Due: Thur. Dec. 4 (Main campus) or Tue. Dec 9 (Distance students)

Problem I. CT Chapter XI, Complement H_{XI}, exercise 2.

Problem II. CT Chapter XI, Complement H_{XI}, exercise 5. Answer (a)-(c), and only the expansion of the ground state in part (d). You do not need to calculate $\langle \mathbf{M} \rangle$ or do the rest of that problem.

Problem III. Consider the spinless hydrogen atom problem with Hamiltonian H_0, and an energy eigenvalue equation expressed in the usual way: $H_0 \,|n\,l\,m\rangle = E_n \,|n\,l\,m\rangle$, where m is the quantum number for the $\hat{z}$-direction component of the electron's orbital angular momentum. Let r be the distance between a point in space and the center of mass of the proton. The Coulomb potential energy term $V(r)$ within H_0 treats the proton as a point particle, with $V(r) \to -\infty$ as $r \to 0$. Alternatively, the proton can be treated as having charge distribution over a spatial region, as considered in the problem below. Ignore spin variables and all other corrections to H_0 discussed in class (ie, ignore fine and hyperfine structure corrections).

In this model we assume that the proton is a **spherical shell** of radius b, with the proton's electric charge and mass uniformly distributed around the surface. In this proton shell model, the Coulomb potential between the electron and proton is

$$V_s(r) = \begin{cases} -q^2/r & \text{for } r > b \\ -q^2/b & \text{for } r \leq b \end{cases}$$

where $q^2 = \frac{e^2}{4\pi\epsilon_0}$, notation for q and e that is consistent with the Field Guide but opposite that of Cohen-Tannoudji. We can relate this model to the familiar hydrogen problem by writing the Hamiltonian for the proton shell model as $H = H_0 + W$, where W is a small perturbation to the spinless hydrogen Hamiltonian H_0, and

$$W = \begin{cases} 0 & \text{for } r > b \\ 2\,E_I\,a_0\,(1/r - 1/b) & \text{for } r \leq b \end{cases}$$

and we have used the relationship $q^2 = \alpha^2\, m_e c^2\, a_0 = 2E_I\, a_0$. In the remaining parts of this problem, let $b/a_0 = 10^{-5}$ (which is approximately correct). We treat $(b/a_0)^2$ as a small parameter for obtaining approximate expressions for the energy eigenvalues of H using stationary perturbation theory.

(a) Evaluate the matrix elements $\langle 1\,0\,0\,|W|1\,0\,0\,\rangle$ and $\langle 2\,0\,0\,|W|2\,0\,0\,\rangle$, expressing each as a power series in (b/a_0) and **retaining only terms up to order** $(b/a_0)^2$**.** In other words, neglect all higher powers of (b/a_0) in your matrix elements. You can use the information on p. 99 of the Field Guide. *BE CAREFUL: set up your integrals correctly, and pay close attention to the limits of integration of the integrals!* To solve the integrals, let e^{-r/a_0} be approximately 1 within the integrals, since the integration is only over values of r less than $b/a_0 \sim 10^{-5}$.

(b) What are the matrix elements $\langle 1\,0\,0\,|W|2\,1\,m\rangle$ and $\langle 2\,0\,0\,|W|2\,1\,m\rangle$ for any m? Justify your answer.

(c) It turns out that each $\langle 2\,1\,m\,|W|2\,1\,m\rangle$ term is much smaller in magnitude than those of part (a), so we'll define $\epsilon \equiv \langle 2\,1\,m\,|W|2\,1\,m\,\rangle$ but do not calculate ϵ. However, $\langle 1\,0\,0\,|W|2\,0\,0\,\rangle \equiv \beta E_I (b/a_0)^2$ is of similar magnitude to the matrix elements of part (a), but you also do not need to determine β. Given all of the above including your results from parts (a) and (b), use the $\{|n\,l\,m\rangle\}$ representation to write the 5×5 sub-matrix of W that corresponds to the five $n = 1$ and $n = 2$ states. Give your answer in terms of E_I, b, a_0, β. You may also use ϵ, or let ϵ be zero.

(d) For this $n = 1$ and $n = 2$ subspace, give expressions for the approximate energy eigenvalues of H, good to first order in the small parameter $(b/a_0)^2$, and letting $\epsilon = 0$. Leave your answer in terms of the parameters given in this problem; do not calculate numerical values here.

(e) In the hydrogen fine structure problem discussed in class (ignoring proton spin), the $2\,^2S_{1/2}$ and $2\,^2P_{1/2}$ states remain degenerate. This degeneracy is removed when the interaction between the atom and the quantum-mechanical nature of the surrounding electromagnetic field is taken into account; this is the Lamb shift, and it leads to a frequency difference between the $2\,^2S_{1/2}$ and $2\,^2P_{1/2}$ levels of about $2\pi \cdot (10^9$ Hz). You should have seen that the finite proton size model also gives a frequency difference between the $2s$ and $2p$ levels. Give a numerical value for that frequency difference, and calculate the ratio of that frequency difference to the frequency difference between the $2\,^2S_{1/2}$ and $2\,^2P_{1/2}$ levels due to the Lamb shift. You can use $E_I \approx \hbar \cdot 2\pi \cdot (3.3 \times 10^{15}$ Hz). Based on your answer, what is more significant to determining accurate energy eigenvalues of hydrogen: the finite size of the proton, or the quantum nature of radiation?

