PHYS3022 APPLIED QUANTUM MECHANICS

SAMPLE QUESTIONS FOR DISCUSSION IN WEEK 6 EXERCISE CLASSES (22 - 26 Feb 2021)

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.

In Week 5 (across the Chinese New Year break), we discussed the effects of spin-orbit interaction and revisited the Zeeman effect in both the strong field and weak field limits.

SQ11: Normal Zeeman Effect: $P \to D$ transitions allowed by $\Delta m_L = 0, \pm 1$
SQ12: The sodium doublet you saw in lab course - The internal magnetic field can be quite large
SQ13: Atomic Units - Getting ready for multi-electron atoms and molecules

SQ11 *Normal Zeeman Effect: $P \to D$ transitions allowed by $\Delta m_L = 0, \pm 1$*

Background: This SQ is about the normal Zeeman effect. It is about a spectral line splitting into three lines when an external magnetic field is applied. In our first encounter of the normal Zeeman effect, the effects of spin is ignored. Even when spin is included, the effect of a strong magnetic field will lead to the normal Zeeman effect. Here, we will ignore the effects of spin for simplicity. Physically, there are cases that the total spin angular momentum of the electrons (multi-electron atoms) sum up to zero and so there will be no spin effects.

The notations here using capital letters look unusual. It is to prepare for cases of multi-electron atoms. So L is the orbital angular momentum of the atom after adding up the contributions of orbital angular momenta from each electron. Thus, P means $L = 1$ with $m_L = 1, 0, -1$ and so on. This is what we discussed under the Term Symbol.

TAs: Consider the possible transitions from an **upper** P to a **lower** D level in a static magnetic field. **Show that** the allowed transitions give two more spectral lines one on each side of the line in the zero field case, according to the selection rules of $\Delta m_L = 0, \pm 1$.

[Remark: We will discuss the physics of multi-electron atoms in Week 6.]

SQ12 *The sodium doublet you saw in lab course - The internal magnetic field can be quite large*

You should have seen the sodium doublet lines in a lab in Physics Laboratory III. They are two closely spaced spectral lines from sodium in the visible range. Although we have not discussed multi-electron atoms yet, it is possible to transfer our knowledge in hydrogen atom to sodium atom, taking the outermost $3s$ electron just as the single electron in hydrogen.

The $3s$ (ground state) is labelled by ($n = 3$, $\ell = 0$, $j = 1/2$). The first excited states are the $3p$ states. Just as in hydrogen, the six states after considering spin-orbit interaction split into two energies, labelled by ($n = 3$, $\ell = 1$, $j = 1/2$) and ($n = 3$, $\ell = 1$, $j = 3/2$). The transitions from these two levels to the ground state are in the visible range. The wavelengths are found to be 589.592 nm and 588.995 nm.

TAs: Without going into the details, which involve using the quantum number j and even an integral $\langle f(r) \rangle$ invoking the radial part of the wavefunction, we know that the sodium atom is effectively a single-electron ($3s$ electron in ground state) hydrogen-like atom. Therefore, the splitting of the $3p$ states can be interpreted as the spin magnetic dipole moment being aligned or anti-aligned with the internal magnetic field B_{int}. As such, the splitting will be $\sim 2\mu_B B_{int}$, where μ_B is the Bohr magnetron (which is also the z-component of the electron's spin magnetic dipole moment). Using the data given above, **estimate** B_{int} and demonstrate that B_{int} is well above 10 Tesla in this case. (Quite a big field!)

[Remark: This is also why we usually see the anomalous Zeeman effect, i.e., we need to treat the spin-orbit interaction first, and then the Zeeman term as a perturbation that will remove the degeneracy behind m_j.]

SQ13 *Atomic Units - Getting ready for multi-electron atoms and molecules*

In the hydrogen atom problem you did in Quantum Mechanics I, you solved the Schrödinger Equation with the Hamiltonian:

$$\hat{H}_{hydrogen} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0 r} \ , \tag{1}$$

which is written in the SI units. In "more professional" contexts (journal articles and quantum chemistry books), it is written as

$$\hat{H}_{hydrogen}^{(atomic\ units)} = -\frac{1}{2}\nabla^2 - \frac{1}{r} \ , \tag{2}$$

which looks simpler and nicer. However, it looks as if all a sudden, the quantities carry no units. Eq. (2) is written in the **Atomic Units**. So, what is going on?

Of course, physics is physics. The physics should not depend on the system of units **if the physics is done correctly**. There are conventions, however. The *atomic units* are commonly used in atomic physics. With some experience in hydrogen (using SI units), it is now time to get to know **the atomic units**.

In atomic units, **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 $e^2/(4\pi\epsilon_0 a_0)$; **angular momentum** is given in units of $\hbar$; and **permittivity** is given in units of $4\pi\epsilon_0$. Thus, all these quantities become just a (dimensionless) number in atomic units.

(a) **Give the SI equivalence** of one unit of each of these quantities (with appropriate units). For example, what does "1" unit of distance correspond to? Etc.

(b) The Hartree (E_h) is the unit of energy in atomic units. In addition to SI units (Joule), physicists also like to use eV for energies. **Give** $1E_h$ in units of eV.

(c) Physicists like to give energies in eV, e.g., the binding energy (representing the strength of chemical bond) of O_2 is 5.1 eV. In more specialized books and data banks on atomic and molecular physics, this quantity is usually expressed in $\mathrm{kJ\cdot mol^{-1}}$ (sometimes even in $\mathrm{kcal\cdot mol^{-1}}$). (i) For the energy of $1E_h$ (which is per atom or per molecule), **what** is the corresponding $\mathrm{kJ\cdot mol^{-1}}$? (ii) Hence, **express** the binding energy of O_2 in $\mathrm{kJ\cdot mol^{-1}}$. It is useful to get a sense on (and remember) a rough conversion factor.

(d) Now, starting from the SI units of the hydrogen atom Hamiltonian in Eq. (1), **show the steps** through which it becomes Eq. (2) in the atomic units.