

EXAMINATION 09-12-2014

ATOMS AND MOLECULES. 18:30-21:30, A. JACOBSHAL 01, # QUESTIONS: 5, # POINTS: 100

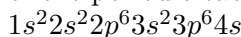
YOU CAN MAKE USE (IF YOU THINK YOU HAVE TO) OF THE FOLLOWING FORMULA'S:

$$g_J = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}$$

$$g_F = \frac{F(F+1) - I(I+1) + J(J+1)}{2F(F+1)} g_J$$

1. POTASSIUM: ELECTRONIC STRUCTURE (20 POINTS)

A. Write down the electron configuration of K, which is first element in the fourth row of the periodic table of the elements.



B. Give the term for the ground state and the first excited state of the Potassium atom. Briefly explain what spin-orbit coupling is and why the ground state is not split but the first excited state is. The light that is emitted as this split excited state decays to the ground state consist of two components with wavelengths of 764.49 and 769.90 nm. Calculate the size of the spin-orbit coupling constant β [in cm^{-1}].

Ground state: ${}^2S_{\frac{1}{2}}$, excited state ${}^2P_{\frac{1}{2}, \frac{3}{2}}$. Spin-orbit coupling leads to a degeneracy in the excited state because the direction of the magnetic moment associated with the orbital angular momentum of the electrons can be parallel or anti-parallel with respect to the magnetic moment associated with the spin of the electrons. The ground state is not split since the orbital angular momentum is zero. From the interval rule we know that the splitting between the $\frac{3}{2}$ and $\frac{1}{2}$ levels is $\frac{3}{2}A$. The energy difference between the two levels is $\Delta E = \frac{1}{764.49 \cdot 10^{-7}} - \frac{1}{769.90 \cdot 10^{-7}} = 91.92 \text{ cm}^{-1}$, which means that $A = 61.28 \text{ cm}^{-1}$.

C. Consider the light from a Potassium lamp, observed by an old spectrometer (that can not resolve the small effects caused by the nuclear spin). In how many components does the ${}^2S_{1/2} - {}^2P_{1/2}$ line split if a weak magnetic field is applied? Calculate the energy shift of each line, with respect to the zero-magnetic field case, expressed in units of $\Delta = \mu_B B$. The g-factors for the ground state and the excited state are 2 and 2/3, respectively. The upper state shifts by $\pm 1/3\Delta$, the ground state by $\pm\Delta$. The transition thus splits in 4 components, with shifts of $\pm 2/3\Delta$ and $\pm 4/3\Delta$.

D. The most abundant isotope of Potassium, ${}^{39}\text{K}$, has a nuclear spin $I = 3/2$. Because of this, the ${}^2P_{3/2}$ component has hyperfine splitting. Draw the splitting schematically, label the hyperfine states with their F quantum number and express the energy separation between these states in terms of the hyperfine constant $A_{4^2P_{3/2}}$.

$\vec{F} = \vec{I} + \vec{J}$ so F can be 0, 1, 2, 3. Using the interval rule we can directly say that the splitting between these lines will be $A, 2A, 3A$.

2. SODIUM: LINEWIDTH AND DOPPLER-FREE SPECTROSCOPY (22 POINTS)

A. The 3s-3p transition in ^{23}Na atoms can be excited by light at a wavelength of 589 nm. The lifetime of the excited state is 16 ns. If we have to stabilise a laser to 1/10th of the natural linewidth, what fractional stability is required?

$\tau = 16 \text{ ns}$, so $\Gamma = 1/\tau = 6.25 \cdot 10^7$. The line width is then $\Delta f = 6.25 \cdot 10^7 / 2\pi = 10^7 \text{ Hz}$. The frequency of the light is $f = c/\lambda = 3 \cdot 10^8 / 589 \cdot 10^{-9} = 5 \cdot 10^{14}$, so that $\Delta f/f = 2 \cdot 10^{-8}$. 1/10th of that is $2 \cdot 10^{-9}$.

B. Consider a gas of Na atoms at a temperature of 300 K. The velocity is distributed according to the Boltzmann distribution: $I(v) = \sqrt{\frac{m}{2\pi kT}} e^{-\frac{1}{2}mv^2/kT}$, where $k=1.38\text{e-}23 \text{ [J/K]}$, or $\text{m}^2 \text{ kg s}^{-2} \text{ K}^{-1}$] is the Boltzmann constant. Combine this formula with the formula for the Doppler-shifted frequency to calculate what the Doppler width (full-width half-max) at $T=300 \text{ K}$ is, in units of MHz. The mass of ^{23}Na is 23 atomic mass units (amu), where $1 \text{ amu} = 1.66\text{e-}27 \text{ [kg]}$.

With $v = \frac{\omega - \omega_0}{\omega_0} c$ one gets $\omega - \omega_0 = \frac{\omega_0}{c} \sqrt{\frac{2 \ln(2) kT}{m}}$. Twice this is the Doppler width $\Delta\omega_D$, and $\Delta f_D = \Delta\omega_D / 2\pi$. For Na at 300 K we find from that formula $\Delta f_D = 1317 \text{ MHz}$.

C. The laser frequency can be locked to an atomic transition using Doppler-free spectroscopy. Sketch a typical setup, and explain the operating principle for a simple two-level system.

See the lecture notes and the book.

D. The ^{23}Na atoms we are considering have a nuclear spin $I = 3/2$. The hyperfine constant $A_{3^2S_{1/2}}$ for the ground state is 885.8 MHz, the hyperfine constant $A_{3^2P_{1/2}}$ for the first excited state is 94.4 MHz. Sketch the absorption of the weak probe beam in the Doppler-free spectroscopy setup for a scan of the laser frequency over the $^2S_{1/2} - ^2P_{1/2}$ transition, where the scan is large enough to include the hyperfine structure in both the ground state and the excited state. Make sure to include the Doppler-broadened part of the absorption at the correct scale! Include cross-over peaks if they arise.

