

## Midterm quiz

### 1 Magnetic versus electric dipolar energy (10 pts.)

- a) By any method you like, e.g. considering kinetic and potential energy plus Heisenberg's uncertainty, find the Bohr radius  $a_0$  of hydrogen (assuming a fixed proton) in terms of the electron's mass  $m$  and charge  $e$ , and  $\hbar$ .
- b) Write down a typical "atomic value" for an electric dipole moment  $d$ .
- c) Find a typical "atomic" value for the electric field strength  $E$ .
- d) Considering the electron as a current loop of radius  $a_0$ , find a typical atomic value for the magnetic moment  $\mu$  (ignore numerical factors).
- e) Find the magnetic field strength  $B$  created by this current loop, again no prefactors required.
- f) Find the ratio of typical magnetic dipolar energy  $\mu B$  to electric dipolar energy  $dE$  in terms of the fine structure constant  $\alpha = e^2/\hbar c$  (in cgs units. SI will make your life harder).

### Solution

In this problem the numerical prefactors can be ignored. Only the powers of  $\alpha$  (the fine structure constant) matter. In the formulae using the SI system sometimes a factor of  $4\pi$  was left. This is to be able to use the substitution  $4\pi\epsilon_0 \rightarrow 1$  to convert from SI to CGS.

- a) We know from the virial theorem that  $\langle T \rangle \sim \langle V \rangle$  so  $\langle p^2/m \rangle \sim \langle e^2/a_0 \rangle_{\text{CGS}} \sim \langle e^2/(\epsilon_0 a_0) \rangle_{\text{SI}}$ . Combining this with the Heisenberg uncertainty principle ( $pa_0 \sim \hbar$ ) for a localized wavepacket we get

$$a_0 \sim \frac{\hbar^2}{me^2} \text{ (CGS)} \sim \frac{4\pi\epsilon_0\hbar^2}{me^2} \text{ (SI)}.$$

- b) The typical distance is the Bohr radius and the typical charge is the electron charge so

$$d \sim e a_0.$$

- c) From Gauss's theorem, the electric field of a charge  $e$  within a region of size  $a_0$  is

$$E \sim \frac{e}{a_0^2} \text{ (CGS)} \sim \frac{e}{4\pi\epsilon_0 a_0^2} \text{ (SI)}.$$

- d) Approximating the orbiting as a current loop one gets  $\mu \sim (IA/c)_{\text{CGS}} \sim (IA)_{\text{SI}}$ . Typical current is  $I \sim e\omega$  with either using  $\hbar\omega \sim (e^2/a_0)_{\text{CGS}} \sim (e^2/\varepsilon a_0)_{\text{SI}}$  or  $p \sim ma_0\omega$ . The typical area is  $a_0^2$ . After some algebra one gets

$$\mu \sim \frac{e\hbar}{mc} (\text{CGS}) \sim \frac{e\hbar}{m} (\text{SI}).$$

- e) Using Ampère's law for the magnetic field  $B \sim (I/ca_0)_{\text{CGS}} \sim (\mu_0 I/a_0)_{\text{SI}}$ . Using that  $c = 1/\sqrt{\varepsilon_0\mu_0}$  if using SI and after a few lines of algebra one gets

$$B \sim \frac{e^2}{\hbar c} \frac{e}{a_0^2} = \alpha E (\text{CGS}) \sim \frac{e^2}{4\pi\varepsilon_0\hbar c} \frac{e}{\varepsilon_0 a_0^2} = \alpha \frac{E}{c} (\text{SI}).$$

- f) Substituting the above results and working through the algebra yields

$$\frac{\mu B}{dE} \sim \alpha^2.$$

## 2 Fine structure in a magnetic field (20 pts)

An atom has orbital angular momentum  $L$ , spin angular momentum  $S$ , and no nuclear spin. The fine structure Hamiltonian is  $H_{\text{FS}} = A\mathbf{L} \cdot \mathbf{S}$ . It is interacting with a magnetic field according to the Zeeman Hamiltonian  $H_Z = -\mu_B (g_S \mathbf{S} + \mathbf{L}) \cdot \mathbf{B}$ . The total angular momentum is denoted  $\mathbf{J} = \mathbf{L} + \mathbf{S}$ .

