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# 1 Theory

To understand the function of an optical dipole-trap one has to understand how far detuned light, more specifically the electric field component, interacts with a neutral atom. There are several models providing different levels of accuracy for the respective application. The atom can be treated rather classically by regarding it as a harmonic oscillator driven by an electric field. It can be treated semiclassically by considering the quantum nature and structure of the atom while still approximating the incoming light as electromagnetic waves. In this model the problem can be solved in second-order perturbation theory. The third approach is treating the atom quantum mechanically as well as the light, now consisting of quantised photons interacting with the atom. For this thesis only the first two approaches are relevant.

## 1.1 The Hamiltonian

The problem of interaction between an atom, laser-light and in the case of this experiment also magnetic fields is represented by different parts in the total hamiltonian. The basis for all calculations is the atomic hamiltonian of the regarded Lithium-atoms  $H_A$ . The atom-light-interaction is represented by the Hamiltonian of the light itself  $H_L$  and the interaction Hamiltonian  $H_{AL}$  while the last contribution is the magnetic field Hamiltonian  $H_M$ .

$$H = H_A + H_L + H_{AL} + H_M \quad (1)$$

## 1.2 Lithium Level-structure

The atomic hamiltonian  $H_A$  corresponds to the energy of the atomic species that is used in our experiment, which is Lithium-6. Lithium is a fermionic alkali-metal, whose electronic structure is mostly dependent of its one valence electron [3]. In this approximation, the *central-field approximation*, the two other bound electrons on the most inner level only contribute to the central electric field, that is supposed to be spherically symmetric. Thus the calculation can follow the well understood model of hydrogen. The ansatz in this case is considering an electron with the reduced mass  $\mu$  in a coulomb-potential.

$$U(\mathbf{r}) = -\frac{e^2 Z}{4\pi\epsilon_0 r} \quad (2)$$

That leads to the Hamiltonian:

$$H_A = \frac{p^2}{2\mu} - \frac{e^2 Z}{4\pi\epsilon_0 r} \quad (3)$$

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Solving the Schrödinger-Equation considering this Hamiltonian leads to a set of wave-functions characterized by the quantum numbers  $N, L, m_L$ ,  $N$  being the main quantum number,  $L$  the angular momentum quantum number and  $m_L$  the projection onto the coordinate axis. The energy-levels for different  $L$  are degenerate, but when the spin of the valence electron is considered this degeneracy is broken and the coupling of this spin to the orbital angular momentum leads to the fine-structure picture in which  $J = l \pm S$  and  $m_J = J, J-1, \dots, -J+1, J$  are the respective quantum numbers. Nevertheless the real Lithium-atom has a substructure arising from interaction of the spin of the core with the angular momentum of the orbit. This effect results in the hyperfinestructure that breaks the degeneracy of the levels with same quantum number  $J$ . In the picture of hyperfinestructure the total angular momentum and the spin of the core  $I$  couple to the new total angular momentum  $F = J \pm I$  with their respective projections  $m_F = F, F-1, \dots, -F+1, F$  that result in a even finer splitting of the lines, and fully characterize a lithium-atom.

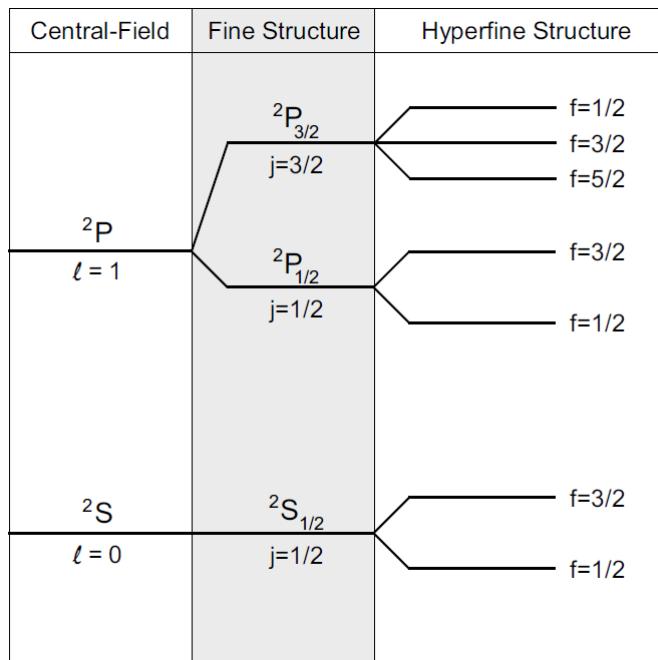


Figure 1.1: Extract of the level structure for Lithium-6 [3]

## 1.3 Magnetic Field

Within the experiment, the regarded atoms are exposed to strong magnetic fields. Therefore, additionally the Zeeman-Effect moves the respective levels contributing to the AC-Stark-Shift. In this approach we simply regard both effects as independent perturbations to the basic Hamiltonian. At strong magnetic fields, as used in the experiment, the Paschen-Back-Effect for hyperfine states dominates and instead of  $F$  and  $m_F$ , the quantum numbers  $J$  and  $m_J$  are still

“good“. Therefore the formula for the shift of each state is given by:

$$\Delta E = g_J m_J \hbar \gamma B \quad (4)$$

With  $\gamma = e/(2m_e)$  and  $g_J$  being the Landé-factor. The results are new values of energy-difference i.e. detuning for the respective transitions that now have a different contribution to the Ac-Stark-Effect.

