Atomic Physics (M1) - T. Roscilde, R. Walder

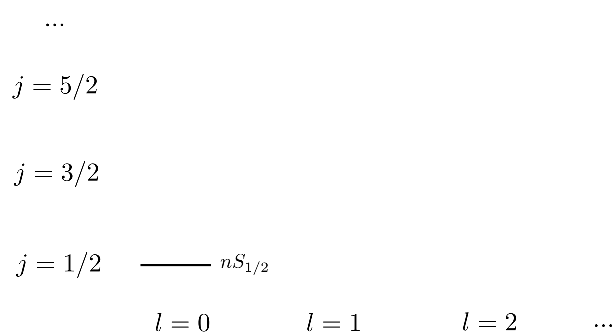
TD2: Fine structure of hydrogen

1 Transitions between the $n = 3$ and the $n = 4$ fine-structure multiplets

We consider the $n = 3$ and the $n = 4$ multiplets of the hydrogen atoms.

1.1

Organize the fine-structure levels of $n = 3$ and $n = 4$ into a table with l on the abscissa and j on the ordinates (below we give the example of the $nS_{1/2}$ level).



1.2

Draw the allowed transition between the $n = 3$ and the $n = 4$ multiplets within the electric-dipole approximation. How many distinct transition lines do you expect to appear?

1.3

CIte at least one transition line which you expect to be split by the Lamb shift.

2 Doppler broadening and spectroscopy of the fine structure

One of the main limitations to the resolution of conventional spectroscopy is represented by the *Doppler broadening* of the transition lines. In this exercise we will examine the impact of such a broadening on the measurement of the fine structure of hydrogen.
We consider a dipole-allowed transition from a lower-energy state $|g\rangle$ with energy E_g to a higher-energy state $|e\rangle$ with energy E_e. The atom can make a $g \to e$ transition by absorbing a photon with energy $\hbar\omega$ and momentum $\hbar\boldsymbol{k}$, or a $e \to g$ transition by emitting the photon. Be $\boldsymbol{p}_\mathrm{i}$ the initial momentum of the atom and $\boldsymbol{p}_\mathrm{f}$ the final one.

2.1

Write down the momentum and energy conservation relations for the absorption and for the emission of the photon.

2.2

Deduce that the absorbed/emitted photon has energy

$$\hbar\omega = \hbar\omega_0 + \hbar\boldsymbol{v}_{\rm i}\cdot\boldsymbol{k} \pm E_{\rm rec} \tag{1}$$

where the + sign applies to absorption and − to emission, $\hbar\omega_0 = E_e - E_g$, $\boldsymbol{v}_i$ is the initial velocity of the atom, and $E_{\rm rec} = \hbar^2k^2/(2M)$ is the so-called recoil energy (M is the atom mass). What does $E_{\rm rec}$ correspond to physically?

2.3

The $\boldsymbol{v}_{\rm i}\cdot\boldsymbol{k}$ term is the so-called Doppler shift. Discuss the sign of the shift if the absorbing atom is moving towards/away from the source of the photons. Discuss briefly how the measurement of the emission spectrum of atoms in outer space can tell us about the expansion of the Universe.

2.4

Justify that, if $v_{\rm i} \ll c$, we can write

$$\hbar\omega \approx \hbar\omega_0\left(1+\frac{v_k}{c}\right) \pm E_{\rm rec}\left(1+\frac{v_k}{c}\right) + \mathcal{O}((v/c)^2) \tag{2}$$

where $v_k = \boldsymbol{v}\cdot\boldsymbol{k}/k$.

2.5

Considering an hydrogen atom, for what frequency is $E_{\rm rec} \sim \hbar\omega$?
(In the following we will always work under the condition $E_{\rm rec} \ll \hbar\omega$, so that we can neglect the term $E_{\rm rec}v_k/c$).

2.6

We consider a hydrogen cloud, faithfully modeled as a classical ideal gas at room temperature ($T = 300$ K). Write down the thermal average velocity $\bar{v}_k$ and estimate $\bar{v}_k/c$. Using your knowledge of the statistical mechanics of an ideal gas, write down the probability distribution $P(v_k)$ of v_k and calculate its variance σ_v^2.

2.7

Draw schematically the distribution $P(\omega)$ for the transition frequency, and discuss why the absorption/emission line for photons detected along the $\boldsymbol{k}$ direction reproduces this distribution. Calculate σ_ω^2 (the Doppler broadening).

In the following we consider specifically the Doppler broadening of the transitions between the fine-structure multiplets $n = 2$ and $n = 3$ of hydrogen.

