

## EXAMINATION 07-11-2014 - ANSWERS

ATOMS AND MOLECULES. 08:30-11:30, K. DUPPENHAL, # QUESTIONS: 6

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. ELECTRONIC AND FINE STRUCTURE (10 POINTS)

- A.** Using the Madelung rule you can find  $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^1$
- B.** The energy is inversely proportional to the wavelength. Convert to wavenumber ( $10^7/\lambda[\text{nm}]$ ), subtract the energies, we find that  $\Delta E = 554.8 \text{ cm}^{-1}$ . Since  $\Delta E = 3/2\beta$  (through the interval rule) we find that  $\beta = 369.9 \text{ cm}^{-1}$ .

### 2. HYPERFINE STRUCTURE, ZEEMAN EFFECT (20 POINTS)

- A.** Just fill in the formula given on the exam to find  $+1/4$  for  $F = 4$  and  $-1/4$  for  $F = 3$
- B.**  $F = 3$  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 (high-field seeking), all the other substates from  $F = 4$  go to a higher energy in a magnetic field (low-field seeking). The lines separate into two sets, with  $m_J \pm 1/2$ , with the hyperfine structure as a perturbation. The states that have their energy decrease with increasing electric field [ $m_J = -1/2$ ] are high-field seekers, the states that have their energy minimum at minimum electric field [ $m_J = +1/2$ ] are low-field seekers.
- C.** see the figure below for the solution

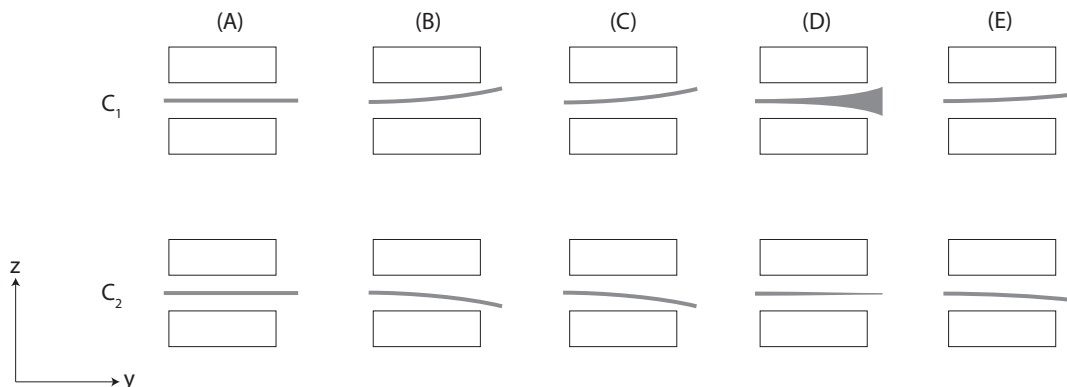


FIGURE 1. A cut-through of various magnet configurations. The atomic beam of Cesium (in the  $F = 3$  level ( $C_1$ ) or in the  $m_F = +4$  state ( $C_2$ )) is deflected or focussed by these magnets.

D. One way would be to add a field-free zone where the  $m_F$  states become degenerate and the population of atoms will redistribute over all  $m_F$  states. Subsequent application of an inhomogeneous magnetic field like (B) or (C) will enable separating the high-field seeking  $m_F = -4$  state from the rest. Another method is to use a non-adiabatic change of the magnetic field: an  $m_F = +4$  atom has its spin aligned with the local magnetic field, so after quickly reversing the magnetic field the atom will be in the  $m_F = -4$  orientation (state).

### 3. RAMSEY SPECTROSCOPY AND LASER COOLING (20 POINTS)

A hyperfine transition in the electronic ground state of Cesium is being used for the definition of the second. This is done using Ramsey spectroscopy on laser-cooled atoms.

