Virial Theorem

The result we obtained from the Rutherford model for the relationship between the kinetic and potential energies of the hydrogen atom was:

$$E = \frac{1}{2}U = - K = -\frac{1}{2}\frac{Z e^2}{4\pi\varepsilon_0 r}$$

This is an example of a more general relationship between kinetic and potential energy called the **Virial Theorem.** This theorem holds both in classical and quantum mechanics and relates the average kinetic and and average potential energies of a system of particles with arbitrary potential interactions. A general proof of the Virial Theorem for quantum mechanics can be found in *Molecular Quantum Mechanics (2nd ed),* P. W. Atkins, Oxford, 1983, pp. 425-426. Application to the coulombic potentials relevant to interactions in atoms and molecules can be found in McQuarrie, pp 229, 252-253.

The purpose of this handout is to state the general form of the Virial Theorem for your edification and use in optional parts of problems #5.

The generalized Virial theorem is:

$$\overline{K} = \frac{1}{2}\overline{\left\{ r\frac{\partial U}{\partial r}\right\}} \quad in\ one\,dimension$$

$$\overline{K} = -\frac{1}{2}\overline{\left\{ \sum_i \vec{F_i}\cdot\vec{r_i}\right\}} \qquad \begin{array}{l} 3D\,(x,y,z) \\ many\,particles\,(i = 1,2,\,...) \end{array}$$

As an example of application of this theorem we use the Coulomb potential in one dimension:

$$U = -\frac{Ze^2}{4\pi\varepsilon_0 r}$$

$$\overline{K} = \frac{1}{2}\overline{\left\{ r\frac{\partial U}{\partial r}\right\}} = \frac{1}{2}\left\{ r\frac{+Ze^2}{4\pi\varepsilon_0 r^2}\right\}$$

$$= \frac{1}{2}\left\{ \frac{Ze^2}{4\pi\varepsilon_0 r}\right\} = -\frac{1}{2}\,\overline{U}$$