Home Work Assignment # 1 4/1/2011

<u>Due:</u> Fri., Apr. 8, 2011.

1. Let us consider the interaction of a Hydrogen atom with a perfectly conducting wall, and contrast it with the problem of Van der Waals (vdW) force between neutral atoms, that we studied last quarter.

Consider a Hydrogen atom at a distance d from a perfect conductor which fills the half space $z < 0$. Let d be much larger than atomic length scales, so that we can safely use a classical, macroscopic description of the metal. The atom interacts with its "electrical image" on the other side of the boundary.
(a) Recall that for the case of two neutral hydrogen atoms, we had shown that the the dipole-dipole interaction energy is given by

$$W = \frac{e^2}{R^3}(X_A X_B + Y_A Y_B - 2Z_A Z_B),$$

where R is the separation between atoms A and B, and (X_A, Y_A, Z_A) and (X_B, Y_B, Z_B) are the positions of the electrons associated with each atom. (You may wish to go through this derivation again).
For the present problem, draw a picture and argue that $X_B = X_A$, $Y_B = Y_A$, $Z_B = -Z_A$, $R = 2d$, and $e^2 \to -e^2$, where A denotes the atom and B its image.
Thus conclude that the interaction energy between the neutral atom and the wall is
$$W = -\frac{e^2}{8d^3}(X_A^2 + Y_A^2 + 2Z_A^2),$$

(b) Use first order perturbation theory to show that, when the atom is in its ground state, the energy of interaction is

$$E_1(d) = -\frac{e^2 a_0^2}{2d^3}.$$

Note that, unlike the case of two atoms where the first order result vanished by symmetry, the atom and its image charge have a non-zero interaction at first order. Thus the energy scales like the inversely as the third power of the distance here in contrast to the inverse sixth power in the case of vdW interaction.

2. The goal of this problem is to understand perturbation theory better using an exactly solvable two-level system.
Consider the Hamiltonian $H = H_0 + H_1$ where

$$H_0 = \begin{pmatrix} \epsilon_1 & 0 \\ 0 & \epsilon_2 \end{pmatrix}, \quad \text{and} \quad H_1 = \begin{pmatrix} 0 & w \\ w^* & 0 \end{pmatrix}.$$

Without loss of generality, assume $\epsilon_1 \geq \epsilon_2$.

(a) Find the exact eigenvalues of H. (i) Expand your results in powers of $|w|$ assuming $\epsilon_1 \neq \epsilon_2$. What is the condition on the validity of this expansion? (ii) What is the exact result in the degenerate case $\epsilon_1 = \epsilon_2$?
(b) Use nondegenerate perturbation theory in H_1 and compare with result of part a(i).
(c) Use degenerate perturbation theory in H_1 and compare with results of part a(ii).

3. Consider again the problem you solved in the Final exam last quarter. An electric dipole $\vec{\mu}$ with a fixed center-of-mass, is free to rotate in the x-y plane with the angular degree of freedom φ. Its dynamics is governed by the Hamiltonian

$$\mathcal{H} = -\frac{\hbar^2}{2I}\frac{d^2}{d\varphi^2} - \mu\mathcal{E}\cos\varphi.$$

The first term is the Hamiltonian of two-dimensional quantum rotor with momentum of inertia I. The second term describes the effect of an external electric field $\mathcal{E}$ along the $\hat{x}$ direction.
Treating the electric field as a perturbation, find the shift in energy (up to second order) and the perturbed wavefunctions (first order).
You had only considered the ground state earlier, now find the effects of $\mathcal{E}$ on *all* the states. Is it necessary to use degenerate perturbation theory? Explain.

4. Read carefully through Shankar Ex. 17.3.4 (p. 470-417). These results will be used in problem 5, but you do <u>not</u> need to hand in the solution.
If you plan on doing any kind of theoretical physics or AMO experiments, I would recommend that you solve this problem even though it is not required for the class.

5. Our goal is to understand the fine structure of the $n = 2$ level of hydrogen. We use below the standard spectroscopic notation $n\ell_j$, where n is the principal quantum number, $s, p, d, \ldots$ denote orbital angular momentum $\ell = 0, 1, 2, \ldots$ and j is the total angular momentum quantum number.

