your name(s)____

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Physics 851 Exercise #10 - Monday, Nov. 8th

You have an electron in a Coulomb potential

$$V(r) = -\frac{e^2}{r}, \quad \frac{e^2}{\hbar c} = \frac{1.0}{137.036}.$$

The reduced mass of an electron is $mc^2 = 0.5107$ MeV and $\hbar c$=197.327 eV·nm.

You will try to solve for the ground state energy using wave functions which are $\ell = 0$ eigenstates of the 3-D harmonic oscillator.

$$\begin{aligned}
\psi_0(\vec{r}) &= \left(\frac{1}{\pi b^2}\right)^{3/4} e^{-r^2/2b^2}, \\
\psi_2(\vec{r}) &= \sqrt{3/2}\left(\frac{1}{\pi b^2}\right)^{3/4} \left(2(r/b)^2/3 - 1\right) e^{-r^2/2b^2}, \\
\psi_4(\vec{r}) &= \sqrt{15/8}\left(\frac{1}{\pi b^2}\right)^{3/4} \left(1 - 4(r/b)^2/3 + 4(r/b)^4/15\right) e^{-r^2/2b^2} .
\end{aligned}$$

Your variational wave function will be

$$\psi(r) = a_0\psi_0(r) + a_2\psi_2(r) + a_4\psi_4(r),$$

with the variational parameters being a_0, a_2, a_4 and b.

Note that we can write the Hamiltonian for $\ell = 0$ spherical waves as:

$$-\frac{(\hbar c)^2}{2mc^2}\left(\partial_r^2 + \frac{2}{r}\partial_r\right) - \frac{e^2}{r}.$$

The expectations of the KE operator are

$$\begin{aligned}
KE_{mn} = \langle\psi_m|\frac{p^2}{2m}|\psi_n\rangle &= -\frac{(\hbar c)^2}{4mc^2b^2}\langle M_r = m+1|(a^\dagger - a)^2|N_r = n+1\rangle \\
&= \frac{(\hbar c)^2}{4mc^2b^2}\left\{\begin{array}{rl}
3, & m=0, n=0 \\
7, & m=2, n=2 \\
11, & m=4, m=4 \\
-\sqrt{6}, & m=0, n=2 \\
0, & m=0, n=4 \\
-2\sqrt{5}, & m=2, n=4
\end{array}\right.
\end{aligned}$$

The expectations of the Coulomb potential are

$$\langle\psi_m|V|\psi_n\rangle = -\frac{e^2}{b\sqrt{\pi}}\left\{\begin{array}{rl}
2, & m=0, n=0 \\
5/3, & m=2, n=2 \\
89/60, & m=4, n=4 \\
-\sqrt{2/3}, & m=0, n=2 \\
\sqrt{3/10} & m=0, n=4 \\
-\frac{11}{6\sqrt{5}}, & m=2, n=4
\end{array}\right.$$

1. Show that for $\ell = 0$ the spherical solutions for the three-dimensional harmonic oscillator are of the form

$$\psi_{n,\ell=0}(r) = \frac{1}{\sqrt{4\pi}r}\phi_{2n+1}(r), \quad n = 0, 1, 2, \cdots$$

where ϕ_n are solutions to the 1-d harmonic oscillator.

2. Using the relations of the previous page, show that when you find the optimum wave function ψ, that

$$\langle\psi|KE|\psi\rangle = -\frac{1}{2}\langle\psi|V|\psi\rangle.$$

Hint: Consider the b-dependence for KE and V.

3. Beginning with the python template,
`https://people.nscl.msu.edu/~pratt/phy851/exercises/fall/exercise10_template.py`
write a program that finds the optimum values of the parameters b, a_0, a_2 and a_4.

4. Plot the wave function alongside the exact solution.

FYI: Multi-dimensional minimization with Newton's method:
If you have a function to minimize, $y(\vec{x})$, you need to find $\vec{x}$ that satisfies all the conditions

$$\partial_i y = 0.$$

If you guess at some value of $\vec{x}$ that fails, i.e. $\partial_i y(\vec{x}) \neq 0$, then you try a new value of $\vec{x}$,

$$\begin{aligned}
\vec{x} &\to \vec{x} + \delta\vec{x}, \\
\delta\vec{x} &= -A^{-1}_{ij}\partial_j y, \\
A_{ij} &= \partial_i\partial_j y.
\end{aligned}$$