PHYS3022 APPLIED QUANTUM MECHANICS

SAMPLE QUESTIONS FOR DISCUSSION IN WEEK 5 EXERCISE CLASSES (11 - 15 Feb 2019)

What are Sample Questions (SQs)? TA will discuss the **SAMPLE QUESTIONS** in exercise classes. The Sample Questions are designed to serve several purposes. They either review what you have learnt in previous courses, supplement our discussions in lectures, or closed related to the questions in an upcoming Problem. You are encouraged to think about (or work out) the sample questions before attending exercise class and ask the TA questions.

SQ11: Labelling atomic states by $(n, \ell, s = 1/2, j, m_j)$, what for?
SQ12: The internal magnetic field in atoms - not a small field
SQ13: Atomic Units - Measuring quantities in atoms/molecules using scales set by hydrogen atom

SQ11 *Labelling atomic states by $(n, \ell, s = 1/2, j, m_j)$, what for?*

Consider the hydrogen atom Hamiltonian $\hat{H}_0$ that carries only the kinetic energy term and the Coulomb potential energy term $-e^2/(4\pi\epsilon_0 r)$. We solved it analytically in Quantum Mechanics I. The solutions are $\psi_{n\ell m_\ell(s)m_s} = R_{n\ell}(r)Y_{\ell m_\ell}(\theta,\phi)\cdot\chi_{m_s}$, where χ_{m_s} is the spin state (e.g. α_z (up spin) for $m_s = 1/2$ and β_z (down spin) for $m_s = 1/2$.

Let's consider $\ell = 1$ (p states). With the spin ($s = 1/2$) of the electron, there are 6 p states. [This is why we have 6 states for $2p$ and also 6 states for $3p$.] For $2p$, say, we can represent the states by the symbol $|n = 2, \ell = 1, m_\ell = 1, 0, -1; s = 1/2, m_s = \pm 1/2\rangle$ or simply $|2, 1, m_\ell; 1/2, m_s\rangle$. These 6 states are degenerate and the corresponding energy is $-13.6/2^2$ eV or -3.4 eV.

With 6 states, we can linearly combine (mix) them to form 6 other states. This is exactly what we did in labelling 6 states by $|n = 2, \ell = 1, s = 1/2; j, m_j\rangle$. Here, $j = \ell + \frac{1}{2} = 3/2$ and $j = \ell - \frac{1}{2} = 1/2$. For a given j, m_j runs from $+j$ to $-j$ in steps of 1. Therefore, there are 6 states.

Formally, we can write

$$|2, 1, 1/2; j, m_j\rangle = \sum_{m_\ell=1,0,-1;\, m_s=1/2,-1/2} C(j, m_j; m_\ell, m_s)|2, 1, m_\ell; 1/2, m_s\rangle \tag{1}$$

where the coefficients $C(j, m_j; m_\ell, m_s)$ are called the Clebsch-Gordan coefficients. Finding the coefficients is beyond the scope of our course. The point here is to convey what is being done when we invoke j and m_j in describing the p states. The states are constructed so that they are orthogonal to each other and they themselves are normalized, i.e.,

$$\langle 2, 1, 1/2; j, m_j|2, 1, 1/2; j', m_{j'}\rangle = \delta_{jj'}\,\delta_{m_j m_{j'}}\ . \tag{2}$$

TA: **Show** that the states $|2, 1, 1/2; j = 3/2\, or\, 1/2, m_j\rangle$ are eigenstates of $\hat{H}_0$ and they are degenerate.

TA: Now, an extra term $\hat{H}'_{so} = f(r)\vec{S}\cdot\vec{L}$ goes into the Hamiltonian when spin-orbit interaction is considered. **Take the 6 states** of $|2, 1, 1/2; j, m_j\rangle$ and form a 6×6 matrix for $\hat{H} = \hat{H}_0 + \hat{H}'_{so}$. In particular, **illustrate** that the matrix is **diagonalized** in this basis set. This is exactly what we did in class notes to handle the spin-orbit interaction.

[Remarks: (a) If we use $|2, 1, m_\ell; 1/2, m_s\rangle$ as the basis set, then the matrix will NOT be that simple. This is why we form Eq. (1) in preparation for handling spin-orbit interaction. (b) The linear combinations in Eq. (1) can be regarded as a procedure in diagonalizing the matrix. (c) The form of the matrix implies that even if we apply the degenerate perturbation theory in the basis of $|2, 1, 1/2; j, m_j\rangle$, it is the same as applying first order non-degenerate perturbation theory in the same basis, as the off-diagonal terms vanish.]

SQ12 *The internal magnetic field in atoms - not a small field*

We can use experimental data to estimate the **internal magnetic field** B_{int} in an atom. Here are two cases.

(a) The transitions between hydrogen $2p$ states to $1s$ state turn out to give two closely spaced lines. The jargon is that there is a doublet.

TA: **From experimental data** of the two lines in hydrogen atom, **estimate** the internal magnetic field strength. Let's not worry about various constants. The spin of an electron is characterized by the Bohr Magneton μ_B. You may simply think about the energy of alignment (anti-alignment) with the internal field to be $-\mu_B B_{int}$ $(+\mu_B B_{int})$.

(b) In sodium atom (a bigger or heavier atom), the transitions between the $3p$ states and $3s$ state also give two closely space lines. These **sodium doublet** lines are well-known as they fall into the visible (yellowish) range. Data say that the wavelengths of the two lines are 588.592 *nm* and 588.995 *nm*.

Although we haven't discussed the physics of atoms beyond the hydrogen, we could transfer our knowledge to sodium by taking the outermost $3s$ electron as the single electron in hydrogen. So the ground state has this outermost electron in $(n = 3, \ell = 0, j = 1/2)$. The electron can be excited to $3p$ states. Due to spin-orbit interaction, the $3p$ states are labelled $(n = 3, \ell = 1, j = 1/2, m_j)$ and $(n = 3, \ell = 1, j = 3/2, m_j)$, as discussed in SQ11.

TA: Use the data to **estimate the internal magnetic field** in sodium atom. The result helps illustrate that the internal field is quite BIG!

SQ13 *Atomic Units - Measuring quantities in atoms/molecules using scales set by hydrogen atom*

Serious discussions on the physics of atoms and molecules usually invoke the **atomic units**. In atomic units, we want to construct **dimensionless** quantities. Therefore, **mass** is given (or measured) in units of the mass of an electron m_e; **charge** is given in units of the charge of a proton e; **distance** is given in units of the Bohr radius a_0; **energy** is given in units of Hartree (which is twice the magnitude of hydrogen ground state energy or simply $e^2/(4\pi\epsilon_0 a_0)$, where a_0 is the Bohr radius; **angular momentum** is given in units of $\hbar$; and **permittivity** is given in units of $4\pi\epsilon_0$. In this system, all these quantities become a (dimensionless) number. For example, the ground state energy of a hydrogen atom is -13.6 eV or just $-1/2$ (a number) when it is expressed in units of Hartree E_h. This SQ introduces the atomic units often used in studying atoms and molecules.

(a) **Give** the SI equivalent of "1" for each of the quantities (with appropriate units) mentioned. **Also give** the equivalent of $1E_h$ ("1 Hartree") in eV.

(b) Based on the expression of the hydrogen ground state energy in terms of m_e, e, $\hbar$, etc., **give** an expression for $1E_h$ in terms of these quantities. **Also give** an expression for the Bohr radius. [You may look up hydrogen atom results for the answers.]

(c) Starting from the SI form of the hydrogen atom Hamiltonian, **illustrate** how the Hamiltonian can be rewritten in atomic units.