The Hamiltonian is given by

$$H = H_0 + H_f$$

where $H_0 = (p^2/2m - e^2/r)$ is the usual non-relativistic part, and the fine structure Hamiltonian

$$H_f = H_K + H_{so} + H_D$$

is the relativistic perturbation. Here

$$H_K = -p^4/(8m^3c^2)$$

arises from the change in mass with velocity,

$$H_{so} = \frac{e^2}{2m^2c^2} \frac{1}{r^3} \mathbf{L} \cdot \mathbf{S}$$

is the spin-orbit interaction between the orbital angular momentum $\mathbf{L}$ and the spin $\mathbf{S}$, and the Darwin term is given by

$$H_D = \frac{\pi e^2 \hbar^2}{2m^2c^2} \delta^{(3)}(\mathbf{r}).$$

(a) Check that the $n = 2$ level is *eight*-fold degenerate, and spanned by the basis $|\ell, m_\ell; s, m_s\rangle$.

(b) Using parity, or otherwise, show that H_f does not connect the $2s$ and $2p$ subspaces. Thus the 8×8 Hamiltonian H_f in the $n = 2$ space breaks up into a 2×2 block and a 6×6 block.

For the calculations below, you are free to use the results for various matrix elements calculated on pages 467 - 471 of Shankar. For the Darwin term you will need the values of the normalized H-atom wavefunctions at the origin, which you can also find in your text book.

(c) First consider the $2s$ states. Since H_K and H_D spin-independent terms, they are simply proportional to the unit matrix in this subspace. Show that

$$\langle H_K \rangle_{2s} = -\frac{13}{128}\alpha^4 mc^2 \quad \text{and} \quad \langle H_D \rangle_{2s} = \frac{1}{16}\alpha^4 mc^2.$$

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(d) Next show that $\langle H_{so} \rangle_{2s} = 0$.

Thus conclude that $2s_{1/2}$ level is shifted (below) its non-relativistic value by an energy $- 5\alpha^4 mc^2/128$.

(e) Next we turn to the $2p$ states. Again H_K and H_D do not depend on the spin, are proportional to the unit matrix in this subspace. Show that

$$\langle H_K \rangle_{2p} = - \frac{7}{384}\alpha^4 mc^2 \quad \text{and} \quad \langle H_D \rangle_{2p} = 0.$$

(f) For the spin-orbit interaction, note that $\mathbf{L} \cdot \mathbf{S}$ is *not* diagonal in the $|\ell = 1, m_\ell; s = 1/2, m_s\rangle$. Hence one needs to find a new basis in which H_{so} is diagonalized. This is the basis of eigenstates of J^2 and J_z where $\mathbf{J} = \mathbf{L} + \mathbf{S}$. Show that the six-fold degeneracy of the $2p$ states is partially removed by H_{so}, resulting in a two-fold degenerate $2p_{1/2}$ level and a four-fold degenerate $2p_{3/2}$ level. (What is the symmetry that leads to these degeneracies?)

(g) Show that the eigenvalues of H_{so} are given by $- \alpha^4 mc^2/48$ (for $j = 1/2$) and $\alpha^4 mc^2/96$ (for $j = 3/2$).

(g) Thus conclude that: (I) the $2p_{1/2}$ level is lowered by $- 5\alpha^4 mc^2/128$, thus resulting in an "accidental degeneracy" between the $2s_{1/2}$ and $2p_{1/2}$ levels (see below). (II) the $2p_{3/2}$ level is higher than the $j = 1/2$ levels. Its energy is lowered by $- \alpha^4 mc^2/128$.

Solving the Dirac equation for Hydrogen atom, one finds that the energy eigenvalue depends only on n and on j. Thus the $2s_{1/2}$, $2p_{1/2}$ degeneracy found above persists to all orders in α within Dirac theory.

Experimentally, there is a *Lamb shift* between these levels, with $2s_{1/2}$ raised with respect to the $2p_{1/2}$ by 1060 MHz, an order of magnitude smaller than the fine-structure splitting of $2p_{1/2}$ and $2p_{3/2}$. The observation of the Lamb shift in 1949 had profound consequences on the development of physics in the second half of the 20th century. It led to the development of Quantum Electrodynamics (QED). In QED, the Lamb shift can be understood in terms of the interaction of the electron with fluctuations of the EM field in vacuum.