September 30, 2010

PHY 741 – Problem Set #11

Continue reading Chapter 5 in **Mahan**; homework is due Monday, October 4, 2010.

Consider an electron of mass M moving in 3 dimensions in a central potential $V(r)$ representing the interaction of that electron with the nucleus and other electrons in an atom, presented by the form for $r \to 0$:

$$V(r) \stackrel{r\to 0}{\equiv} -\frac{Ze^2}{r}$$

and by the form for $r \to \infty$:

$$V(r) \stackrel{r\to \infty}{\equiv} -\frac{qe^2}{r}.$$

Here Z represents the nuclear charge and q is usually 1 or 2 depending on whether the atom is neutral or positively charged. It is convenient to write the Schrödinger equation in terms of the scaled variables:

$$\rho \equiv \frac{r}{a} \quad \text{where } a \text{ is the Bohr radius} \quad a \equiv \frac{\hbar^2}{Me^2}.$$

$$\epsilon \equiv -\frac{E}{E_{Ry}} \quad \text{where } E_{Ry} \text{ is the Rydberg constant} \quad E_{Ry} \equiv \frac{\hbar^2}{2Ma^2} \equiv \frac{e^2}{2a}.$$

1. Show that the radial Schrödinger equation to determine the radial component of the wavefunction $R(\rho)$ can be written

$$\left\{ \frac{d^2}{d\rho^2} + \frac{2}{\rho}\frac{d}{d\rho} - \frac{l(l+1)}{\rho^2} - \frac{2Ma^2}{\hbar^2}V(\rho) - \epsilon \right\} R(\rho) = 0.$$

2. Consider the limit $\rho \to \infty$, where the dominant terms in the equation simplify to

$$\left\{ \frac{d^2}{d\rho^2} + \frac{2}{\rho}\frac{d}{d\rho} + \frac{2q}{\rho} - \epsilon \right\} R(\rho) = 0.$$

   In general, the value of ϵ needs to be determined numerically. Show that, if it were known, the radial wavefunction would take the form:

$$R(\rho) = \mathcal{N} \rho^{q/\sqrt{\epsilon}-1} \mathrm{e}^{-\sqrt{\epsilon}\rho} \left(1 + \sum_{n=1} \frac{C_n}{\rho^n} \right),$$

   where $\mathcal{N}$ and $\{C_n\}$ are constant coefficients.

3. Now consider the limit $\rho \to 0$, where the dominant terms in the equation simplify to

$$\left\{ \frac{d^2}{d\rho^2} + \frac{2}{\rho}\frac{d}{d\rho} - \frac{l(l+1)}{\rho^2} + \frac{2Z}{\rho} \right\} R(\rho) = 0.$$

   Find the leading power series for $R(\rho)$ in this limit.