Phys 551 Homework 1

1. Quantum-defect theory and Bates-Damgaard approximation

One can crudely approximate the wavefunction of the valence electron in an alkali-metal atom by a hydrogen wavefunction with Z = 1 assuming that the rest of the nuclear charge is screened by inner electrons. However, the hydrogenic energy levels do not match observed energies in alkali-metal atoms. A simple extension of this approach is to allow the quantum number n to be non-integer, $n^* = n-\delta(l)$, where $\delta(l)$ is known as a quantum defect. It is a function of the angular momentum l but not n. For large l, $\delta(l) \to 0$ because the wavefunction is far away from the core. $\delta(l)$ is determined empirically by matching the hydrogen energy levels $E = -\text{Ry} / n^{*2}$ to the experimental values. The resulting wavefunctions are solutions of the Schrödinger equation with the usual Coulomb potential but for a non-integer value of n^*. They can be used for calculation of various atomic parameters with reasonable accuracy. Bates-Damgaard approximation is a calculation of the radial transition matrix elements using this approach.

a) Find the quantum defects for s, p and d states in potassium.
b) Calculate the radial matrix element <e|r|g> for 4s-4p, 4s-5p and 4d – 5p transitions in potassium in the Bates-Damgaard approximation.

You will need more general form of the hydrogen radial wavefunctions for non-integer n^*. They are known as Coulomb wave functions and can be expressed in terms of Whittaker functions or hypergeometric functions. These wavefunctions diverge at the origin, but have proper behavior at large r. One can also use asymptotic expansions available for large r. Check that your wavefunctions agree with the usual hydrogen wavefunctions for integer n.

2. Magnetic field insensitive hyperfine transitions.

It is well known that $F= I–1/2 \to F= I+1/2$ transition for $m = 0$ is insensitive to magnetic field to first order ($d(E_+–E_-)/dB = 0$) at zero field and is used for atomic clocks. For I >1/2 there are other first order magnetic field-insensitive transitions at a finite magnetic field. For the Hamiltonian $H = A\ \mathbf{I}\cdot\mathbf{S} + g\mu_B\ \mathbf{B}\cdot\mathbf{S}$ with I = 3/2 and A = 1 GHz find all field-insensitive transitions. Calculate the magnetic field corresponding to each one and the spin wavefunction in the |F,m> basis.