PHY 491

HW Assignment #2; September 12-19, 2011

1. Calculate the ground state energy of a hydrogen atom using the variational principle.

   Assume that the variational form for the wave function is a Gaussian of the form $Ne^{-\left(\frac{r}{\alpha}\right)^2}$, where *N* is the normalization constant and α is a variational parameter. How does this variational energy compare with the exact ground state energy?

   We will need these integrals:

   $$\int_0^\infty xe^{-x^2}\,dx = \frac{1}{2};\ \int_0^\infty x^2e^{-x^2}\,dx = \frac{\sqrt{\pi}}{4};\ \int_0^\infty x^4e^{-x^2}\,dx = \frac{3\sqrt{\pi}}{8}$$

2. Use the virial theorem which states that $2 < T > = < \vec{r}.\vec{\nabla}V >$, and show that for the hydrogen atom

   $$\left\langle \psi_{nlm} \middle| \frac{1}{r} \middle| \psi_{nlm} \right\rangle = \frac{1}{n^2 a}$$

3. Use Feynman-Hellmann theorem which states that $\frac{\partial E_n}{\partial \lambda} = \left\langle \psi_n \middle| \frac{\partial H}{\partial \lambda} \middle| \psi_n \right\rangle$, to show that for a hydrogen atom

   $$\left\langle \psi_{nlm} \middle| \frac{1}{r} \middle| \psi_{nlm} \right\rangle = \frac{1}{n^2 a}$$

   $$\left\langle \psi_{nlm} \middle| \frac{1}{r^2} \middle| \psi_{nlm} \right\rangle = \frac{1}{(l+\frac{1}{2})n^3 a^2}$$

4. Using the 1st order perturbation results for $E_{mv}^{(1)}$, where *mv* denotes mass velocity and $E_{so}^{(1)}$, where *so* denotes spin-orbit show that

   $$E_{mv}^{(1)} + E_{so}^{(1)} = E_{fs}^{(1)} = \frac{(E_n)^2}{2mc^2}\left(3 - \frac{4n}{j+1/2}\right),$$

   where *fs* denontes fine structure and *j* is the total angular momentum, orbital plus spin.