PHYS3022 APPLIED QUANTUM MECHANICS

SAMPLE QUESTIONS FOR DISCUSSION IN WEEK 10 EXERCISE CLASSES (22 - 26 March 2021)

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 Set. Students should be able to do the homework problems independently after attending the exercise class. **You should attend one exercise class session.** You are encouraged to think about (or work out) the sample questions before attending exercise class and ask the TA questions.

Progress: In Week 9, we discussed the QM of stimulated absorption and emission, Einstein's A and B coefficients. Taking Einstein's result on how the A and B coefficients are related, we also found a QM formula for the spontaneous emission rate. This indirect approach by-passed the necessity of quantizing the EM fields (photons and photons' ground state - the vacuum). The life time τ of an excited state is related to spontaneous emission rate as $1/A$. We also discussed briefly the idea behind lasers, although a detailed study of lasers require more quantum mechanics. This ends the Module on Atom/Matter-Light Interaction. We will discuss the Physics of Molecules in Week 10.

SQ20 - Quantum mechanics gives quantitatively the life time of hydrogen 2p state (see also SQ19)
SQ21 - Natural Broadening of a Spectral Line

SQ20 *Life time of hydrogen 2p state - Quantum Mechanics is a quantitative theory!*

In SQ19 (Week 9), TA calculated the vector $\overline{\mathbf{r}_{2p,1s}}$ for a hydrogen atom analytically and considered the allowed transitions for different incident light polarizations. The quantity $\overline{\mathbf{r}_{2p,1s}}$ also goes into the formulas of the transition rates and thus the A and B coefficients. Here, we apply the result and obtain quantitatively the life time of a hydrogen atom 2p state. The key point here is to illustrate that Quantum Mechanics is a theory that gives quantitative results for measurable quantities.

The flow of ideas is as follows: QM gives the stimulated emission transition rate $\lambda_{2\to1}$. Einstein introduced his B and A coefficients in 1917, prior to the establishment of QM. The A-coefficient is related to spontaneous emission (difficult to handle within Schrödinger's QM) and the B-coefficient is related to stimulated processes. In QM, the formula of $\lambda_{2\to1}$ for stimulated processes gives a formula of the B-coefficient. Einstein gave a relation between the A-coefficient and the B-coefficient. Therefore, we can obtain a QM formula for the A-coefficient too. The life time of an excited state is how long on average it will last if it is "undisturbed". The life time τ of an excited state is related to spontaneous emission and the A-coefficient through $1/A$. In summary, $\lambda_{2\to1}$ (QM) $\to$ formula of B-coefficient $\to$ formula of A-coefficient via relation between A-coefficient and B-coefficient (Einstein) $\to$ lifetime $\tau = 1/A$.

Here, we consider the life time of a 2p state of hydrogen atom. We will use the result in SQ19 to get at the life time of the 2p state of $(2, 1, +1)$. For spontaneous emission, it can make a transition to the ground state (final state) of $(1, 0, 0)$. In this case, the matrix element involved is $\overline{\mathbf{r}_{1s,2p}}$ (from 2p to 1s) rather than $\overline{\mathbf{r}_{2p,1s}}$ evaluated in SQ19.

(a) By referring to SQ19, **give** $\overline{\mathbf{r}_{1s,2p}}$ without doing any calculation. Note that it is a vector.

(b) What we need is $|\overline{\mathbf{r}_{1s,2p}}|^2$, which is a scalar. **Evaluate it** and give the answer in terms of Bohr radius squared.

(c) A formula of the A-coefficient (spontaneous emission) was found by using Einstein's result of relating A to B and then the QM result of the B-coefficient. The formula consists of three factors: a bunch of constants, ω^3 dependence, and $|\overline{\mathbf{r}_{1s,2p}}|^2$ dependence. So, (i) **evaluate** the quantity $|\overline{\mu_{1s,2p}}|^2 = e^2|\overline{\mathbf{r}_{1s,2p}}|^2$ and give the result **in SI units**, i.e., in $\mathrm{C}^2\mathrm{m}^2$ where C is Coulomb and m is meter. This is related to the electric dipole moment squared. (ii) **Evaluate** ω_{21} (or simply call it ω) from the energy differences of the 2p and 1s states.

(d) For the 2p $(2, 1, +1)$ state, the $(1, 0, 0)$ state is the *only* transition down in energy. This makes the calculation easier, because we don't need to consider several possible final state. The **life time** is then given by $\tau = 1/A$. Thus we need to calculate A. The formula was given in class notes. There are some constants involving $\hbar$, c, and ϵ_0 in A. Plug in all the numbers to **find** A (in SI units) and the **lifetime** due to the electric dipole mechanism. **The answer is a number** in **seconds**. The result is worthy of remembering as it is typical of a state that can make a transition downward via electric dipole radiation. **You should appreciate that quantum mechanics works to give a precise number for a property of a quantum state.**

