

EXAMINATION 07-11-2013 WITH ANSWERS

ATOMS AND MOLECULES

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. ENERGY LEVELS (25 POINTS)

In Figure 1, on the next page, you see two sets of electronic energy levels. The energy levels are indicated with lines. Not all levels are given, just the most important ones. They are roughly, but not exactly, drawn to scale (with energy on the vertical axis). One of the two is a one-electron system, the other one is a two-electron system. Indicate the following in these figures (either on your own paper, or on the question sheet):

A. Which one is the two-electron system, and which one is the one-electron system?

The picture on the right is a one-electron system with doublets due to spin-orbit coupling. The singlet and triplet states on the left picture indicate that these are energy levels of a two-electron system.

B. The two-electron system is Calcium. From your knowledge of the periodic table of elements, give the electron configuration of the Calcium atom.

A system of singlet and triplet states is the result of 2 s electrons; Calcium is indeed from the second column of the periodic table. You might think that Calcium has two p electrons: this does, however, not result in a singlet ground state. Two d electrons is in principle also possible, but we have never dealt with this system in the lectures so it is highly unlikely... Good answer: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$ but $3s^2$ or $5s^2$ also gets full points, in case you forgot that Calcium has 20 electrons (and 20 protons and 20 neutrons).

C. Label the energy levels of the Calcium system with term symbols, and also indicate the electron configuration (only the changing part) for these energy levels.

Ground state $4s^2 \ ^1S_0$, above it $4s5s \ ^1S_0$. Then, to the right of these two levels: $4s4p \ ^1P_1$, and $4s5p \ ^1P_1$. Then in the next column the D state: $4s4d \ ^1D_2$. The three levels that are given from the triplet manifold must then be the $4s4p \ ^3P_{0,1,2}$

D. Indicate a strong allowed transition and an inter combination line in one of these energy level schemes.

Intercombination lines connect the singlet and triplet system, like $^1S_0 - ^3P_1$. A strong transition is a $\Delta J = \pm 1$ transition like $^1S_0 - ^1P_1$.

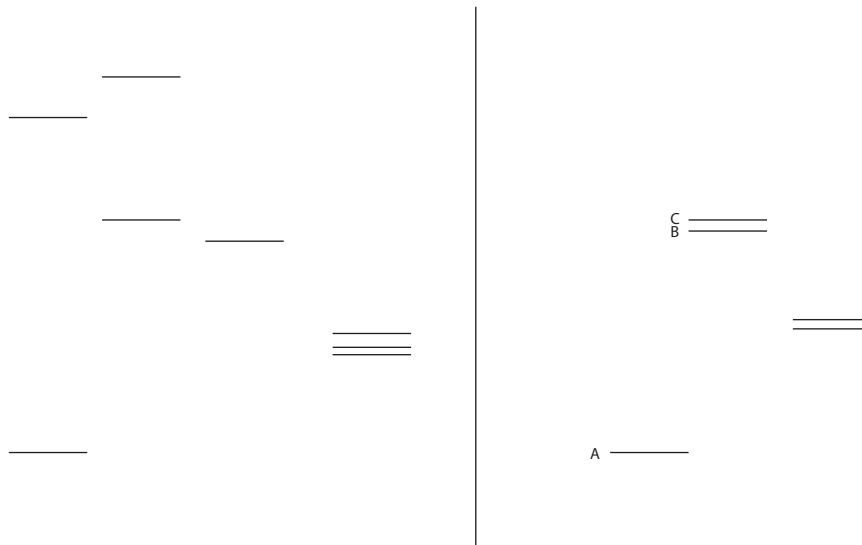


FIGURE 1. Two sets of energy levels: one for a one-electron system, one for a two-electron system.

E. The set of three lines close together on the left-figure are split by spin-orbit coupling. The spin-orbit coupling constant in this case is 52 cm^{-1} . Use the interval rule, and your knowledge of the quantum numbers for this case, to calculate the spacing between these three levels.

Interval rule: $(J'' - J') = \beta J'$. The J 's must be 0,1,2 so the splitting is 2β and β , 104 and 52 cm^{-1} respectively.

F. Consider the light from a glowing gas of the element on the right. This light is observed by an old spectrometer (that can not resolve the small effects caused by the nuclear spin). In how many components does the line between level A and B 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 $\Delta = \mu_B B$.

Identify which levels these are: single electron system: single s electron, $^2S_{1/2}$ ground state and $^2P_{1/2,3/2}$ excited states. Calculate the splitting of the upper level and the lower level: $^2P_{1/2} : \pm\frac{1}{3}\Delta$, $^2S_{1/2} : \pm\Delta$. They do not shift by the same amount: thus 4 possible transitions, with shifts $\pm\frac{2}{3}\Delta, \pm\frac{4}{3}\Delta$

G. An odd isotope of this element has a nuclear spin $I = 3/2$. Because of this, level C 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 .

Write down the possible F levels: ($3/2-3/2$ to $3/2+3/2$ is 0,1,2,3). Apply the interval rule to find $3A, 2A, A$ for the splittings.

2. RAMSEY SPECTROSCOPY (25 POINTS)

Now we turn to the ground state of the Cesium atom, which is the element on the sixth row of the first column in the periodic table. This state is being used as the definition of the second. The only stable isotope of Cesium has a nuclear spin of $F = 7/2$.

A. Calculate the g_F factors for the two hyperfine components of the ground state.

Just fill in the formula given on the exam to find $+1/4$ for $F = 4$ and $-1/4$ for $F = 3$

B. Make a sketch of the splitting of the ground state of Cesium in low magnetic fields, and label the lines according to their m_F . Then indicate in the same figure the splitting in large magnetic fields, and show the connection between the two regimes.

