3.5: Some Useful Expressions

Listed below are a number of equations which give the dependence of $\bar{r}$, $\overline{PE}$ and $\overline{KE}$ on the quantum numbers n, l and m. They refer not only to the hydrogen atom but also to any one-electron ion in general with a nuclear charge of Z. Thus He^+ is a one-electron ion with $Z = 2$, Li^{+2} another example with $Z = 3$.

The average distance between the electron and the nucleus expressed in atomic units of length is:

$$\bar{r}_{n,l,m} = \frac{n^2}{Z}\left[1+\frac{1}{2}\left\{1-\frac{l(l+1)}{n^2}\right\}\right]$$

Note that $\bar{r}_{n,l,m}$ is proportional to n^2 for $l = 0$ orbitals, and deviates only slightly from this for l ¹ 0. The value of $\bar{r}_{n,l,m}$ decreases as Z increases because the nuclear attractive force is greater. Thus $\bar{r}_{1,0,0}$ for He^+ would be only one half as large as $\bar{r}_{1,0,0}$ for H.

$E_n = -\frac{Z^2}{n^2}K = -\frac{Z^2}{2n^2}$ au	$K = \frac{2\pi^2 me^4}{h^2} = \frac{e^2}{2a_0}$
$\left(\overline{PE}\right)_{n,l,m} = -\frac{2Z^2}{n^2}K$	$\left(\overline{KE}\right)_{n,l,m} = -E_n = +\frac{Z^2}{n^2}K$