[Remarks: You just saw that typical life time is $\sim 10^{-9}$ s for states with allowed electric dipole transitions downward. If such a transition is forbidden (meaning "electric-dipole forbidden"), the life time becomes much longer as transitions will have to invoke higher multipoles. Physicists have manipulated atoms and measured some exceptionally long life time. An example of very long life-time excited state of the 1st excited state of the Helium Atom 2 $^2\mathrm{S}_1$. It is the spin triplet state that we discussed. Since the ground state is a spin singlet and electric dipole mechanism does not involve a change in spin state, the spin triplet state has nowhere to go downward in energy by the electric dipole mechanism. The experimentally measured lifetime is 7870 seconds, a result that can be calculated accurately by QED. See Hodgman *et al.* in Phys. Rev. Lett. **103**, 053002 (2009). Another example is a metastable state in Mg with lifetime of 2050 seconds (see Jensen *et al.* Phys. Rev. Lett. **107**, 1130 (2011)). There are more extreme cases. When electric dipole transition is forbidden, then comes magnetic dipole, electric quadrupole, magnetic quadrupole, electric octupole processes, etc. An excited state in $^{172}\mathrm{Yb}^+$ ion was found to have a life time of 10 years via the electric octupole transition. See Roberts *et al.* in Phys. Rev. Lett. **78**, 1876 (1997). Of course, one needs to find a way to excite the atom to such a state before one can study it.]

SQ21 *Natural Line Broadening of a Spectral Line*

Background: We consider the measured intensity from spontaneous emissions from a collection of atoms, which are excited into state 2 by some way at time $t = 0$. The measured emitted intensity will not have the form of $I(\omega) \propto \delta(\omega - \omega_{21})$, but with a certain width about ω_{21}. This is called line broadening. It is an experimental fact. There are many reasons that contribute to line broadening. There may be collisions between the atoms, and the atoms are also moving around with different speeds and therefore there are Doppler's effect. These causes can be controlled (dilute system and cool atoms down). The cause to be discussed here,

however, cannot be avoided. This is why the consequence is called **natural line broadening**, as it happens naturally.

The Signal detected: From $t = 0$ onwards, there will be spontaneous emission and therefore we will detect $I(t)$ as the signal. Each transition gives a photon of $\omega_{21} = (E_2 - E_1)/\hbar$, but $I(t) \propto N_2(t)$, the number of atoms in state 2 at time t that drops with time as $N_2(t) \sim e^{-At} = e^{-t/\tau}$. Considering $I(t) \propto |\mathcal{E}|^2 = \mathcal{E}^*(t)\mathcal{E}(t)$, the electric field $\mathcal{E}(t)$ in the signal can be represented by

$$\begin{aligned} \mathcal{E}(t) &= 0 \quad for\ t < 0 \\ \mathcal{E}(t) &= \mathcal{E}_0\, e^{-i\omega_{21}t} e^{-t/2\tau} \quad for\ t > 0 \end{aligned} \tag{1}$$

It is from $\mathcal{E}(t)$ as given in Eq. (1) that we get the spectrum $I(\omega)$ (how the intensity distributed in ω) studied experimentally. The idea is $\mathcal{E}(t) \rightarrow \mathcal{E}(\omega)$ by a Fourier Transform and then $I(\omega) \propto \mathcal{E}^*(\omega)\mathcal{E}(\omega)$. Done! The TAs will carry out the idea.

(a) **Show that**

$$\mathcal{E}(\omega) \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathcal{E}(t) e^{i\omega t} dt = \frac{1}{\sqrt{2\pi}}\, \mathcal{E}_0\, \frac{i}{(\omega - \omega_{21}) + \frac{i}{2\tau}} \tag{2}$$

(b) Hence, **show that**

$$I(\omega) \propto \frac{\mathcal{E}_0^2}{2\pi} \frac{1}{(\omega - \omega_{21})^2 + \frac{1}{4\tau^2}} \tag{3}$$

(c) **Show that** the result can be written as

$$I(\omega) = \frac{I_{peak}}{4\tau^2}\ \frac{1}{(\omega - \omega_{21})^2 + \frac{1}{4\tau^2}} = \frac{I(\omega_{21})}{4\tau^2}\ \frac{1}{(\omega - \omega_{21})^2 + \frac{1}{4\tau^2}} \tag{4}$$

where I_{peak} is the peak value of I and the peak is at $\omega = \omega_{21}$.

(d) **Find** the ω' (on either side of ω_{21}, doesn't matter which side) that will give the half-width at half maximum. Hence, **determine how the full width at half maximum** FWHM $\Delta\omega$ **is related to** τ.

(e) Finally, **rewrite** the result as

$$I(\omega) = I(\omega_{21})\ \left[\frac{\frac{1}{4\tau^2}}{(\omega - \omega_{21})^2 + \frac{1}{4\tau^2}}\right] = I(\omega_{21})\ \left[\frac{(\frac{\Delta\omega}{2})^2}{(\omega - \omega_{21})^2 + (\frac{\Delta\omega}{2})^2}\right] \tag{5}$$

The function in the brackets is the **Lorentzian spectral line-shape function**. **Sketch** the function as a function of ω and **illustrate** the key features (peak, FWHM).

Important Remarks: Eq. (5) is an important result. $I(\omega)$ is a Lorzentian centered at ω_{12}. From an experimental spectrum, one can fit (there are softwares to do it) the Lorentzian shape to a peak and obtain ω_{21} and $\Delta\omega$. Then, $\Delta\omega$ is related to τ and thus the lifetime of the excited state. The value of τ can also be used into the transition rate formulas. This is very nice. Recall that we only considered an ideal situation. As mentioned, there are other line broadening sources, e.g. Doppler's broadening will give a Gaussian line shape. The same method is used in other experiments, e.g. identifying resonance particles (short lifetime particles) in particle physics.