Physics 487 – Homework #4

due Friday 1 pm

Reading for week 5 : Griffiths §6.1 and 6.2

Problem 1 : Full Wavefunction = ψ(Space) × χ(Spin)   *adapted from Griffiths 4.55*

The electron in a hydrogen atom is in the following state :

$$\psi = R_{21}\left(\sqrt{\frac{1}{3}}\, Y_1^0\, \chi_+ + \sqrt{\frac{2}{3}}\, Y_1^1\, \chi_- \right)$$

where the basis states for the spinors are, as usual,

$$\chi_+ \equiv \chi_{(m_S=+1/2)} \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } \chi_- \equiv \chi_{(m_S=-1/2)} \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

(a) If you measured L^2, what values might you get, and what is the probability of each?

(b) same question for L_z (c) same question for S^2 (d) same question for S_z

(e) same question for J^2 where $\vec{J} \equiv \vec{L} + \vec{S}$ (f) same question for J_z

(g) If you measured the position of the electron, what is the probability density for finding it at (r, θ, ϕ) ?

(h) If you measured both the z component of the spin *and* the distance from the origin (note that these are compatible observables), what is the probability density for finding the electron with spin up at radius r ?

Problem 2 : Helium Ground State Energy   (b) *adapted from Griffiths 5.11*

(a) The helium atom consists of two electrons bound by a doubly-charged nucleus. The most crude approximation you can make to its Hamiltonian is the sum of two hydrogen-like Hamiltonians, i.e. one for each of the two electrons, treating them as if they are interacting with just the Z (nuclear charge) = 2 nucleus and not at all with each other (also no spin-orbit interaction or other corrections to the Bohr model). Making use of the hydrogenic energy eigenstates and eigenvalues,

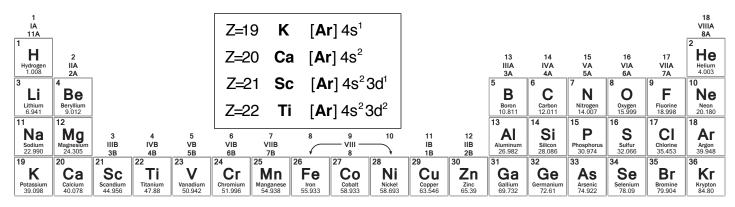$$\psi_{nlm}(\vec{r}) = R_{nl}(r)\, Y_{lm}(\theta,\phi) \quad \text{and} \quad E_n = -\frac{(Z\alpha)^2}{2n^2}(m_e c^2),$$

from our 486 formula sheet, calculate the energy of the helium ground state in the approximation that Helium ≈ two non-interacting electrons sitting in the field of a Z=2 nucleus. Express your result in eV.

(b) The measured energy of the helium ground state is –79 eV, so the non-interacting-particle approximation is not very accurate (almost 40% tighter binding than –79 eV). Almost all of the discrepancy with experiment can be accounted for by adding the **electron-electron repulsion term, V_{ee}**, to the Hamiltonian. Calculate the expectation value $\langle V_{ee} \rangle$ of this interaction for the helium ground state. After you apply $\langle V_{ee} \rangle$ correction, you should be about 5% away from the experimental ground state energy instead of 40% → as we said during our discussion of the Hund rules, V_{ee} is the dominant correction to the Bohr model for multi-electron atoms.

▶ INTEGRATION GUIDANCE: Calculating $\langle V_{ee} \rangle$ requires calculating $\langle 1/|\vec{r}_1 - \vec{r}_2| \rangle$. See Griffiths problem 5.11(a) for assistance on how to set up this multi-dimensional integral.

Problem 3 : The Fourth Row

The electronic configurations of the first four elements in the fourth row of the periodic table are in the box :

Z=19	**K**	$[\textbf{Ar}]\,4s^1$
Z=20	**Ca**	$[\textbf{Ar}]\,4s^2$
Z=21	**Sc**	$[\textbf{Ar}]\,4s^2 3d^1$
Z=22	**Ti**	$[\textbf{Ar}]\,4s^2 3d^2$

(Periodic table)

▶ Recall from chemistry: The word **valence** comes from the Latin word for "power". A **valence electron** is "an electron available for chemical bonding", i.e. an electron in a partly-filled shell. The **noble gases** He, Ne, Ar, … have *no* valence electrons, and so are tightly-bound systems that hardly interact with other atoms. To simplify electronic configurations, it is common to lump together all the chemically-inactive electrons from the nearest noble gas into a single symbol, as you see in the box above. Expanded out, the e^- configuration for potassium is $1s^2\,2s^2\,2p^6\,3s^2\,3p^6\,4s^1$; it's much simpler to absorb all those filled shells into one symbol: $[\text{Ar}]\,4s^1$.

(a) Consider potassium (K). Its ground state is $^2S_{1/2}$ = the "doublet-S-½". Explain briefly why this is the <u>only</u> possible ground state given the electron configuration K = $[\text{Ar}]\,4s^1$.

(b) As you see from the box, scandium (Sc) has only <u>one valence electron</u>. First, list all possible $^{2S+1}\mathcal{L}_J$ states given that the valence electron is in the d-shell. Then decide which of your states has the lowest energy and explain your decision qualitatively (no calculation needed).

(c) Titanium (Ti) has <u>two valence electrons</u>, as you can see from its electron configuration in the box above. As it happens, the ground state of Ti has total orbital angular momentum quantum number $L = 3$. Let's align a ground-state Ti atom so that its M_L quantum number is –1. *Ignoring spin entirely*, express this state, $\left|3,-1\right\rangle_{LM}$, as a superposition of states $\left|m_1 m_2\right\rangle$ using Clebsch-Gordan tables.

(d) The ground state of Ti is the "triplet-F-2" state, $^3F_2$. Explain the <u>triplet</u> part: why does the system reach its lowest energy when its total spin is 1? Please explain more deeply than simply quoting one of the Hund rules, you need to explain the *reason* behind that Hund rule.

(e) What is your favourite element?