QM Spring 2020: In-Class Presentation

1. **Finite Size Effects of the Nucleus** The hydrogen-like atom is usually described by the Hamiltonian

$$H_0 = \frac{\vec{P}^2}{2m} - \frac{Ze^2}{r}. \tag{0.0.1}$$

The $1/r$ form of the potential indicates we are treating the nucleus as a point charge $Z|e|$. Suppose we wish to capture the effects on atomic energy levels due to the internal structure of the nucleus. For simplicity, let us assume the nucleus is a perfect sphere; but allow its charge density $\rho(r, \theta, \phi)$ to be arbitrary – we may hence decompose

$$\rho(r, \theta, \phi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{+\ell} \rho_\ell^m(r) Y_\ell^m(\theta, \phi), \qquad \text{for } 0 \leq r \leq R \tag{0.0.2}$$

$$= 0 \qquad \text{for } r > R. \tag{0.0.3}$$

Use perturbation theory to approximate the first order shift in the Bohr energy levels $E_n = -m(Ze^2)^2/(2n^2)$ due to these $\{\rho_\ell^m\}$.

2. **Inter-Electron Interactions** Consider an atom with Z protons and Z electrons. The interactions between nucleus and the electrons may be modeled as the usual

$$H_0 = \sum_{k=1}^{Z} \left(\frac{\vec{p}_k^2}{2m} + V(|\vec{x}_k|) \right), \tag{0.0.4}$$

where $\vec{p}_k$ and $\vec{x}_k$ are the momentum and position of the kth electron. Let us now attempt to include the mutual interactions of the electrons

$$H_1 = \frac{1}{2} \sum_{a \neq b=1}^{Z} \frac{e^2}{|\vec{x}_a - \vec{x}_b|}. \tag{0.0.5}$$

For an arbitrary V assume the un-perturbed energy eiegen wave functions take the form

$$\langle \vec{x}_k | \, \ell, m \rangle = R_\ell(r) Y_\ell^m(\theta, \phi). \tag{0.0.6}$$

Can you express the first order shift in energies due to H_1 in terms of these $R_\ell(r)$? Calculate these shifts for $\ell = 0, 1, 2$ for the usual Coulomb potential

$$V(r) = -\frac{Ze^2}{r}. \tag{0.0.7}$$

Finally, for such a Coulombic potential, can you use the variational method to estimate the ground state energy of such a Z-proton/electron system?