- What are the “good” quantum numbers at low magnetic field ( $\mu_B B \ll A$ )?
- What are the “good” quantum numbers at high magnetic fields ( $\mu_B B \gg A$ )?
- What are the energy levels of the atom in zero magnetic field  $B = 0$ ?
- What are the energy levels at very high field?
- At low magnetic fields one observes a linear Zeeman effect whose description involves the Landé  $g$ -factor. Derive the Landé  $g$ -factor in terms of  $g_s$ ,  $S$ ,  $L$  and other good quantum number(s) at low field. In terms of  $g$ , and relevant quantum number(s), write down the expression for the Zeeman energies at low field.

## Solution

Throughout this problem one energy scale is much larger than the other and that should be considered first with the other being neglected or treated as a small perturbation. In real life the fine structure is in many cases much stronger than the Zeeman effect for alkali atoms. For example for potassium, the fine structure splitting is on the order of a THz which corresponds to  $10^6$  G or 100 T magnetic fields which is way far from attainable in an atomic physics lab. This is not the case when the Zeeman energy is compared to the hyperfine energy.

- As the system is symmetric for rotations about the magnetic field axis  $m_J$  is always a good quantum number. When the spin-orbit coupling dominates then  $J$ ,  $L$  and  $S$  are also conserved quantities therefore good quantum numbers.
- When the strong magnetic field sets the quantization axis, then  $L$  and  $S$  decouple and rotate around the  $\mathbf{B}$  field axis independently. Therefore the good quantum numbers are  $L$ ,  $S$ ,  $m_L$ ,  $m_S$ .  $m_J = m_L + m_S$  is still a good quantum number but it is redundant.
- The Hamiltonian can be written as  $\mathbf{A} \mathbf{L} \cdot \mathbf{S} = \frac{A}{2}(\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2) = \frac{A}{2}(J(J+1) - L(L+1) - S(S+1))$ . Here  $J$  runs between  $|L - S| \leq J \leq L + S$  and each  $J$  value has multiplicity of  $2J + 1$ .
- At very high field the Zeeman energy is  $-\mu_B(g_S m_S + m_L)B + A m_L m_S$ . The first term is the Zeeman energy, and the second is the first order perturbation correction due to the fine splitting. The vectors  $\mathbf{L}$  and  $\mathbf{S}$  rotate very fast around  $\mathbf{B}$  therefore the components in the vectors  $\mathbf{L}$  and  $\mathbf{S}$  perpendicular to  $\mathbf{B}$  average out to zero and only their projections to  $\mathbf{B}$  matter. Doing the math properly writing  $\mathbf{L} \cdot \mathbf{S}$  in terms of  $m_L, m_S$  and raising and lowering operators also gives this result in first order.
- Again the largest term in the Hamiltonian should be considered first which sets the appropriate basis to use. As  $L$  and  $S$  rotate rapidly around  $J$ , first they need to be projected to  $J$  and then to  $B$  when calculating the Zeeman energy. This gives

$$-\mu_B g_J m_J B = -\mu_B \left[ g_S \frac{(\mathbf{S} \cdot \mathbf{J})(\mathbf{J} \cdot \mathbf{B})}{|\mathbf{J}|^2} + \frac{(\mathbf{L} \cdot \mathbf{J})(\mathbf{J} \cdot \mathbf{B})}{|\mathbf{J}|^2} \right].$$

Using that  $\mathbf{J} \cdot \mathbf{B} = m_J$  and that  $\mathbf{S} \cdot \mathbf{J} = \mathbf{S} \cdot \mathbf{L} + \mathbf{S} \cdot \mathbf{S} = \mathbf{S} \cdot \mathbf{L} + |\mathbf{S}|^2$  one gets

$$\begin{aligned} g_J &= g_S \frac{(|\mathbf{J}|^2 + |\mathbf{S}|^2 - |\mathbf{L}|^2)}{2|\mathbf{J}|^2} + \frac{(|\mathbf{J}|^2 + |\mathbf{L}|^2 - |\mathbf{S}|^2)}{2|\mathbf{J}|^2} \\ &= g_S \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)} + \frac{J(J+1) + L(L+1) - S(S+1)}{2J(J+1)} \\ &= \frac{g_S + 1}{2} + \frac{g_S - 1}{2} \frac{S(S+1) - L(L+1)}{J(J+1)} \end{aligned}$$