A. see the figure below for the solution

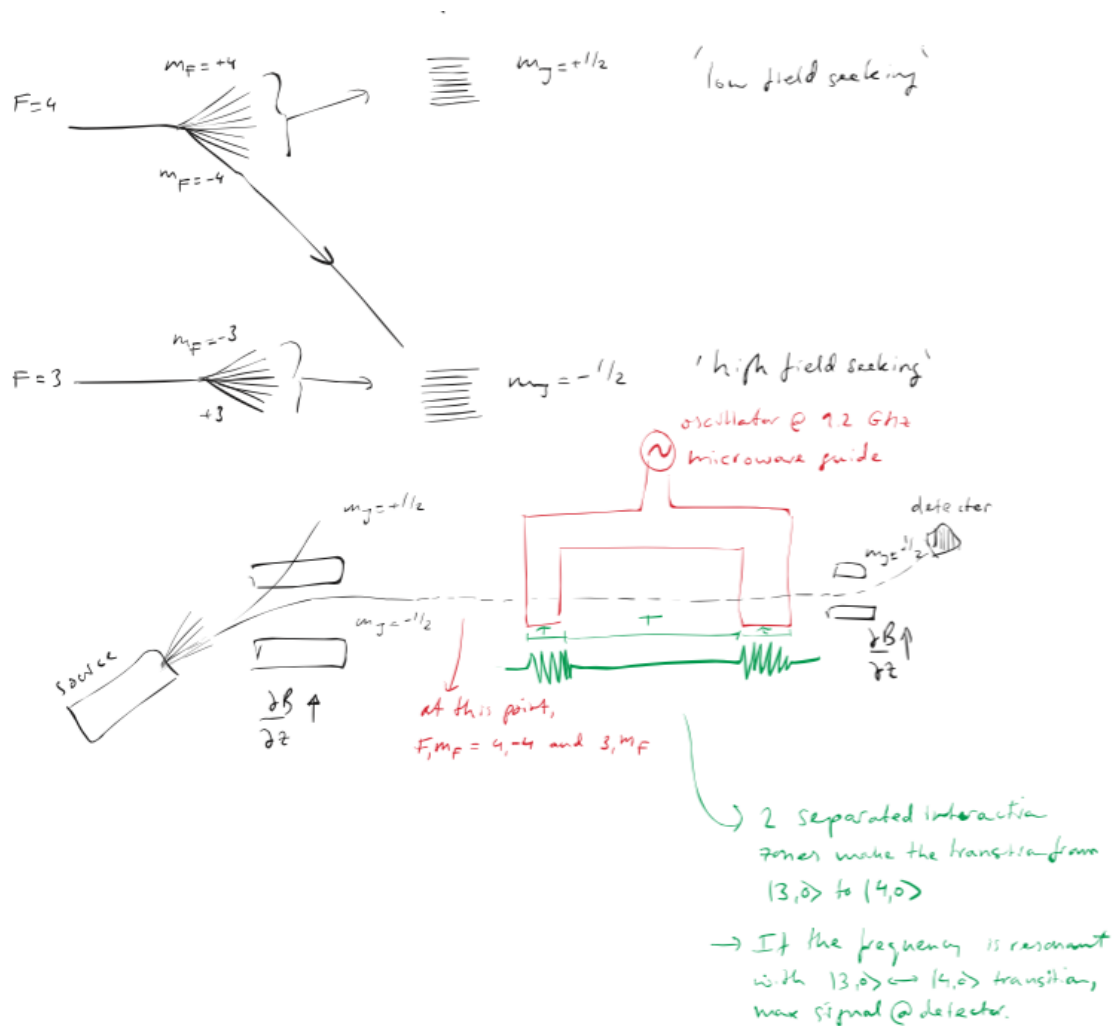


FIGURE 2. The sketch of the setup

B. 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.

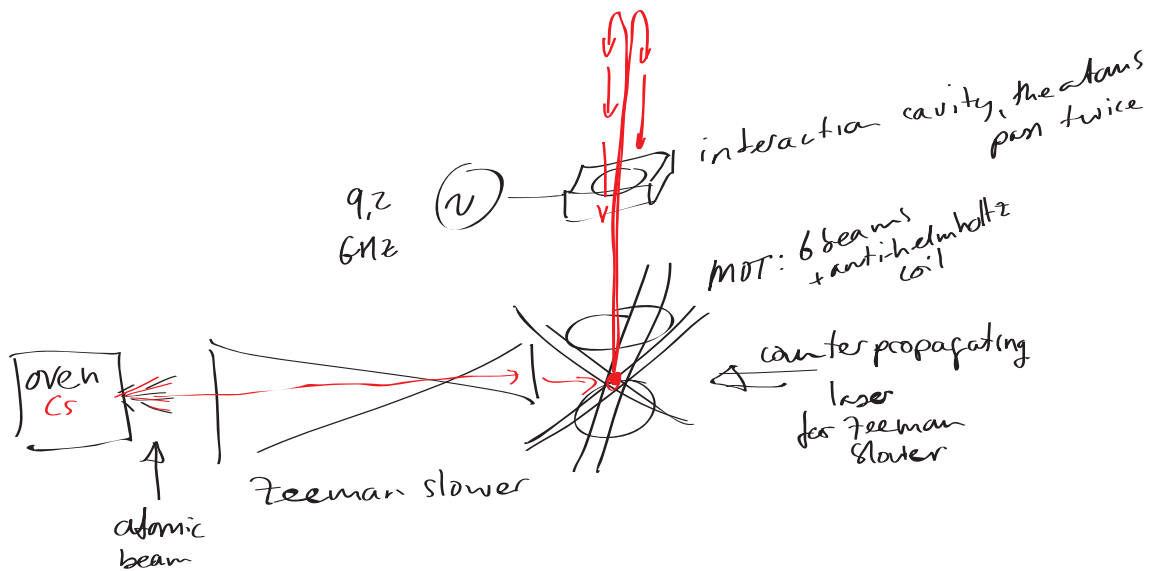


FIGURE 3. The sketch of the fountain setup

C. The Ramsey scheme is implemented by having the atoms pass the same cavity twice, once when they go up, the second time when they go down.

D. The total sequence of steps from oven to BEC is: Oven - Zeeman Slower - MOT - Molasses (for sisyphus cooling) - Dipole trap or magnetic trap (for evaporative cooling) - trick to prevent Majorana losses (orbiting trap or optical plug) - BEC

#### 4. DOPPLER-FREE SATURATION SPECTROSCOPY (20 POINTS)

The lasers used in the laser cooling experiments have to be precisely kept at the required wavelength. This is done using Doppler-free spectroscopy. For this question we consider transitions between the hyperfine-split states  $^2S_{1/2}$  and  $^2P_{3/2}$  of Cesium.

