AtomsMoleculesExam2022 solutions

7 November 2022

1 Electronic, fine, and hyperfine structure (18 points)

1.1 A

Using the interval rule for fine structure we know that $\Delta E_{so} = E_J - E_{J-1} = J\beta$. See the figure for the level structure, the 7p level splits in a p1/2 and p3/2 and the energy difference is given by the difference of the 817.2 nm and 718.2 nm lines,

Thus,
$$\beta = \frac{2}{3} \cdot 1686.8cm^{-1} = 1125cm^{-1}.$$

1.2 B

For the size of the hyperfine splitting we can use the interval rule, but for the shift relative to the fine structure level, we need $E_{hfs} = \frac{A}{2}(F(F+1) - I(I+1) - J(J+1))$. This results in the level structure in the figure.

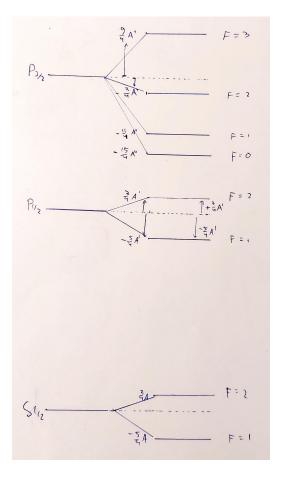


Figure 1: 1 A and B, Francium fine- and hyperfine structure

1.3 C

The difference between the two isotopes is a different dipole moment, which changes the size of A, and a different nuclear spin, which changes the F quantum numbers. With I=5 we get F=9/2 and F=11/2 for the s and p1/2,

and F=7/2, 9/2, 11/2, 13/2 for the p3/2. This also changes the size of the splitting. The student must provide a sketch of this difference.

2 2. Zeeman Effect

2.1 A

The sketch shows two hyperfine levels that split in 9 and 7 levels under the Zeeman effect, so this must be m_F levels corresponding the F=4 and F=3. The level is 6s so J=1/2. This gives a **nuclear spin of I=7/2** in order to give rise to these F=3,4 hyperfine levels.

2.2 B

See figure. In low field the lines can be classified by the m_F quantum numbers, and in high field by m_J , where the $m_J = -1/2$ are high-field seeking levels and the $m_J = 1/2$ are low-field seeking levels.

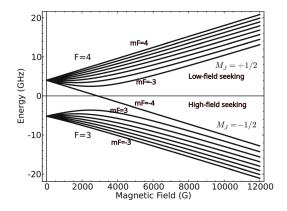


Figure 2: 1 A and B, Francium fine- and hyperfine structure

2.3 C

These specific m_F levels are used since they have the most negligible shift (at least to first-order Zeeman shift), making the clock more stable. See Fig's 6.13 and 6.14 in Foot.

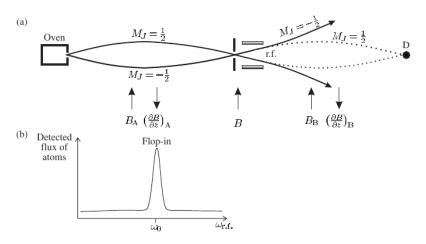


Fig. 6.15 (a) The trajectories of atoms in an atomic-beam apparatus similar to that shown in Fig. 6.14, but magnetic field gradients in the A and B regions have the same direction. Atoms only reach the detector if their M_J quantum number is changed in the C region by the interaction with radio-frequency radiation. This is known as the flop-in arrangement and gives a signal as in (b).

Figure 3: 1 A and B, Francium fine- and hyperfine structure

3 3. Doppler-free spectroscopy

3.1 A

The lifetime is 16 ns, so the natural linewidth is $1/\tau = 1/16$ ns = 63 MHz.

3.2 B

The FWHM Doppler width can be calculated by $\Delta f_D = 1.7 \frac{u}{\lambda}$ where u is the most probable velocity defined by $u = 2230ms^{-1} * \sqrt{\frac{T}{300K} \cdot \frac{1a.m.u.}{M}}$. The mass number of 23Na is 23, and we get for the velocity u = 465 m/s and the Doppler width at 589 nm $\Delta f_D = 1.7 \frac{u}{\lambda} = 789MHz$.

3.3 C

See figure.