### 3 Microwave dressing of molecules (20 pts)

The rotational Hamiltonian of a molecule is  $H = B\mathbf{J}^2$ , where  $B$  is the rotational constant. In the molecule frame, the “permanent” dipole moment of the molecule is  $d$ . We would like to induce a strong dipole moment in the lab frame, but instead of using a large static electric field we will use microwaves tuned to rotational transitions. For simplicity, we will consider  $\pi$ -polarized microwaves, i.e. the electric field will oscillate along the  $z$ -direction, our quantization axis. So the perturbation is

$$V = -\mathbf{d} \cdot \mathbf{E}(t) = -dE \cos \vartheta \cos(\omega t)$$

- a) Starting with the molecule in the rotational ground state  $|J=0, m_J=0\rangle$ , which excited state can the microwave reach and what is the resonant frequency  $\omega_0$  for this transition?
- b) Derive the coupling matrix element between  $|0,0\rangle \equiv |\downarrow\rangle$  and the excited state (denoted  $|\uparrow\rangle$ ). This can be written as  $\hbar\omega_R \cos \omega t$  with Rabi frequency  $\omega_R$  that you will find. Note that  $\cos \vartheta = \sqrt{\frac{4\pi}{3}} Y_{10}(\theta, \phi)$ .
- c) Using the rotating wave approximation, derive a time-independent  $2 \times 2$  Hamiltonian matrix describing the evolution in the presence of the microwave drive.
- d) Find the eigenstates (in the rotating frame, i.e. time-independent) in the case of a resonant drive  $\omega = \omega_0$ .
- e) Find the dipole moment in these two eigenstates.
- f) Starting in the state  $|0,0\rangle$ , sketch the dipole moment versus time. Choose a scale where  $dE$  is a good fraction of  $\omega_0$ , so that all relevant behavior is visible. At what times is the dipole moment at its largest magnitude? *Note: Just a proper sketch suffices, you don't need to give the wavefunction as a function of time, although you might want to write that down if you are stuck, and derive the dipole moment vs. time.*
- g) Instead of the behavior in f), we would like to find a microwave dressing scheme that smoothly “turns on” the molecule’s dipole moment permanently. Can you propose a method that achieves this? Is there an adiabaticity criterion you need to fulfill, and if so, what is it?

## Solution

- a) The selection rules set the possible final states for the given perturbation. The (MW) photon carries one  $\hbar$  angular momentum so it can only change the molecule  $J$  state by 1. One may also say that the given coupling Hamiltonian is a vector operator and according to the Wigner-Eckart theorem any transition can only have  $\Delta J = \pm 1$  ( $\Delta J = 0$  is forbidden due to parity) and there is no  $J < 0$  state so  $\Delta J = 1$ . As we are considering  $\pi$ -polarized drive in this problem, the  $m_J$  state cannot be changed so the only available state is  $|J = 1, m_J = 0\rangle$ . The resonance frequency is the energy difference of the states  $\hbar\omega_0 = \Delta E = B(1 \cdot (1 + 1) - 0) = 2B$ .

- b) It was given that  $\hbar\omega_R \cos \omega t = \langle \uparrow | V | \downarrow \rangle = \int d\Omega (-dE \cos \vartheta \cos \omega t) Y_{10}^*(\theta, \phi) Y_{00}(\theta, \phi)$ . One way to evaluate this is to use the given formula for  $\cos \vartheta$  and use that  $Y_{00}$  has to be  $1/\sqrt{4\pi}$  because of wavefunction normalization and that the  $Y_{J,m_J}$  functions are normalized. Then the above integral can be written as  $\int d\Omega (-dE \sqrt{4\pi/3} Y_{10}(\theta, \phi) \cos \omega t) Y_{10}^*(\theta, \phi) \sqrt{1/4\pi} = -dE/\sqrt{3} \cos \omega t$ . This gives the Rabi frequency

$$\hbar\omega_R = -dE/\sqrt{3}$$

- c) To move into the rotating frame the states are written as  $|\uparrow\rangle_{\text{rot}} = e^{-i\omega t/2} |\uparrow\rangle$  and  $|\downarrow\rangle_{\text{rot}} = e^{i\omega t/2} |\downarrow\rangle$ . Transforming the Hamiltonian gives an operator with a time independent part and fast oscillating terms with rate  $2\omega$ . In the rotating wave approximation the latter are neglected and we get

$$H_{\text{RWA}} = \frac{\hbar}{2} \begin{pmatrix} \omega - \omega_0 & \omega_R \\ \omega_R & -(\omega - \omega_0) \end{pmatrix}$$