This is roughly similar like the spectrum on page 176 of Foot, but with three instead of 6 peaks in the doppler-broadened background, since there are two possible transitions with a cross-over peak in the middle. The separation between the ground state levels is $2A$, which gives us 1772 MHz, and the excited state is also split by $2A$, which is 189 MHz. The crossover-peak of the top levels is in between those two peaks (also a peak). The cross-over peak in the middle of the scan due to the ground state splitting is not visible, since it falls outside the doppler-broadened range.

3. SISYPHUS COOLING (23 POINTS)

A. Draw the M-substates of a $J = 1/2$ ground state and the possible transitions to a $J = 3/2$ excited state. Explain why the transition rates are not all equal. Which ones are the strongest?

The answer to these questions is essentially given at page 205 of Foot.

B. Assume we are starting with a gas of atoms distributed equally over both M_J ground states. What is the effect on the ground-state population if we excite these atoms for some time using right-handed circularly polarised laser light (making σ^+ transitions with $\Delta M_J = +1$)?

C. Indicate the AC Stark shift of the 2 ground state and 4 excited state substates, for the following four configurations: if we were to use right (left) handed polarised laser light of a red (blue) detuned laser.

D. Sketch the polarisation gradient that is obtained in the standing light field of two counter-propagating linearly polarised laser beams, with the linear polarisation orthogonal to each other. It is useful to decompose the local electric field vector into two orthogonal components.

E. Explain how all components that you described above can lead to a cooling effect. What can you say about the velocity class for which this cooling mechanism works?

4. THE QUANTUM ZENO EFFECT (20 POINTS)

A. We consider a two-level system, with levels denoted $|1\rangle$ and $|2\rangle$, energies E_1 and E_2 , and with individual wave functions $|\psi_1\rangle$ and $|\psi_2\rangle$. Write down the general time-dependent form of the two-level wavefunction Ψ .

$$\Psi = c_1(t) |\psi_1\rangle e^{-i\omega_1 t} + c_2(t) |\psi_2\rangle e^{-i\omega_2 t}, \text{ with } c_1(t) = \cos\left(\frac{\Omega}{2}t\right) \text{ and } c_2(t) = -i\sin\left(\frac{\Omega}{2}t\right).$$

B. At $t = 0$ the population is all in the ground state $|1\rangle$. We start driving the system with an electromagnetic wave tuned to the energy difference of the two levels. Assume there is no spontaneous decay from the excited state. Explain the temporal evolution of the population in the two levels. What is the population in the two levels if we would do a measurement at $\Omega t = \pi/2$?

Bloch oscillation, at Bloch frequency Ω . If we stop at $\Omega t = \pi/2$, and we would do a measurement, we would find half of the atoms in level $|1\rangle$ and the other half in $|2\rangle$, because $P(|1\rangle) = P(|2\rangle) = \cos^2\left(\frac{\Omega t}{2}\right) = \cos^2\left(\frac{\pi}{4}\right) = \frac{1}{2}$.

C. Suppose that we add another measurement of the population in the levels half-way through this process, i.e. at $\Omega t = \pi/4$. Calculate the population you measure at this moment, and show the effect of this additional measurement on the measurement at $\Omega t = \pi/2$.

We find for the population at $\Omega t = \pi/4$ that $P(|1\rangle) = \frac{1}{2} + \frac{\sqrt{2}}{4} \approx 0.85$ and that $P(|2\rangle) = \frac{1}{2} - \frac{\sqrt{2}}{4} \approx 0.15$. At $\Omega t = \pi/2$ the probabilities have now changed due to the observation at $\Omega t = \pi/4$: $P(|1\rangle) \approx 0.75$ and $P(|2\rangle) \approx 0.25$.

D. What requirements have to be met for the Quantum Zeno effect to be observable in an experiment?

The spontaneous decay has to be negligible; the system has to be allowed to evolve coherently for at least the time of the measurement, and spontaneous decay leads to decoherence.

5. SPIN-ORBIT COUPLING IN MOLECULES (15 POINTS)

A. Explain the difference (in terms of angular momentum coupling) between a ${}^3\Pi_0, {}^3\Pi_1$ and a ${}^3\Pi_2$ electronic state.

$\Lambda = 1; S = 1; \Sigma = -1, 0, 1. \Omega = 1$ if $\Sigma = 0$: the spin S and the angular momentum Λ are perpendicular. If $\Omega = 0, 1$ and $\Sigma = -1, 1$: the spin and angular momentum are antiparallel and parallel, respectively.

B. Give the term labels for the fine-structure split components of the possible molecular states with $L = 2, S = 1$. What is the separation in energy between the possible fine-structure levels of these states?

$$\Lambda = 0, 1, 2 \Rightarrow {}^3\Sigma_1, {}^3\Pi_{0,1,2}, {}^3\Delta_{1,2,3}. W = A\Lambda\Sigma$$

C. Complete the following table.

Electronic state	Λ	S	Σ	Ω
$^1\Sigma$				
$^3\Pi_1$				
	3	1		4
	1	1	1	
$^2\Delta_{5/2}$	1	1	-1	

TABLE 1. The question

Electronic state	Λ	S	Σ	Ω
$^1\Sigma_0$	0	0	0	0
$^3\Pi_1$	1	1	0	1
$^3\Phi_4$	3	1	1	4
$^3\Pi_2$	1	1	1	2
$^3\Pi_0$	1	1	-1	0
$^2\Delta_{5/2}$	2	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{5}{2}$

TABLE 2. The answers