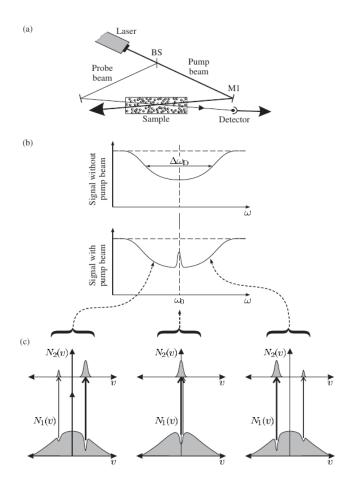


Figure 4: 3C - A saturated absorption spectroscopy experiment. The beam splitter BS, e.g. a piece of glass, divides the laser power between a weak probe and a stronger pump beam. The figure shows a finite angle of intersection between the weak probe beam and the stronger pump beam in the sample; this arrangement makes it straightforward to detect the probe beam after the cell but it leaves some residual Doppler broadening. Therefore saturated absorption experiments often have the pump and probe beams exactly counter-propagating and use a partially-reflecting mirror at M1 to transmit some of the probe beam to the detector (while still reflecting enough of the pump beam). (b) A plot of the probe intensity transmitted through the sample as a function of the laser frequency. With the pump beam a narrow peak appears at the atomic resonance frequency. (c) The population densities of the two levels N1 (v) and N2 (v) as a function of velocity for three different laser frequencies: below, equal to, and above the atomic resonance, showing the effect of the pump and probe beams.

4 4. Slowing and cooling with lasers

4.1 A

The scattering rate is $R_{scatt} = \Gamma \rho_{22}$. We know that $\rho_{22} = \frac{1-w}{2}$ and from the optical Bloch equations we can get w for maximum intensity $(\Omega \to \infty)$. In that case w $\to 0$. Therefore $\rho_{22}^{max_intensity} = 1/2$. We need one more step, from scattering rate R to the scattering force F. For each photon scattering we have a force equal to the photon momentum $\hbar k$. Thus we arrive at the maximum scattering force $F_{max} = \hbar k \Gamma/2$.

4.2 B

This was a tutorial question, copy-paste of the solution:

The faster an atom can scatter, the higher is the scattering rate and so it can lose energy faster. So, it determines the length of the Zeeman slower. The shape of the Zeeman slower depends on the velocity change.

$$v = v_0 - at \Rightarrow t = (v_0 - v)/a,$$

$$z = v_0 t - \frac{1}{2} a t^2,$$

$$= \frac{v_0 (v_0 - v)}{a} - \frac{a (v_0 - v)^2}{2a^2},$$

$$= \frac{v_0^2 - v^2}{2a}.$$

$$L = \frac{v_0^2}{2a}.$$

$$v = v_0 \sqrt{1 - z/L}.$$
(1)

If you do the deceleration faster than feasible by max acceleration the process will no longer be adiabatic and atoms will not follow the field gradient. This determines the maximum acceleration that you can apply to decelerate the atoms in the least possible time.

$$\hbar\omega(1 - v/c) = \hbar\omega_0 + \mu_B B(z)$$

$$B(z) = \frac{\hbar\omega - \hbar\omega_0}{\mu_B} + \frac{\hbar\omega}{\mu_B c} v(z),$$

$$\mu_B + \mu_B c^{*(z)},$$

$$= B_{bias} + \frac{\hbar \omega v_0}{\mu_B c} \sqrt{1 - z/L}.$$

So the maximum velocity that can be captured is determined by

$$B_0 = \frac{\hbar \omega v_0}{\mu_B c}$$

4.3 C

(Give at least 2 criteria, examples:) Suitable for laser cooling: transition frequency reachable by available lasers. Transition should be closed or easily repumped. Etc..

5 5 Molecules

5.1 A

$$H = -\frac{\hbar^{2}}{2M_{A}}\nabla_{A}^{2} - \frac{\hbar^{2}}{2M_{B}}\nabla_{B}^{2} + \frac{e^{2}}{4\pi\epsilon_{0}}\frac{2A2_{B}}{R_{AB}} - \frac{\hbar^{2}}{2m_{e}}\sum_{i}^{2}\nabla_{i}^{2} + \frac{e^{2}}{4\pi\epsilon_{0}}\left(\frac{1}{2}\sum_{i}\sum_{j\neq i}^{2}\frac{1}{r_{j}} - \sum_{i}^{2}\frac{2}{r_{B}} - \sum_{i}^{2}\frac{2}{r_{B}}\right)$$

$$+ \frac{1}{2M_{A}}\nabla_{A}^{2} - \frac{\hbar^{2}}{2M_{B}}\nabla_{B}^{2} + \frac{e^{2}}{4\pi\epsilon_{0}}\frac{2A2_{B}}{R_{AB}} - \frac{\hbar^{2}}{2m_{e}}\sum_{i}^{2}\nabla_{i}^{2} + \frac{e^{2}}{4\pi\epsilon_{0}}\left(\frac{1}{2}\sum_{i}\sum_{j\neq i}^{2}\frac{1}{r_{j}} - \sum_{i}^{2}\frac{2}{r_{B}} - \sum_{i}^{2}\frac{2}{r_{B}}\right)$$