$F = 3$ has a negative g_F factor, so the m_F 's are reversed ($m_F = -3$ will be on the top). All m_F 's from $F = 3$ and the lowest $M_F = -4$ from $F = 4$ level go to a lower energy in a magnetic field (low-field seeking), all the other substates from $F = 4$ go to a higher energy in a magnetic field (high-field seeking). The lines separate into two sets, with $m_J \pm 1/2$, with the hyperfine structure as a perturbation.

C. Indicate in the figure that you just made which states are low-field seeking and which states are high-field seeking.

see answer above

D. Draw a schematic diagram of a Ramsey setup making use of separated oscillatory fields. Label the essential components, and indicate the relevant quantum numbers (F, m_F) for Cesium atoms in various parts of the setup. Also draw the typical spectrum that is obtained.

You can look this up in the lecture notes. Don't confuse Rabi (a single interaction zone, flop-in and flop-out) with the Ramsey setup (two interaction zones, separated in time and space).

E. Explain how this experiment works using pictures of a Bloch sphere with the state vector that describes the state of the Cesium atom. Use these pictures to explain the minima and maxima in the spectrum that is obtained.

Initially the state vector points up ($F=3$ state). Then the first $\pi/2$ pulse brings it to a superposition of the $F=3$ and $F=4$ states. As time progresses, the state vector rotates in the horizontal plane, until the atom reaches the second interaction zone. The second $\pi/2$ pulse either brings the system to the $F=4$ state or back to the $F=3$ state (or somewhere in between), depending on the relative phase of the external reference and the superposition, that builds up during the time in between the two interaction zones. Depending on the final detection step, selecting either high- or low-field seeking states, the maximum would correspond to $F=3$ atoms or $F=4$ atoms, and vice-versa.

F. Explain how the apparatus described in **E** benefits from the use of cold atoms, and give the reasons why such a machine is better suited as a frequency standard compared to a Hydrogen maser.

The increased interaction time offered by cold (=slow) atoms means that the time between the two interaction zones is increased: as a result of this a small frequency difference between the external reference source and the atomic level system leads to a larger phase difference. As a result the spacing between the maxima will be reduced, and the precision with which the central maximum can be determined is increased.

3. NON-DESTRUCTIVE PHOTON DETECTION (20 POINTS)

We start with an atom that has 3 states labelled $|i\rangle$, $|g\rangle$ and $|e\rangle$. There is a cavity, with or without a photon, that is tuned to resonance with the transition $|g\rangle \longleftrightarrow |e\rangle$. In this question we investigate how we can use the atoms to probe whether a photon is present in the cavity, without destroying the photon.

A. The atom has to be prepared in a superposition of states for this trick to work. Which states are coupled, and how is this done? Give the initial atomic wave function and the wave function after preparation.

Initially prepare in $|g\rangle$, and couple using a $\pi/2$ pulse to $|i\rangle$. Wavefunctions can be found in the lecture notes.

B. What kind of interaction of the atom and the photon can take place in the cavity that can be detected but does not lead to destruction of the photon? Give the wave function after passage through the cavity if the photon is present, and if it is not.

A 2π pulse can be applied, coupling $|g\rangle$ and $|e\rangle$. Effectively a photon is absorbed and emitted again. The only difference this makes is a minus sign for the $|g\rangle$ part of the wavefunction.

C. How does the final detection step work? Give the wave function following the detection step if the photon is present and if it is not.

Again a $\pi/2$ pulse coupling $|g\rangle$ and $|i\rangle$. The resulting wavefunction can be found in the lecture notes.

4. MOLECULAR SPECTRA (15 POINTS)

A. Make a schematic drawing of the first four rotational levels in a vibrational ground state $v'' = 0$ and the first excited state $v' = 1$.

Draw twice four horizontal lines, in two sets, above each other. Make sure that they are not equidistant for rotational levels: the spacing increases with increasing J .

B. Assuming these vibrational states to be in the same electronic potential, indicate the allowed transitions between these rotational levels, and give these transitions the appropriate labels.

$\Delta J \pm 1$ are P and R branches. General form of the labels: $P(J'')$, $R(J'')$.

C. How does the situation change if the vibrational states are in different electronic states? Indicate possible new transitions, and label them.

Now also the Q branch is allowed, $\Delta J = 0$.

D. What is the reason for the frequency difference between the P, Q and R branch? Which approximation is therefore not valid here?

The rigid rotor approximation is not valid anymore, because the difference is being caused by the dependence of the rotational constant on the vibrational quantum number.

5. DIATOMIC MOLECULES IN AN EXTERNAL MAGNETIC FIELD (15 POINTS)

A. Give a drawing of the relevant vectors and their projections (\vec{J} , \vec{R} , Ω , Λ , Σ) for a Hund's case (a) molecule.

You can look this up in the Demtröder textbook, or the lecture notes.

B. Give the magnetic moment μ_{Ω} of these molecular states: a) $^1\Pi$ b) $^3\Sigma$ c) $^2\Pi_{3/2}$ d) $^2\Pi_{1/2}$
 $\mu_{\Omega} = 2\mu_S + \mu_L$: you find 1, 2, 2, 0 μ_B

C. Without a magnetic field, the magnetic moment μ_{Ω} precesses around \vec{J} to form a magnetic moment μ_J . In an external field, \vec{J} precesses around \vec{B} . Knowing this, derive the effective time-averaged value of the magnetic dipole moment of a rotating molecule in an external magnetic field, μ_{eff} .

You can look this up in the Demtröder textbook, or the lecture notes.