A. see the figure below for the solution

B. see the figure below for the solution

C. see the figure below for the solution

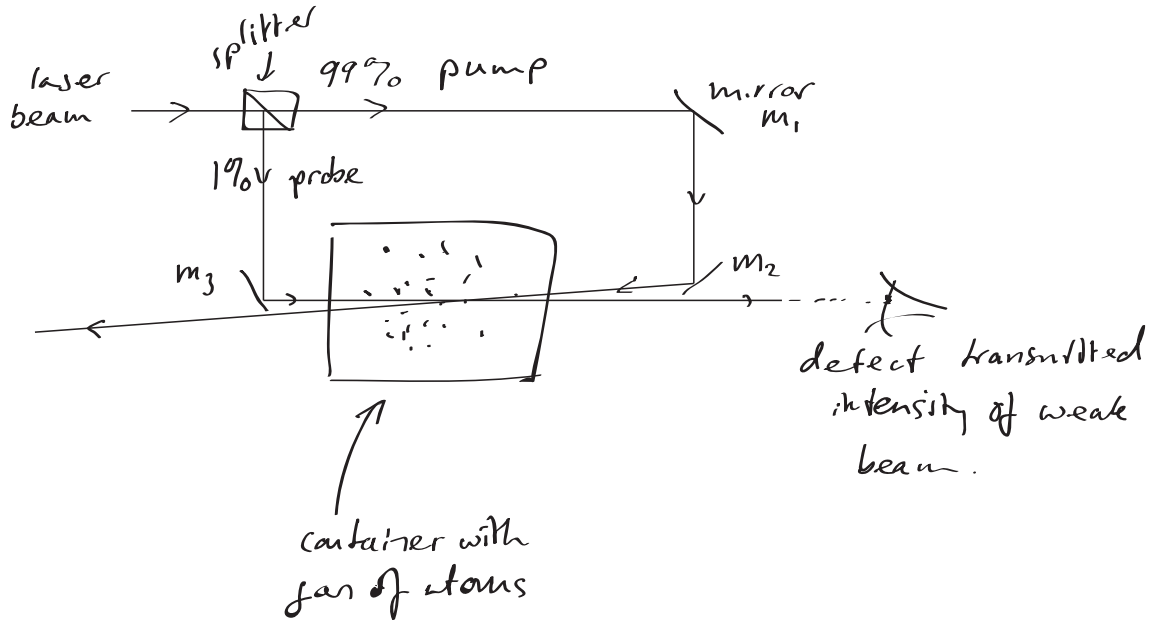


FIGURE 4. The sketch of the doppler free detection setup

## 5. QUANTUM COMPUTATION (10 POINTS)

**A.** The  $C$  stands for Control. This means that the spin-flip operation on ion #2 can be controlled by the state of ion #1. This is done in ion traps by coupling the motion of the ions: if the ions are brought into an excited motional state by ion #1, the resonance frequency for the spin-flip of ion #2 is different.

**B.** This is similar to the non-destructive photon detection, in which the  $2\pi$  excitation is performed by the cavity. So the procedure is identical to the follow solution for that problem:

We have 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  $|g\rangle \longleftrightarrow |e\rangle$ . Given the atom is in  $|i\rangle$  initially

Prepare a  $\frac{\pi}{2}$  pulse coupling  $|i\rangle$  and  $|g\rangle$ ,  $|i\rangle \xrightarrow{\frac{\pi}{2}} |g\rangle$

$$\Psi = \cos\left(\frac{\pi}{4}\right) |i\rangle - i \sin\left(\frac{\pi}{4}\right) |g\rangle = \frac{1}{\sqrt{2}} |i\rangle - \frac{i}{\sqrt{2}} |g\rangle$$

This is the wave function if there is no photon coupling  $|g\rangle$  and  $|e\rangle$  present.

If there is a photon coupling  $|g\rangle$  and  $|e\rangle$  present for a time  $t$  such that  $t = \frac{2\pi}{\Omega}$ ,  $|g\rangle \xrightarrow{2\pi} |e\rangle$ :

$$\frac{1}{\sqrt{2}} |g\rangle \Rightarrow -\frac{1}{\sqrt{2}} |g\rangle$$

$$\Rightarrow \Psi = \frac{1}{\sqrt{2}} |i\rangle + \frac{i}{\sqrt{2}} |g\rangle$$

After the cavity, apply another  $\frac{\pi}{2}$  pulse coupling  $|g\rangle$  and  $|i\rangle$ ,  $|g\rangle \xrightarrow{\frac{\pi}{2}} |i\rangle$  on both the no-photon wave function and the photon wave function:

Then the no-photon wave function becomes

$$\Psi = \frac{1}{\sqrt{2}} \left( \frac{1}{\sqrt{2}} |i\rangle - \frac{i}{\sqrt{2}} |g\rangle \right) - \frac{i}{\sqrt{2}} \left( \frac{1}{\sqrt{2}} |g\rangle - \frac{i}{\sqrt{2}} |i\rangle \right)$$

### Doppler-free spectroscopy

Strong pump beam can be resonant with  $|g_2\rangle \rightarrow |e\rangle$  (or  $|g_1\rangle \rightarrow |e\rangle$ ) and transfer the population from  $|g_2\rangle \rightarrow |g_1\rangle$  (or the other way around).

