Physics 531
Problem Set #2 – Due Tuesday, Feb. 8, 2005

Problem 1: Hydrogenic atoms and characteristic scales.

Consider the "hydrogenic" atoms - that is bound-states of two oppositely charged particles:

(i) The hydrogen atom: Binding of an electron and proton.

(ii) Heavy ion: Single electron bound to a nucleus of mass *M*, charge *Ze* (say Z=50).

(iii) Muonium: Muon bound to a proton

(iv) Positronium: Bound state of an electron and a positron (anti-electron)

(a) For each, using the charges, *reduced* mass, and the unit $\hbar$, determine the characteristic scales of:

Length, energy, time, momentum, internal electric field, and electric dipole moment. Please give numerical values as well as the expressions in terms of the fundamental constants.

(b) Now add the speed of light *c* into the mix. Find characteristic velocity in units of *c*, magnetic field, and magnetic moment. Show that for the particular case of hydrogen the characteristic velocity is $v/c = \alpha = \frac{e^2}{\hbar c}(cgs) \approx \frac{1}{137}$, the "fine-structure" constant, and that the Bohr radius, Compton wavelength, and "classical electron radius", differ by powers of α according to,

$$r_{class} = \alpha \lambda_{compton} = \alpha^2 a_0$$

(c) What is the characteristic magnetic field and magnetic dipole moment?

Problem 2: Radial Expectation Values for Hydrogen

(a) By brute force, show that mean radius a one-electron atom in the hydrogenic orbital $|n,l,m\rangle$ is

$$\langle r\rangle_{nl} = n^2 \frac{a_0}{Z}\left[1+\frac{1}{2}\left(1-\frac{l(l+1)}{n^2}\right)\right] \text{ (independent of q-number } m\text{)}$$

(b) For "circular" states (the ones with zero radial momentum, n_r=0), and in the "correspondence limt" ($n\to\infty$) show that we retrieve Bohr's result,

$$\langle r\rangle \to n^2 \frac{a_0}{Z}.$$

Though any expectation value can be calculated by tedious method in part (a), a trick to due Feyman and Hellman, saves a lot of work (note this was part of Feyman's undergrad thesis!).
The radial Hamiltonian is a function of various "parameters", $m_e, e, l \equiv \xi$,

$$\hat{H}(m_e,e,l) = \frac{-\hbar^2}{2m_e}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2m_e r^2} - \frac{Ze^2}{r}$$

Mathematically, is well defined for arbitrary assignment or real numbers to any ξ.

(c) Defining the radial eigenstate as $\hat{H}(\xi)|n_r,\xi\rangle = E_{n_r}(\xi)|n_r,\xi\rangle = -\frac{1}{2(n_r+l+1)^2}\frac{Z^2me^4}{\hbar^2}|n_r,\xi\rangle$,

show that $\langle n_r,\xi|\frac{\partial \hat{H}(\xi)}{\partial\xi}|n_r,\xi\rangle = \frac{\partial E_{n_r}(\xi)}{\partial\xi}$ (Feyman-Hellman theorem)

(d) Using the Feynman-Hellman theorem, show that

- $\left\langle \frac{1}{r}\right\rangle_{n,l} = \frac{Z}{a_0 n^2}$ (use $\xi = e^2$). Relate this to the Viral Theorem.
- $\left\langle \frac{1}{r^2}\right\rangle_{n,l} = \frac{Z^2}{a_0^2}\frac{1}{n^3(l+1/2)}$ (use $\xi = l$).
- $\left\langle \frac{1}{r^3}\right\rangle_{n,l} = \frac{Z}{a_0}\frac{1}{l(l+1)}\left\langle \frac{1}{r^2}\right\rangle_{n,l}$.

For this final case prove and then use the expectation value of the commutator,

$$\left\langle\left[\frac{d}{dr},\hat{H}(\xi)\right]\right\rangle_{nl} = 0.$$

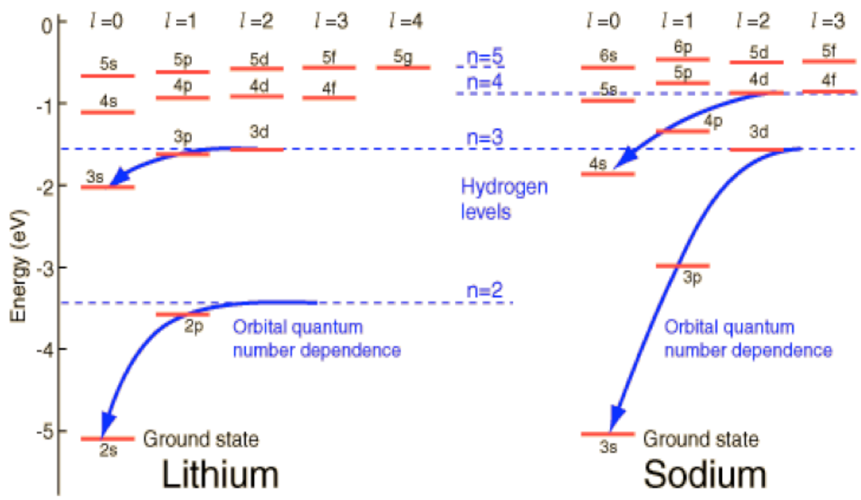
Problem 3: Spectrum of Alkali Atoms

We have seen that the spectrum of hydrogen has an "accidental" degeneracy – states with the same principle quantum number *n*, but different angular momentum quantum number *l* are degenerate. This was an artifact of the pure $1/r$ Coulomb potential associated .

In a multielectron atom things are, of course, more complicated. Each electron moves in the combined attractive field of the nucleus and repulsive field of the other electrons. The Pauli principle must also be accounted for. This many-body problem cannot be solved exactly. Much of the middle part of the course will be devoted to solving this.

One coarse approximation is the "mean-field" approximation, whereby every electron moves in the average field of all the other particles. The mean field is spherically symmetric, and thus, the quantum numbers *n* and *l* are still good. This approximation is especially good for alkalis (group IA in the period table) since they have one valence electron around a stable "noble atom-like core". They are thus vaguely hydrogenic if the valence electron does not "penetrate" the core.

Consider the spectrum of Li and Na, two alkali atoms, shown below:



Clearly, states with different *l* are no longer degenerate.

(a) Using the discussion above and your knowledge of the hydrogenic wave functions, explain the qualitative behavior of these spectra.

(b) Let us take an artificial (but exactly solvable) model of the mean field of the other electrons as having a $1/r^2$ dependence, so that $V(r) = -\frac{e^2}{r} + \frac{A}{r^2}$. Show that wave functions are hydrogenic in form, and the eignevalues are:

$$E(n_r, l) = -\Re\left[n_r + \frac{1}{2}\left(1 + \sqrt{(2l+1)^2 + 8mA/\hbar^2}\right)\right]^{-2}$$, where $\Re$ is the Rydberg constant.

Hint: Show that the radial equation leads to the same hypergeometric function.

(c) Expand in the $8mA/\hbar^2 << 1$. Show that you get the correct result to first order perturbation. Sketch an energy-level diagram.