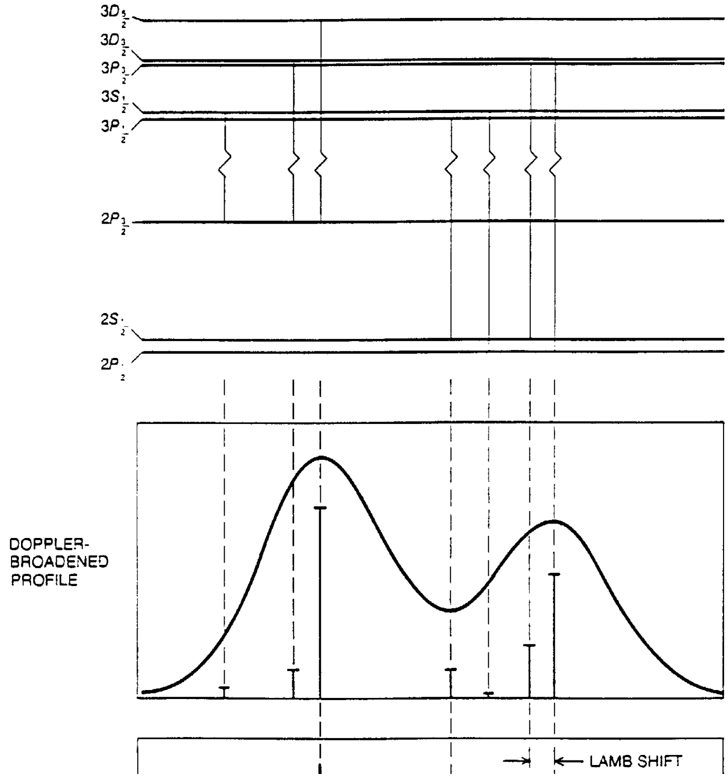


Figure 1: Doppler-broadened structure of the $(n = 2) \to (n = 3)$ line. From T. W. Hänsch, A. L. Schawlow and G. W. Series, Scientific American (1975).

2.8

Estimate numerically ω_0, σ_ω and $E_{\rm rec}$. Comment the results. What kind of radiation can one use to excite this transition?
[*Suggestion*: to compare with the literature values, express (angular) frequencies as $\omega = 2\pi f$, where f is the actual frequency].

2.9

Be $E'_{nj} = E_n + \Delta E_{nj}$ the hydrogen energy level with fine-structure corrections. For a transition conserving the j quantum number, find the general expression for the transition-line energy $\delta E'_{nj} = E'_{(n+1)j} - E'_{nj}$. Be $\delta E^{(\rm fs)}$ the fine-structure correction to the transition energy $\delta E'_{nj}$. Calculate it explicitly for $n = 2$, $j = 1/2$ and for $n = 2$, $j = 3/2$, and quote two transitions with these quantum numbers.

2.10

Compare the Doppler broadening to the fine-structure splitting between the two above transitions. Is the splitting experimentally observable? And is the Lamb shift between $2S_{1/2}$ and $2P_{1/2}$ ($\omega(2S_{1/2} \to 2P_{1/2}) = 2\pi * 1057$ MHz) observable? Compare with the data in Fig. 1.

2.11

To observe the Lamb shift, Lamb and Retherford (1947) addressed instead a direct transition between $2S_{1/2}$ and $2P_{1/2}$, namely a transition *within* the fine-structure multiplet. What kind of radiation does one need in this case? How big is the Doppler broadening for this transition? Is it still true that $\hbar\omega_0 \gg E_{\rm rec}$?

3 Z dependence of the fine-structure correction

We consider a system in which an electron is bound to a nucleus containing Z protons, with a (non-relativistic) Hamiltonian $\mathcal{H}_0 = p^2/2M + V(r)$ where $V(r) = -Ze^2/(4\pi\epsilon_0 r)$. The fine structure corrections to the Hamiltonian are

$$\begin{aligned} \mathcal{H}_{\rm SO} &= \frac{1}{2m^2c^2}\,\frac{1}{r}\frac{dV}{dr}\,\boldsymbol{L}\cdot\boldsymbol{S} \\ \mathcal{H}_{\rm rel} &= -\frac{p^4}{8m^3c^2} \\ \mathcal{H}_{\rm D} &= \frac{\hbar^2}{8m^2c^2}\nabla^2 V(r)\ . \end{aligned} \tag{3}$$

3.1

Discuss the dependence on Z of the expectation values $\langle\mathcal{H}_{\rm SO}\rangle_{nlsjm_j}$, $\langle\mathcal{H}_{\rm rel}\rangle_{nlsjm_j}$ and $\langle\mathcal{H}_{\rm D}\rangle_{nlsjm_j}$, calculated on the unperturbed eigenstates $|nlsjm_j\rangle$ of $\mathcal{H}_0$, and show that they all scale with the same power of Z.

3.2

How much bigger are the fine-structure corrections on the orbitals of the He^+ ion and of the Li^{2+} ion with respect to those of H?

Appendix

Selection rules for dipole-allowed transitions among fine-structure levels:
$\Delta l = \pm 1$, $\Delta j = 0, \pm 1$.

Fine structure corrections to the hydrogen energy level

$$\Delta E_{nj} = -E_n \frac{\alpha}{n^2}\left(\frac{3}{4} - \frac{n}{j+1/2}\right) \tag{4}$$

For a nucleus with Z protons

$$\left\langle\frac{1}{r}\right\rangle_{nl} = \frac{Z}{n^2 a_0} \qquad \left\langle\frac{1}{r^2}\right\rangle_{nl} = \frac{Z^2}{n^3 a_0} \qquad \left\langle\frac{1}{r}\right\rangle_{nl} = \frac{Z^3}{n^3\ l(l+1/2)(l+1)\ a_0^3} \tag{5}$$