The probe beam will be resonant with  $|g_1\rangle$  (or  $|g_2\rangle$ ) and therefore find an increase of the ground state population, leading to a decreased transmission.

—————  $|e\rangle$

—————  $|g_2\rangle$   
 —————  $|g_1\rangle$

The spectrum will look like this:

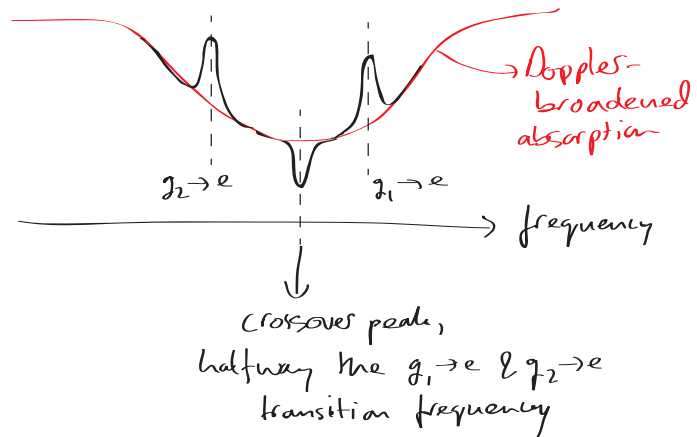


FIGURE 5. The sketch of how cross-over peak arise

$$= \frac{1}{2} |i\rangle - \frac{i}{2} |g\rangle - \frac{i}{2} |g\rangle - \frac{1}{2} |i\rangle = -i |g\rangle$$

and the photon present wave function becomes,

$$\Psi = \frac{1}{\sqrt{2}} \left( \frac{1}{\sqrt{2}} |i\rangle - \frac{i}{\sqrt{2}} |g\rangle \right) + \frac{i}{\sqrt{2}} \left( \frac{1}{\sqrt{2}} |g\rangle - \frac{i}{\sqrt{2}} |i\rangle \right)$$

$$= \frac{1}{2} |i\rangle - \frac{i}{2} |g\rangle + \frac{i}{2} |g\rangle + \frac{1}{2} |i\rangle = |i\rangle$$

Here the outcome depends on photon present/not. Hence the system works.

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

- A. See the figure below.
- B.  $\mu_\Omega = 2\mu_S + \mu_L$ : you find 1,2,2,0  $\mu_B$
- C. See the figure below

