your name(s)____

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Physics 851 Exercise #10

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

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

Here, M_r and N_r are quantum numbers for radial Schrödinger equation, remembering that radial wave function ϕ has to go to zero after substitution $\phi \to \psi$, i.e. ϕ is an odd function.

The expectations of the Coulomb potential are

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

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.

Solution:
From Chapter 4, Eq. (56) you know that you can define $u_{\ell=0}(r) = r\psi_\ell(r)$, and that the Schrödinger equation for u_ℓ is the standard 1-d equation.

$$(-\frac{\hbar^2}{2m}\partial_r^2 + V(r))u_\ell = Eu_\ell,$$

with $V(r)$ being the harmonic oscillator potential. BUT, there is also the B.C. that $u_\ell(r = 0) = 0$. Thus the solutions are the H.O. solutions with $n = 1, 3, 5, 7...$, i.e. the solutions with odd reflection symmetry.

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

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

Solution:
From the previous page,

$$\begin{aligned} KE &= \frac{1}{b^2}\text{garbage}, \\ V &= \frac{-1}{b^2}\text{trash}, \\ \partial_b(KE + V) &= \frac{2}{b}KE - \frac{1}{b}V = 0, \\ KE &= -V/1. \end{aligned}$$

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

Solution:
energy should come out to -12.85 eV, and $b = 0.0591$ fm, $a_2/a_0 = 0.1623$, $a_4/a_0 = 0.184$.

4. Plot the wave function alongside the exact solution.