**PHYS3022 APPLIED QUANTUM MECHANICS**

**SAMPLE QUESTIONS FOR DISCUSSION IN WEEK 8 EXERCISE CLASSES (16 - 20 March 2020)**

**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.

SQ18: The internal magnetic field in atoms - not a small field
SQ19: Strong-field Zeeman Effect: Paschen-Back Effect
SQ20: Atomic Units - Measuring quantities in atoms/molecules using scales set by hydrogen atom

SQ18 *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 $\mu_B$. 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 heavier atom), the transitions between the $3p$ states and $3s$ state also give two closely space lines. Note that sodium atom is hydrogen-like, as the core electrons completed filled the $1s$, $2s$, and $2p$ states. These **sodium doublet** lines are well-known as they fall into the visible (yellowish) range, as you saw them in PHYS2722 lab. 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 yet, 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 expected of spin-orbit interaction.

TA: **Use the data to estimate the internal magnetic field** in sodium atom. The result helps illustrate that the internal field is not small.

SQ19 *Strong-field Zeeman Effect: Paschen-Back Effect*

Consider the strong-field Zeeman effect. From class notes, we discussed that the 6 degenerate $p$ states (say $2p$) split into 5 levels according to the $m_\ell$ and $m_s$ values. Let's say the external magnetic field is much stronger than the internal magnetic field that the spin-orbit interaction effort can be ignored entirely.

TA: Consider the Lyman $2p \to 1s$ line of a hydrogen atom under a strong external magnetic field. Let the energy difference in the absence of field be $\Delta E_{Lyman-\alpha}$. [The first line in the Lyman series if called the Lyman-$\alpha$ line.] **Make a sketch showing** how the $2p$ and the $1s$ states split in the external field. The selection rules are $\Delta m_s = 0$ and $\Delta m_\ell = 0, \pm 1$. **Applying the selection rules, indicate** that the Lyman-$\alpha$ line splits into three lines and **find the energy differences** that give rise to the three lines.

SQ20 *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) Starting from the SI form of the **hydrogen atom Hamiltonian**, **illustrate** how the Hamiltonian can be rewritten in atomic units.