## Werkcollege test #5, 01-10-2014

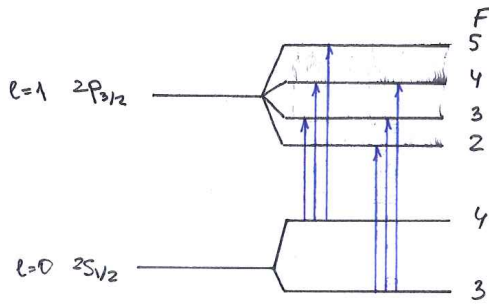
### Solutions

A. Cs ;  $I = 7/2$

$$\vec{F} = \vec{I} + \vec{J}; \quad F = |I - J|, \dots, I + J$$

$${}^6S_{1/2}: J = 1/2 \Rightarrow F = 3, 4$$

$${}^6P_{3/2}: J = 3/2 \Rightarrow F = 2, 3, 4, 5$$

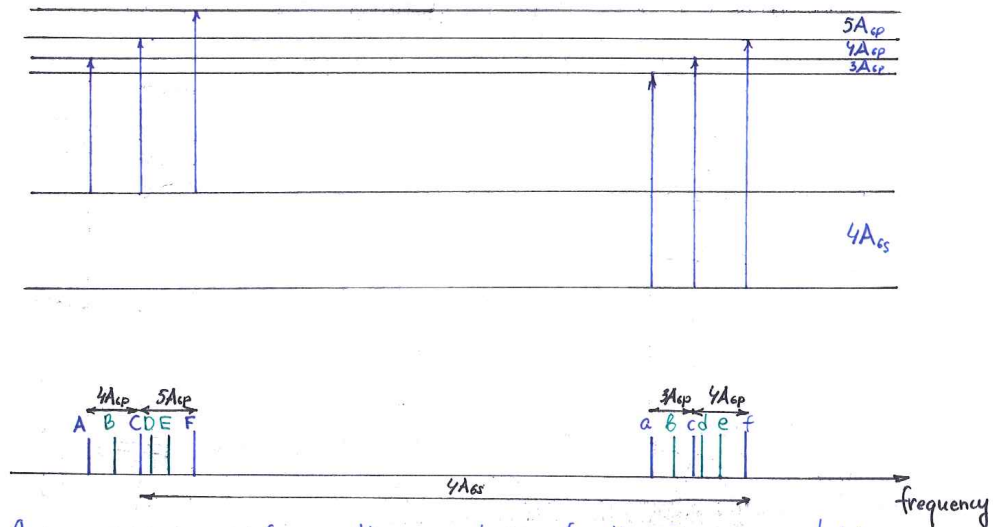


From interval rules ( $E_{F+1} - E_F = A(F+1)$ ) one can find energy splitting in terms of hyperfine constant A.

Electric dipole transitions:  $\Delta l = \pm 1$ ;  $\Delta F = \pm 1, 0$

There are 6 possible transitions according to selection rules

B.

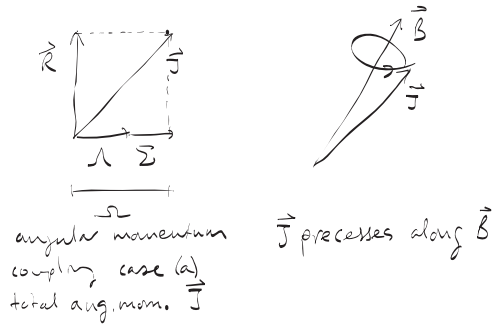


As we can see from the analysis of the frequency differences, B, D, E, B, d, e are cross-over resonances.

$$\left. \begin{aligned} f_C - f_A = f_F - f_C = 4A_{6P_{3/2}} &\Rightarrow A = \frac{1}{4} \cdot 201,5 = 50,4 \text{ MHz} \\ f_F - f_C = 5A_{6P_{3/2}} &\Rightarrow A = \frac{1}{5} \cdot 251,4 = 50,3 \text{ MHz} \\ f_C - f_A = 3A_{6P_{3/2}} &\Rightarrow A = \frac{1}{3} \cdot 151,5 = 50,5 \text{ MHz} \end{aligned} \right\} \Rightarrow A_{6P_{3/2}} = 50,4 \text{ MHz}$$

$$f_F - f_C = 4A_{6S_{1/2}} \Rightarrow A = \frac{1}{4} [(f_F - f_A) + (f_A - f_F) + (f_F - f_C)] = \frac{1}{4} (353 + 85,2 + 251,4) = 229,2 \text{ MHz}$$

FIGURE 6. The solution to the cross-over puzzle in Cs doppler-free spectroscopy



The magnetic moment along the molecular axis is  $\mu_z = (\Lambda + 2\Sigma) \mu_B$

factor 2 difference because of g-factors (gyromagnetic ratio)

Examples

state	magnetic moment
$^1\Sigma$	$\mu_m = 1 \mu_B$
$^3\Sigma$	$\mu_m = 2 \mu_B$
$2^1\Sigma_{3/2}$	$\mu_m = 2 \mu_B$
$2^1\Sigma_{1/2}$	$\mu_m = 0$ ( $m_L$ and $m_S$ opposite signs)