Problem IV: The Variational Method. CT Complement E_{XI} contains details and background about the topic of this problem. You may find it useful to consult CT, although it is not necessary for you to read the complement for the completion of the following problem.

The *variational method* is a useful approximation method for energy eigenvalue problems that are difficult or impossible to solve analytically. It is complementary to perturbation theory, with different strengths and weaknesses (see the first and last paragraphs of Complement E_{XI}). It is especially useful in placing an upper bound on the ground state energy of a given system: *for* ***any*** *"trial" wavefunction ψ or trial ket $|\psi\rangle$, the* ***true*** *ground state energy E_0 is no bigger than $\langle H\rangle = \langle\psi|H|\psi\rangle/\langle\psi|\psi\rangle$*. In other words,

$$E_0 \leq \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$$

for absolutely any physically acceptable $|\psi\rangle$. This is a very useful and powerful principle: even if you don't know the energy eigenstates of a problem, you can *guess* a trial solution $|\psi\rangle$, and be sure that the true ground state energy eigenvalue is no bigger than the mean energy that you calculate using $\langle H\rangle = \langle\psi|H|\psi\rangle/\langle\psi|\psi\rangle$. **Before proceeding, convince yourself that this must be true!**

In this problem, you will examine a particle in a 1-D gravitational potential well above a repulsive surface (such as a floor or desk). Let $V(z)$ be the gravitational potential energy of a "point" particle of mass m at a distance z above the surface:

$$V(z) = \begin{cases} \infty & z \leq 0 \ \text{(the surface)} \\ mgz & z > 0 \ \text{(the gravitational field)}, \end{cases}$$

where $g = 9.8$ m/s^2 is the acceleration due to gravity, and all other forces are neglected. $V(0) = \infty$ is representative of the repulsive nature of the surface. You will now use the variational principle to place an an upper bound on the true ground state energy of the system.

(a) First, sketch the potential well $V(z)$ vs. z, and also make a qualitative sketch of the ground-state wavefunction (which should go to zero at $z = 0$, approach zero for large z, and have no nodes).

(b) Write the one-dimensional Hamiltonian for this problem.

(c) In order to estimate $\langle H \rangle$ for a ground-state particle, you need to make a **guess** for the functional form of the ground-state wavefunction that you have sketched. A simple guess is $\psi(z) = A(z/b)e^{-z/b}$, where A is the normalization coefficient and b is a constant with units of length. Using this trial wavefunction, first normalize ψ by finding A in terms of b. Also, sketch $\psi(z)$ vs. z. The sketch should look something like your sketch from part (a).

(You may find it helpful to use the formula $\int_0^\infty u^n e^{-au} du = n!/a^{n+1}$.)

(d) Determine $\langle z \rangle$, and express your answer in terms of b. From this answer, you should be able to see how b relates to a mean particle position above the surface for this trial wavefunction.

(e) Evaluate $\langle H \rangle$, and write your answer in terms of the constants and the variable b. Make sure the dimensional units of your answer make sense!

(f) Find an expression for the value of b that minimizes $\langle H \rangle$. Your answer should contain $\hbar, m, g$, and a numerical constant.

(g) Now suppose that the particle is a ^{87}Rb atom, with $m = 1.5 \times 10^{-25}$ kg. Using your answer from part (f), find a numerical value for b in units of meters.

(h) Using the answers from (g) and (e), determine a numerical value for $\langle H \rangle$. By the variational principle, the true gravitational ground-state energy of the atom can be no larger than this answer.

(i) Express your answer from (h) as a temperature by dividing $\langle H \rangle$ by Boltzmann's constant $k_B = 1.4 \times 10^{-23}$ J/K. The temperature that you get is an approximate upper bound on how cold a ^{87}Rb atom needs to be before it will have a significant probability of being found in the gravitational ground state. (Note: laser cooling methods reach temperatures on the μK scale, evaporative cooling methods can reach nK temperatures.)

(j) Suppose that the "point particle" has a mass of 100 kg. What is b for this mass? What is the associated $\langle H \rangle / k_B$?

From this answer, you should see that it makes no sense to talk about macroscopic objects (like people) in relation to the ground state of the gravitational potential (or any other reasonable potential well). Even disregarding the temperature calculation, a 100-kg mass can not be considered a "point particle" on a length scale comparable to b. (A 100-kg mass with a radius of b would have a density that far exceeds the density of a black hole, $\sim 10^{19}$ kg/m^3.)