Practice Problems Related to Atomic Structure

This is a somewhat more extensive than normal numerical problem. We show in the notes that because, obviously, no energy state has a lower expected energy than the ground eigenstate, any trial wavefunction gives an upper bound to the ground state energy if the expected energy of that wavefunction is minimized over the wavefunction's parameters. Here we'll give you an opportunity to explore a couple of different wavefunction families.

For the first class, let the wavefunction family be a Gaussian, $\psi = C \exp(-r^2/2r_0^2)$.

1. Determine the normalization constant C.

2. Determine the integrand that needs to be integrated to get the expected energy (explicitly, i.e., do the derivatives).

3. Perform the integral and minimize the energy as a function of r_0. How close do you get to the true answer?

For the second class we will take a power law with a core, $\psi = C/(r^n + r_0^n)$.

4. What values of n are allowed? Note that n does not have to be an integer.

5. For $n = 4$ and $n = 5$, determine (numerically is fine) the normalization constant C.

6. For $n = 4$ and $n = 5$, determine the integrand.

7. Do the integral numerically for $n = 4$ and $n = 5$, and minimize the energy with respect to r_0 in each case; how close do you get?