→ rotational molecule - no external field  
molecular axis ( $\hat{z}$ ) precesses around  $\vec{J}$

$$\langle M_J \rangle = \mu_B \cos(\angle \hat{z}, \vec{J}) = (\Lambda + 2\Sigma) \mu_B \frac{\Lambda + \Sigma}{\sqrt{J(J+1)}}$$

→ external field;  $\vec{J}$  precesses around  $\vec{B}$ ;  
time-averaged  $\mu_{eff}$  of a rotating mol in ext. field:

$$\mu_{eff} = \mu_B \cos(\angle \vec{B}, \vec{J}) = \frac{(\Lambda + 2\Sigma)(\Lambda + \Sigma)}{J(J+1)} \mu_B$$

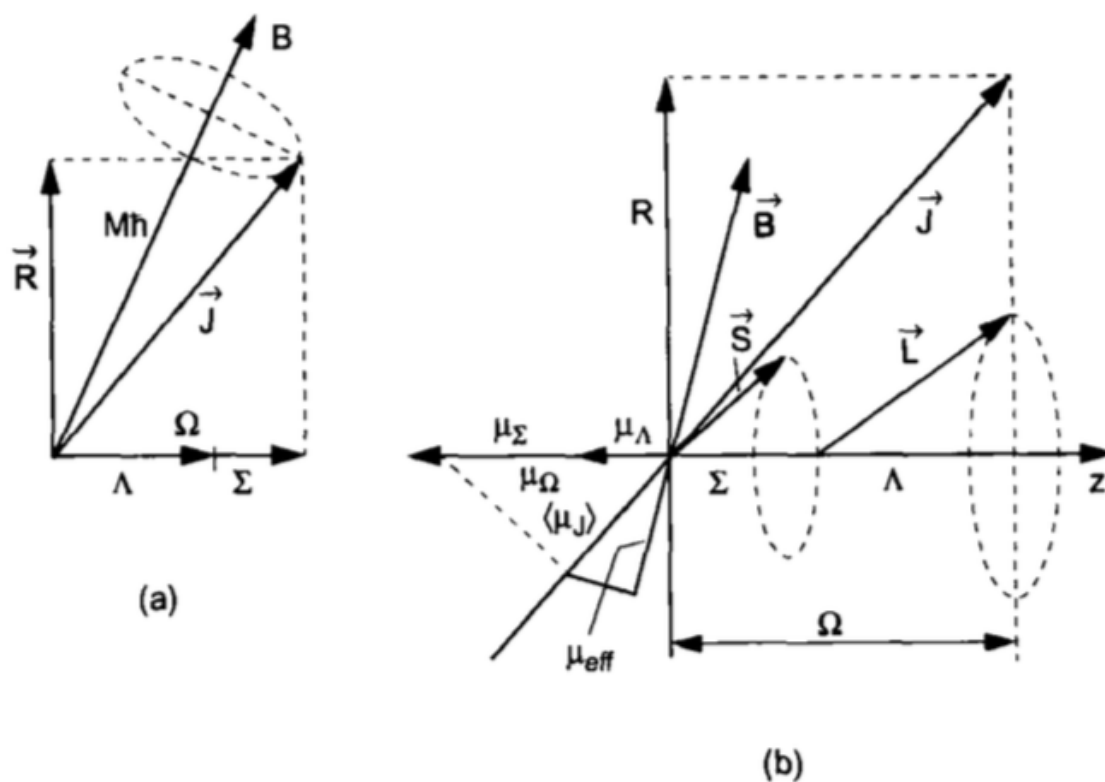
where  $M$  is the projection of  $J$  on  $B$ .

strongly dependent on  $J$ !

Energy:

$$E(J, B) = E_0 + \mu_{eff} \cdot B$$

FIGURE 7. Molecules in magnetic fields.



**Fig. 10.1** a) Coupling of angular momenta and b) coupling of magnetic moments with an external magnetic field in Hund's coupling case a).

FIGURE 8. Molecules in magnetic fields.