PHY801: Survey of Atomic and Condensed Matter Physics
Michigan State University

Homework 2

2.1. Calculate the ground state energy of a hydrogen atom using the variational principle. Assume that the variational 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?

You will need these integrals:

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

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

$$< \psi_{nlm}|\frac{1}{r}|\psi_{nlm} >= \frac{1}{n^2 a_B}\ .$$

2.3. Use the Hellmann-Feynman theorem, which states that

$$\frac{\partial E_n}{\partial \lambda} =< \psi_n|\frac{\partial H}{\partial \lambda}|\psi_n >$$

to show that for a hydrogen atom

$$< \psi_{nlm}|\frac{1}{r}|\psi_{nlm} >= \frac{1}{n^2 a_B}\ ,$$

$$< \psi_{nlm}|\frac{1}{r^2}|\psi_{nlm} >= \frac{1}{(l+\frac{1}{2})n^3 a_B^2}\ .$$

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

$$E_{mv}^{(1)} + E_{so}^{(1)} = E_{fs}^{(1)} = \frac{(E_n^0)^2}{2mc^2}\left(3 - \frac{4n}{j+\frac{1}{2}}\right)\ ,$$

where fs denotes fine structure and j is the total angular momentum containing orbital angular momentum plus spin.
