Heidelberg University Winter Term 2023/24 Lecturer: Prof. Dr. Matthias Bartelmann Head tutor: Dr. Michael Zacharias

## **Problem Sheet 4**

Discussion in the tutorial groups in the week of November 13, 2023

## 1. Comprehension Question.

- (i) Summarise in your own words the steps and approximations leading to the common cross section for radiative quantum transitions.
- (ii) What is a "forbidden line", and how could it be allowed?
- (iii) Describe broadening mechanisms of spectral lines and what shape of the line profile they produce.
- 2. Hydrogen ionisation cross section. Consider the bound-free transition between the hydrogen ground state (n, l, m) = (1, 0, 0) and the free state of the electron. The momentum of the free electron follows the de-Broglie relation  $\vec{p} = \hbar \vec{k}$ .
  - (a) Calculate the dipole matrix element  $\vec{d}_{nm}$  for this transition using the wave functions

$$\langle x|m\rangle = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{x}}$$

$$\langle x|n\rangle = \frac{1}{\sqrt{\pi a_B}} e^{-r/a_B}$$

and the Fourier transform

$$\mathcal{F}[\mathrm{e}^{-r/a_B}](k) = \frac{8\pi a_B^3}{(1+a_B^2 k^2)^2}$$

of the exponential. We set the Bohr radius  $a_B := \hbar/(\alpha m_e c)$  with the finestructure constant  $\alpha = e^2/\hbar c$ .

(b) Explain why the cross section

$$\sigma_{\omega} = 4\pi^2 r_e c f_{nm} \delta_D(\omega_{nm} - \omega)$$

needs to be multiplied by the number of free electron states

$$\frac{m_e V}{2\pi^2 \hbar} k \mathrm{d}\omega$$

so that the frequency-integrated cross section becomes

$$\sigma = \frac{2r_em_ec}{\hbar}Vkf_{nm}.$$

(c) Calculate the oscillator strength  $f_{nm}$  and express  $\omega_{nm}$  by k,  $a_B$ , and the Rydberg energy Ry =  $\alpha^2 m_e c^2/2$ . Plug it in to obtain the cross section  $\sigma$ .

3. Excited state. The cross section for a transition between an initial state  $|n\rangle$  and a final state  $|m\rangle$  was derived as

$$\sigma_{mn}=\frac{4\pi}{3c\hbar}\omega_{mn}\left|\vec{d}_{mn}\right|^2\delta_D(\omega_{mn}-\omega),$$

where  $\vec{d}_{mn} = \langle m | e \hat{x} | n \rangle$  is the dipole matrix element and  $\omega_{mn} = (E_m - E_n)/\hbar$  is the frequency corresponding to the energy difference between the states  $|m\rangle$  and  $|n\rangle$ . The delta distribution  $\delta_D(x)$  assures that only those photons contribute to the cross section that have the correct frequency.

(a) Consider the one-dimensional harmonic oscillator with energy levels  $E_n = \hbar\omega(n + 1/2)$  and corresponding wave functions

$$\Psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n\left(\sqrt{\frac{m\omega}{\hbar}} x\right) \exp\left(-\frac{m\omega}{2\hbar} x^2\right)$$

with the Hermite polynomials

$$H_n(x) = (-1)^n \mathrm{e}^{x^2} \frac{\mathrm{d}^n}{\mathrm{d}x^n} \mathrm{e}^{-x^2}$$

Calculate the cross section  $\sigma_{10}$  for the transition from the ground state (n = 0) to the first excited state (n = 1). *Hint:* It may be helpful to use

$$\int_{-\infty}^{\infty} \mathrm{d}x \, x^2 \mathrm{e}^{-\alpha x^2} = - \int_{-\infty}^{\infty} \mathrm{d}x \, \frac{\partial}{\partial \alpha} \mathrm{e}^{-\alpha x^2}.$$

(b) Consider now an infinitely deep potential well of length L with energy levels

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

with  $n \in \mathbb{N}$  and wave functions

$$\Psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \cos\left(\frac{n\pi}{L}x\right) & \text{if } n \text{ is odd} \\ \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right) & \text{if } n \text{ is even} \end{cases}$$

with  $x \in [-L/2, L/2]$ . What is the cross section  $\sigma_{21}$  for the transition from the ground state (n = 1) to the first excited state (n = 2)?

Compare the factor in front of the delta distribution with that for the harmonic oscillator.

4. **Title (classroom assignment)**. Besides their natural line width, emission lines with transition frequency  $\omega_0$  are broadened due to collisions of the emitting atoms and their thermal velocities. The collisional broadening leads to a line shape that is described by a Lorentz profile

$$\Phi_{\Gamma_c}(\omega-\omega_{12}) = \frac{1}{\pi} \frac{\Gamma_c/2}{(\omega-\omega_{12})^2 + \Gamma_c^2/4}$$

where  $\Gamma_c = \sigma \langle nv \rangle$  is the collision rate,  $\sigma$  is the cross section for collisions, *n* is the number density of atoms, *v* their velocity and  $\langle \cdot \rangle$  indicates the thermal average. The Doppler broadening leads to the Gaussian profile function

$$\Phi_D = \frac{c}{\sqrt{2\pi\omega_0\sigma_v}} \exp\left[-\frac{c^2}{2\sigma_v^2} \left(\frac{\omega-\omega_0}{\omega_0}\right)^2\right],$$

where  $\sigma_v$  is the velocity dispersion.

- (a) Estimate the line width for Doppler broadening from the full width at half maximum (FWHM)  $\Delta \omega_D$  from the Gaussian profile, defined by  $\Phi_D(\omega_0 \pm \Delta \omega_D/2) = \Phi_D(\omega_0)/2$ , as a function of temperature *T*.
- (b) Estimate the line width  $\Delta \omega_c$  due to collisions from the FWHM of the Lorentz profile  $\Phi_{\Gamma_c}(\omega)$  as a function of *T*. Assume that  $\sigma$  is set by the Bohr radius  $a_B = \hbar/(\alpha mc)$  and that the density does not depend on temperature. *Hint:* What is the relation between the line width  $\Delta \omega_c$  and the collision rate  $\Gamma_c$ ?
- (c) How can the results from (a) and (b) be combined to determine the density of an emitting medium?
- (d) Calculate the ratio  $\Delta \omega_c / \Delta \omega_D$  for the H $\alpha$  line (6563Å) emitted from a cloud of atomic hydrogen with  $n = 16 \text{ cm}^{-3}$ .