$$+ \frac{1}{2M_{A}}\nabla_{A}^{2} - \frac{\hbar^{2}}{2M_{B}}\nabla_{B}^{2} + \frac{e^{2}}{4\pi\epsilon_{0}}\frac{2A2_{B}}{R_{AB}} - \frac{\hbar^{2}}{2m_{e}}\sum_{i}^{2}\nabla_{i}^{2} + \frac{e^{2}}{4\pi\epsilon_{0}}\left(\frac{1}{2}\sum_{i}\sum_{j\neq i}^{2}\frac{1}{r_{j}} - \sum_{i}^{2}\frac{2}{r_{B}}\right)$$

$$+ \frac{1}{2M_{A}}\nabla_{A}^{2} - \frac{\hbar^{2}}{2M_{B}}\nabla_{B}^{2} + \frac{e^{2}}{4\pi\epsilon_{0}}\frac{2A2_{B}}{R_{AB}} - \frac{\hbar^{2}}{2m_{e}}\sum_{i}^{2}\nabla_{i}^{2} + \frac{e^{2}}{4\pi\epsilon_{0}}\left(\frac{1}{2}\sum_{i}\sum_{j\neq i}^{2}\frac{1}{r_{j}} - \sum_{i}^{2}\frac{2}{r_{B}}\right)$$

$$+ \frac{1}{2M_{A}}\nabla_{A}^{2} - \frac{\hbar^{2}}{2M_{B}}\nabla_{B}^{2} + \frac{e^{2}}{4\pi\epsilon_{0}}\frac{2A2_{B}}{R_{AB}} - \frac{\hbar^{2}}{2m_{e}}\sum_{i}^{2}\nabla_{i}^{2} + \frac{e^{2}}{4\pi\epsilon_{0}}\left(\frac{1}{2}\sum_{i}\sum_{j\neq i}^{2}\frac{1}{r_{i}} - \sum_{i}^{2}\frac{2}{r_{B}}\right)$$

$$+ \frac{1}{2M_{A}}\nabla_{A}^{2} - \frac{\hbar^{2}}{2M_{B}}\nabla_{B}^{2} + \frac{e^{2}}{4\pi\epsilon_{0}}\frac{2A2_{B}}{R_{AB}} - \frac{\hbar^{2}}{2m_{e}}\sum_{i}^{2}\nabla_{i}^{2} + \frac{e^{2}}{4\pi\epsilon_{0}}\left(\frac{1}{2}\sum_{j\neq i}^{2}\frac{1}{r_{i}} - \sum_{i}^{2}\frac{2}{r_{B}}\right)$$

$$+ \frac{1}{2M_{A}}\nabla_{A}^{2} - \frac{\hbar^{2}}{2M_{B}}\nabla_{B}^{2} + \frac{e^{2}}{4\pi\epsilon_{0}}\frac{2A2_{B}}{R_{AB}} - \frac{\hbar^{2}}{2m_{e}}\sum_{i}^{2}\nabla_{i}^{2} + \frac{e^{2}}{4\pi\epsilon_{0}}\left(\frac{1}{2}\sum_{j\neq i}^{2}\frac{1}{r_{j}} - \sum_{i}^{2}\frac{2}{r_{B}}\right)$$

$$+ \frac{1}{2M_{A}}\nabla_{A}^{2} - \frac{\hbar^{2}}{2M_{B}}\nabla_{A}^{2} - \frac{\hbar^{2}}{2M_{B}}\nabla_{A}^$$

See figure 5.1. In this specific case, Za=20 and Zb=9, and the number of electrons should correspond to that.

5.2 B

The Born-Oppenheimer approximation separates the motion of the nuclei and the motion of the electrons, which relies on the fact that the mass of the nucleus is much larger than that of the electrons.

5.3 C

In the rigid rotor approximation the rotational level energies are $B_e J(J+1)$, while the nonrigid rotor includes terms to account for a change in R with $-D_e J^2 (J+1)^2$. See Figures 5 and 6.

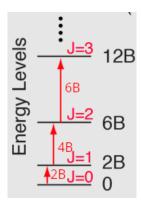


Figure 5: Rotational levels for a rigid rotor.

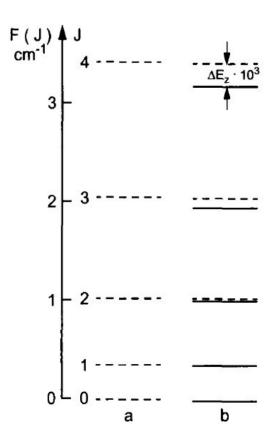


Figure 6: Deviation from rigid rotor (left) on the right.