PHYS-4601 Homework 18 Due 10 Mar 2016

This homework is due in the dropbox outside 2L26 by 11:59PM on the due date. You may alternately email a PDF (typed or black-and-white scanned) or give a hardcopy to Dr. Frey.

1. **Estimating Helium Better** *Griffiths 5.11 clarified*

   In this problem, we will estimate the ground state energy of a helium atom. We treat the electron repulsion as a first-order correction to the attraction between the electrons and the nucleus.

   (a) Consider the states of a single electron around a helium nucleus (which has twice the charge of a proton). Argue that the "helium Bohr radius" $a_{\mathrm{He}} = a/2$, where a is the usual Bohr radius, and that therefore the single-electron ground state wavefunction is given by

   $$\langle \vec{x} | n=1, \ell=0, m=0\rangle = \sqrt{\frac{8}{\pi a^3}} e^{-2r/a} \ . \tag{1}$$

   Next assume that the two electron helium groundstate is $|n=1,\ell=0,m=0\rangle_1 |n=1,\ell=0,m=0\rangle_2 |s=0,m_s=0\rangle$, where the total spin state is the antisymmetric singlet. (The spatial wavefunction is given by Griffiths eqn [5.30].) Briefly argue that the energy of this state, in the absence of electron repulsion, is given by Griffiths eqn [5.31].

   (b) Now find $\langle |\vec{x}_1 - \vec{x}_2|^{-1}\rangle$ in this state, as follows:

      1. Use the trick of setting the z axis for $\vec{x}_2$ along $\vec{x}_1$ and the law of cosines to see $|\vec{x}_1 - \vec{x}_2| = \sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta_2}$.
      2. Do the angular integrals for $\vec{x}_2$, noting that

         $$\int_0^\pi d\theta \sin\theta f(\cos\theta) = \int_{-1}^1 dx f(x) \ .$$

         Your result will have square roots of perfect squares, which are equal to absolute values. *Be careful of that!*
      3. Carry out the r_2 integral in two parts, $0 < r_2 \le r_1$ and $r_1 < r_2 < \infty$.
      4. Now do the $\vec{x}_1$ integrals.

   Hint: The "exponential integrals" formula in the back cover of Griffiths will be helpful.

   (c) Use your result to find the change in ground state energy ΔE at first order in perturbation theory. Write ΔE in terms of the Bohr radius a and estimate its value in eV. Then add this to the energy from part (a) to get a rough estimate of the He ground state energy. *Hint*: Remember that the hydrogen ground state energy is $-\hbar^2/2ma^2 = -13.6$ eV.

2. **Not-Quite-Square Well**

   Consider a particle moving in a 1D well of potential

   $$\begin{cases} V_0 x/a & 0 < x < a \\ \infty & \text{otherwise} \end{cases} \ . \tag{2}$$

   Assume that $\epsilon = ma^2 V_0/\hbar^2 \ll 1$. Recall that the energy eigenfunctions and eigenvalues are

   $$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \ , \quad E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2 \ , \quad n = 1, 2, \cdots \ . \tag{3}$$

(a) Show that the first order contribution to the energy is $E_n^1 = V_0/2$ for all n.

(b) Now consider the ground state of the system. Recalling that the first order correction to the ground state can be written as

$$|\psi_1^1\rangle = \sum_{n=2}^{\infty} c_n |\psi_n^0\rangle \ , \tag{4}$$

use Maple's `seq` and `int` commands to make a list of the coefficients c_n for $n = 2, \cdots 10$. Attach a copy of your Maple code. You should work in units where $a = 1$ and express your answer in terms of the parameter ϵ.

(c) Use Maple to plot the uncorrected ground state wavefunction and the wavefunction with first order terms (including corrections from the $n = 2, \cdots 10$ states) on the same plot. In order to see the difference, use an exaggerated value of $\epsilon = 3$.

3. **Finite Proton in Hydrogen** *related to Griffiths 6.29*

In modeling the hydrogen atom with the Coulomb potential, we have treated the proton as a point charge. In this problem, consider the proton to be a shell of charge of radius R. Throughout, make approximations appropriate for $R \ll a$ with a the Bohr radius.

(a) First, let the proton be a uniform spherical shell of charge, so the electron experiences a potential

$$V(r) = -\frac{e^2}{4\pi\epsilon_0} \times \begin{cases} 1/R & \text{for } r < R \\ 1/r & \text{for } r > R \end{cases} \ . \tag{5}$$

What is the change in the hydrogen ground state energy due to the finite size of the proton to lowest order in R/a? Note that the perturbation Hamiltonian is the difference between this potential and the Coulomb potential.

(b) Assume $R \approx 10^{-15}$ m. How large is the shift in energy as a fraction of the hydrogen ground state energy? Work to 1 significant figure. Is this large or small compared to the hyperfine structure splitting?

(c) Next, suppose the proton charge is not uniformly distributed, so

$$V(r) = -\frac{e^2}{4\pi\epsilon_0} \times \begin{cases} 1/R(1+\cos\theta) & \text{for } r < R \\ 1/r & \text{for } r > R \end{cases} \ , \tag{6}$$

where θ is the polar angle. Is the energy of the ground state the same or different than for the potential (5)?

(d) **This part cancelled.**