- d) The eigenstates of a purely off diagonal 2x2 matrix (one proportional to the  $\sigma_x$  Pauli matrix) are

$$|\Psi_{\pm}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$$

- e) In the rotating frame  $\langle d \rangle = \langle \Psi_{\pm} | d_z | \Psi_{\pm} \rangle = \left( \frac{\langle \uparrow |_{\text{rot}} \pm \langle \downarrow |_{\text{rot}}}{\sqrt{2}} \right) d \cos \vartheta \left( \frac{|\uparrow\rangle_{\text{rot}} \pm |\downarrow\rangle_{\text{rot}}}{\sqrt{2}} \right) = \pm d/\sqrt{3}$ . Going back to the lab frame gives the  $|\uparrow\rangle / |\downarrow\rangle$  states  $e^{\pm i\omega t/2}$  prefactors in front of them which eventually gives  $\langle d \rangle_{\text{lab}} = \pm d/\sqrt{3} \cos \omega t$ .

- f) The coupling between the two states gives Rabi oscillations between the two molecular states with frequency  $\omega_R$ . This gives a  $\pm \sin \omega_R t$  envelope to the dipole moment. In the lab frame there is a fast  $\cos \omega t$  oscillation due to the energy splitting between the two bare states. So the dipole moment is

$$d(t) = \frac{d}{\sqrt{3}} \cos \omega_R t \cos \omega t.$$

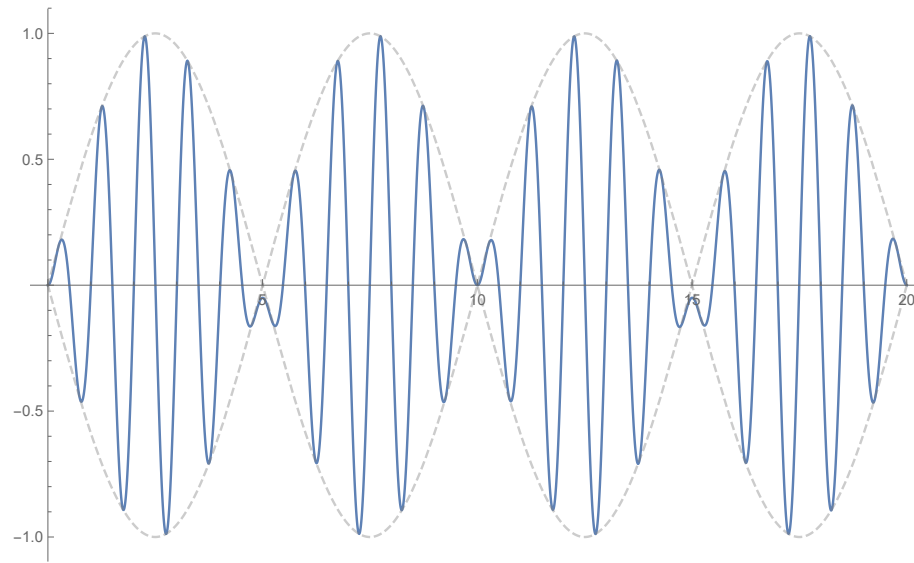


Figure 1: The molecule's dipole moment. The used parameters were  $\omega_0 = 2\pi$  and  $\omega_R = 2\pi \times 0.1$ .

See also Fig (1).

- g) Due to the energy splitting between the two molecular states there is no way to get rid of the fast  $\cos \omega t$  oscillations but the slow  $\cos \omega_R t$  oscillations can be eliminated by either turning off the drive after a  $\pi/2$  pulse or using a Landau-Zener sweep, stopped on resonance. The former requires a Rabi frequency and timing stability such that  $\delta \omega_R t \ll 1$  and  $\omega_R \delta t \ll 1$ . In the case of the Landau-Zener sweep the MW detuning is smoothly tuned from a large value to zero. This requires less precise control but more time,  $\dot{\omega} \ll \omega_R^2 \sim (dE)^2$ .