Concepts

- The angular part of the wave functions ($\Theta\Phi$) describe the three dimensional shape of the solutions to the Schrödinger Equation .
 - For example, if $l = 0$ and $m = 0$ we discovered that the resulting solution would be spherical in shape because it was independent of both θ and ϕ .
 - For $l = 1$ and $m = 0$ we obtained a solution that resembled a p_z -orbital: it has a θ dependence but was independent of ϕ .
 - In general, when $m \neq 0$, the angular portion of Ψ will have an imaginary component. To avoid this, we take linear combinations of the two solutions ($\pm m$) to obtain the real wave functions.
- The radial solutions, $R(r)$ lead to two important results: the energy and the functional form of $R(r)$.
- We find that the energy depends on a new quantum number, n in the following way:

$$E \propto -\frac{m_e e^4 Z^2}{2\hbar^2 n^2}$$

with the following important observations:

1. The energy only depends on n .
 2. The energy is inversely proportional to n^2 , or $E \propto \frac{1}{n^2}$.
 3. The energy is negative ($E < 0$).
 4. As n gets very large, the energy approaches zero: $n \rightarrow \infty$, $E \rightarrow 0$.
- The general solutions for $R(r)$ have the following form:

$$R_{nl}(r) = F_{nl}(r)e^{\frac{Zr}{na_o}} = F_{nl}(r)e^{-\rho/n}$$

where a_o is the Bohr radius and is found from a bunch of physical constants and $\rho = \frac{Zr}{a_o}$. $F_{nl}(r)$ is a polynomial that is damped by an exponential function $e^{-\rho/n}$. Solutions are dependent on both n and l which means there are degenerate states that have the same energies (identical n 's) yet different solutions ($R_{nl}(r)$).

- Exact solutions that include all constants for the radial and angular parts can be found on the handout distributed in class. Notice the form for all $R(r)$ is the same as described above.
- There are both radial and angular nodes in the wave functions of the hydrogen atom. These occur when either the radial or angular solution is zero. As the energy (n) increases, the number of total nodes also increases.

Related Exercises in Levine

Exercises 18.1, 18.6, 18.10