Makroskopische Quantenzustände und kalte Gase

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Problem Set No 1 Date: 24 April 2018

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30 Punkte, weil Sie Zeit bis zur nächsten Übung am 15. Mai haben.

Problem 1.1 – Critical review of the Wigner-Eckart formula (7 points)

In the book 'Dispersion Forces II' by Stefan Y. Buhmann (Springer 2013), you can find an Appendix with a collection of formulas for the electric dipole matrix elements (see the Moodle for a copy). In particular, the dependence on the angular momentum quantum numbers j, m (or J, M for the total angular momentum) can be worked out without knowing the electronic wave functions in full detail. This is the contents of the so-called Wigner-Eckart theorem.

(0) Read the chapter and find the errors in the sentences. Don't be scared by the formulas.

(1) The formulas provide a way to compute the polarisability tensor of simple atomic levels (with small angular momentum):

$$\alpha_n(\omega) = \frac{1}{\hbar} \sum_k \left\{ \frac{\mathbf{d}_{nk} \otimes \mathbf{d}_{kn}}{\omega_{kn} - \omega - \mathrm{i}0} + \frac{\mathbf{d}_{kn} \otimes \mathbf{d}_{nk}}{\omega_{kn} + \omega + \mathrm{i}0} \right\} \tag{1.1}$$

that we discussed in the lecture. Use the final result of the Appendix to check a statement like: 'The polarisability of the Zeeman state $|J, M\rangle = |\frac{1}{2}, \pm\frac{1}{2}\rangle$ does not depend on M and is isotropic. Well, at least when the applied field is far from resonance, i.e., ...'

(2) I have the strong feeling that Eq.(B.22) is wrong because the two lines do not sum up give a diagonal (isotropic) polarisability, as stated in Eq.(B.26). Look up the question on the Moodle and check this. If the error persists, go through the calculations leading to Eq.(B.22) and correct the signs or numbers. (You are allowed to correct the Moodle formula.)

Problem 1.2 – Compute electronic wave functions (8 points)

On the Moodle, you can find a Python script that defines the radial and angular wave functions in the hydrogen atom.

(1) Download the script and try to execute it on a computer you have access to. Share the information how you made it with the fellow students.

(2) Make a plot of the radial charge density of a highly excited orbital (a Rydberg state). (Similar plots can be found at the web site of Michael Komma.)

(3) Compute numerically the expectation value of the radial coordinate for a few quantum numbers and compare with the exact formula

$$\langle nl|r|nl\rangle = \frac{3a_0 n^2}{2}\left(1 - \frac{l(l+1)}{3n^2}\right), \tag{1.2}$$

Python can use the integration routine '`quad`' for 'quadrature'. Check carefully the normalisation of both the radial and the angular parts of the wave function.

(4) Rydberg orbitals show many similarities with planetary motion (celestical mechanics). Recall your classical mechanics lecture and find a formula that gives the 'eccentricity' (or the ratio of major and minor axes) for an elliptic orbit in the Coulomb potential. Express your result in terms of the quantum numbers n, l, m. An interesting quantity is also the 'perinucleus' (i.e.: the distance of closest approach to the nucleus) of the elliptic orbit.

Problem 1.3 – Do the experiment: typical numbers (15 points)

Experiments with Rydberg atoms can be performed in the gas phase, using a two-photon excitation. You are invited to check a few numbers for the 'first step', taking as an example the D-line of your favorite alkali atom. It connects the energy levels $n\mathrm{s}$ and $n\mathrm{p}$ of the valence electron (*Leuchtelektron*). For Li, Na, $n = 2, 3$.

(1) In the lecture, we have talked about homogeneous and inhomogeneous linewidth of an absorption line. Find typical numbers for the 'natural linewidth' of the D-line. (Recall: the inverse of the radiative lifetime $\gamma = \gamma_{n\mathrm{p}}$ of the upper level.) Express your result in meV, MHz, cm^{-1}, and K.

(2) Consider a gas at room temperature and give an estimation for the (inhomogeneous) Doppler broadening kv_{th}. At which temperature is this smaller than the natural linewidth?

(3) When an atom absorbs or emits a photon (wave vector $\mathbf{k}$), a recoil momentum (*Rückstoß*) $\hbar k = h/\lambda$ appears. Compute the corresponding 'recoil velocity' v_{rec} for the D-line and find a temperature where $v_{\mathrm{rec}} \approx v_{\mathrm{th}}$. This is about the limit that can be reached with laser cooling, a more realistic value is $k_B T \approx \hbar\gamma$. Compare the two temperatures.

(4) The two states $n\mathrm{s}$ and $n\mathrm{p}$ form what is called as closed 'two-level system'. (Well, we ignore for the moment the fine, hyperfine and Zeeman sub-structures.) As a result, the dipole moment of the atom is no longer linear in the electric field when an intense laser is applied, an effect called 'saturation'. A typical number is the saturation intensity I_{sat}. Find typical values and show that for $I = I_{\mathrm{sat}}$, the electric field E_L of the laser satisfies $d_{n\mathrm{p},n\mathrm{s}} E_L \sim \hbar\gamma$ (keyword 'Rabi frequency'). As a rough estimate, $d_{n\mathrm{p},n\mathrm{s}} \approx e a_0$.

(5) From electrodynamics, you remember that the dielectric function of a dilute gas with polarisability $\alpha(\omega)$ is given by

$$\varepsilon(\omega) \approx \varepsilon_0 + \frac{N}{V}\alpha(\omega) \tag{1.3}$$

where N/V is the number density of atoms. Make the connection to the refractive index and from its imaginary part to the absorption A (in $1/\mathrm{m}$, not a conventional notation) to show that

$$A(\omega) \approx \frac{2\pi N}{\lambda V} \,\mathrm{Im}\, \frac{\alpha(\omega)}{\varepsilon_0} \tag{1.4}$$

In a frequency range near an atomic resonance, the following (isotropic, two-level) approximation may be used:

$$\alpha(\omega) \approx \frac{\pi\varepsilon_0 \lambda\!\!\!^{-}{}_D^3 \gamma}{\omega_D - \omega - \mathrm{i}\gamma/2} \tag{1.5}$$

where $\lambda\!\!\!^{-}{}_D = \lambda_D/(2\pi)$ and ω_D correspond to the D-line. Find an estimate for the 'resonant absorption cross section' of the gas.

(6) Complete the following narrative: a laser beam with intensity $\ldots\mathrm{mW}/\mathrm{cm}^2$ and cross section S corresponds to a flux of ... photons per second. The absorption cross section of an atom multiplied by the photon ... (per second and unit area) gives the photon absorption rate (events per second). Once the atom has absorbed a photon, it stays in the ... state for ... lifetime $1/\gamma$ on average. This gives for a laser intensity of $\ldots\mathrm{mW}/\mathrm{cm}^2$ and an atomic density of $\ldots\mathrm{cm}^{-3}$ an average density of excited atoms of $\ldots\mathrm{cm}^{-3}$. What is typical distance between excited atoms?