Note and Problems for Midterm 1 on Wednesday February 14

Topic 1: Solution of **time-independent Schrodinger equation**:

$-\frac{\hbar^2}{2m}\frac{d^2\psi_0}{dx^2}+V\psi_0=E_0\psi_0$ (1D), where is the potential energy.

For hydrogen, **3D** in Spherical Coordinate:

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi_{nlm_\ell}}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi_{nlm_\ell}}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi_{nlm_\ell}}{\partial\phi^2},$$

$$+\frac{2m}{\hbar^2}\left(E_n+\frac{e^2}{4\pi\varepsilon_0}\frac{1}{r}\right)\psi_{nlm_\ell}=0$$

Study question 1 of assignment 1, and question 2 of assignment 2.

Topic 2: Interpretation of Quantum Mechanics: Linear Combination/superposition states, also called arbitrary states, and probability distribution.
Study question 1 and 2 of assignment 1.

Topic 3: Hydrogen-like orbitals, and electronic configurations of atoms, spectroscopic notation, ground-state (lowest energy) of atoms, Unsold Theorem, addition of angular momentum, Hund's rules (three rules), Pauli Exclusion Principle.

Study Question 4, Problem 4 of Chapter 8 of assignment 1; Question 2 and 3 of assignment 2; problem 8, 16 and 18 of chapter 8 (assignment 2).

Topic 4: Fine-structure (fs) of atoms and the Zeeman Effect.

Study Question 2 of Assignment 3, and **Problem 21**, **25**, **36**, and **37** of chapter 8 (assignment 3).

Problems to do in preparation for midterm 1

Problem 1

Consider a Bohr hydrogen (neglect spin), whose energy is given by the formula $E_n=-\frac{13.6eV}{n^2}$, $n=1,2,3...$, in the stationary state $n=3$, $\ell=2$, $m_\ell=1$.

A) Write down the explicit form of wave function (in r,θ,ϕ) for this hydrogen state.

B) Find the **most probable distance** of the electron from the proton. **Hint**: minimize the probability distribution $P_{n\ell}(r)=r^2R_{n\ell}^2$.

C) A physicist conducts an experiment on a hydrogen atom in the state $n = 3,\ \ell = 2,\ m_\ell = 1$, which will determine the **energy**, **magnitude of the orbital angular momentum**, **z-component of the orbital angular momentum**. What values for the abovementioned quantities will he obtain? Express your answers in eV for energy, and $\hbar$ for angular momentum.

D) Consider now an electron in the linear combination state $0.8\psi_{100} + 0.6\psi_{211}$. If the physicist measures the **z-component of the orbital angular momentum**, what **values** would he obtain, and with what **probabilities**?

Problem 2

Using table 7.1 and 7.2, write down the hydrogen wavefunction $\psi_{2,0,0} = R_{2,0}Y_{0,0}$. Verify by direct substitution that it is the solution of the time-independent Schrodinger equation:

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial \psi_{nlm_\ell}}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi_{nlm_\ell}}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi_{nlm_\ell}}{\partial\phi^2}.$$

$$+\frac{2m}{\hbar^2}\left(E_n + \frac{e^2}{4\pi\varepsilon_0}\frac{1}{r}\right)\psi_{nlm_\ell} = 0$$

Hint: Use $a_0 = \dfrac{4\pi\varepsilon_0\hbar^2}{me^2}$, and $E_n = -\dfrac{m}{2\hbar^2}\left(\dfrac{e^2}{4\pi\varepsilon_0}\right)^2\dfrac{1}{n^2}$

Problem 3

Consider a hydrogen atom in an orbital angular momentum state $\ell = 3$.

A) For now **neglect** the **electron's spin**, what are the possible values of the **magnitude** of the orbital angular momentum L and the possible values of the **z-component** of the orbital angular momentum L_z?

B) What would be the value of the **x-component** L_x?

C) Now consider the **electron's spin**, $\vec{S}$. In this case we must find the **total angular momentum**, $\vec{J} = \vec{L} + \vec{S}$. Find the possible values of the magnitude of the total angular momentum J and the possible values of the z-component of the total angular momentum J_z?

Problem 4

Electronic configurations

(A) Write the electronic configuration ($n\ell$) of the ground state and the first excited state of carbon (Z = 6).

(B) Write the electronic configuration ($n\ell$) of the ground state and the first excited state of Xeon (Z = 54).

Problem 5

The ground state of Neon (Ne)

a) Neon has an atomic number of Z = 10. Write down its ground state configuration

b) Find the **term symbol (spectroscopic notation)** of the **ground state** of **Neon**.
REMARK: For this question you are expected to justify your answer with Hund's rules and the class discussion on the effects of core and valence electrons on the angular momentum (orbital, spin, and total) of an atom. Another hint is that only electrons in **unfilled subshells** contribute to the total angular momentum.

Problem 6

Fine Structure of Lithium (Li) atomic number Z = 3

a) Write down the **ground-state** electronic configurations of Li. Derive the **term symbol (spectroscopic notation, see equation sheet)** of the ground state.

b) The lowest excited states of lithium involve a **single electron in an unfilled 2p subshell**. This will result in two states (doublets). Use the rule of addition of angular momentum to derive the **term symbol (spectroscopic notation)** of these **two excited states**. Briefly explain why there are two states. Draw the energy-level diagram involving the **ground state** (part a) and the **two excited states**.

c) As you should know the excited states of part b will split into two states of different energy. The energy difference between these two states is $\Delta V_{fs} = 2\mu_B B_{\text{int}}$ (see equation sheet), where $\vec{B}_{\text{int}}$ is the **internal magnetic field**. **Briefly explain** the physics origin of the **internal magnetic field** and the energy difference. Suppose $\vec{B}_{\text{int}}$ points in the + z direction and has magnitude $B_{\text{int}} = 0.4T$, calculate the energy difference ΔV_{fs} in eV.