## 1.4 AC-Stark-Shift

The AC-Stark-Shift arises from the interaction of electric fields with the regarded atom. Before treating this problem quantum-mechanically in terms of our Hamiltonian (1.1), we look at the problem in a classical model, that already results in a formula, that is very accurate in certain systems.

### 1.4.1 Lorentz Oscillator Model

Classically the problem of light-matter-interaction can be described in terms of an atomic dipole moment induced by an oscillating electric field, following [8]. The atom is hereby described as a damped harmonic oscillator driven by the field. Intuitively one can think of the electrons and the core being pulled away from each other by the electric force, resulting in an oscillation against each other. The potential arising from these conditions is the following<sup>1</sup>:

$$U = -\frac{1}{2} \langle \mathbf{p} \cdot \mathbf{E} \rangle \quad (5)$$

Here  $\mathbf{p}$  is the induced dipole moment,  $\mathbf{E}$  the electric field. The time-average is introduced since the electric field in an electro-magnetic wave is oscillating very fast and the atom “feels” an effective potential averaged over the oscillation. If we only consider the real part of  $\mathbf{p} \cdot \mathbf{E} \propto \cos^2$ , the time average is  $\langle \mathbf{p} \cdot \mathbf{E} \rangle = 1/2 \operatorname{Re}(\alpha) E^2$ . One can rewrite (5) in terms of the Intensity  $I = 1/2\epsilon_0 c E^2$ :

$$U = -\frac{1}{2\epsilon_0 c} \operatorname{Re}(\alpha) I \quad (6)$$

To calculate the exact potential one has to obtain a value for  $\alpha$ . In this classical description an electron is considered bound to the core elastically with the oscillation eigenfrequency  $\omega_0$

<sup>1</sup>The force on a dipole is given by [7]:

$$\mathbf{F} = (\mathbf{p} \cdot \nabla) \mathbf{E}$$

We know that the following holds:

$$\nabla(\mathbf{p} \cdot \mathbf{E}) = \mathbf{p} \times (\nabla \times \mathbf{E}) + \mathbf{E} \times (\nabla \times \mathbf{p}) + (\mathbf{p} \cdot \nabla) \mathbf{E} + (\mathbf{E} \cdot \nabla) \mathbf{p}$$

We consider the trap to consist of a retro-reflected laserbeam, that is in phase, so the B-field-component of the electromagnetic wave is considered to be 0 as well as  $\nabla \times \mathbf{E} = -\partial \mathbf{B}/\partial t = 0$ . In our case the dipole-moment is not constant but  $\mathbf{p} = \alpha \mathbf{E}$  and thus becomes:

$$\nabla(\mathbf{p} \cdot \mathbf{E}) = \alpha \mathbf{E} \times (\nabla \times \mathbf{E}) + \alpha \mathbf{E} \times (\nabla \times \mathbf{E}) + (\alpha \mathbf{E} \cdot \nabla) \mathbf{E} + \alpha (\mathbf{E} \cdot \nabla) \mathbf{E}$$

which becomes:

$$\begin{aligned} \nabla(\mathbf{p} \cdot \mathbf{E}) &= 2\alpha(\mathbf{E} \cdot \nabla) \mathbf{E} = 2(\mathbf{p} \cdot \nabla) \mathbf{E} \\ \Rightarrow \mathbf{F} &= \frac{1}{2} \nabla(\mathbf{p} \cdot \mathbf{E}) \end{aligned}$$

To get the corresponding potential one has to integrate the force. For a rapidly oscillating field we further have to take the time average to get an effective value for the trapping potential.

$$U = -\frac{1}{2} \langle \mathbf{p} \cdot \mathbf{E} \rangle$$

corresponding to the optical transition frequency. In our practical case that is the frequency of the Lithium-D2-Line. In a real atom, there are of course multiple resonances, corresponding to multiple states of the electron, thus this approximation yields only for certain cases in which the system can also be regarded as a quantummechanical two-state-system. We will later see, that while this approach leads to a very accurate calculation for the Lithium ground state, it can not at all be applied to the calculation of the trapping potential for the first excited state, since there exists no single dominant transition, but multiple resonances, all contributing to the respective energy-shift, in contrast to the groundstate.

The polarizability now can be calculated by solving the equation of motion of a driven and damped harmonic oscillator.

$$\ddot{x} + \Gamma_\omega \dot{x} + \omega_0^2 x = -\frac{eE(t)}{m_e} \quad (7)$$

for that the solution can be calculated using basic tools for differential-equation-solving. The result is then:

$$\alpha = \frac{e^2}{m_e} \frac{1}{\omega_0^2 - \omega^2 - i\omega\Gamma_\omega} \quad (8)$$

With

$$\Gamma_\omega = \frac{e^2\omega^2}{6\pi\epsilon_0 m_e c^3} \quad (9)$$

We can substitute  $e^2/m_e = 6\pi\epsilon_0 c^3 \Gamma_\omega / \omega^2$  and define the on-resonance damping rate  $\Gamma := (\omega_0/\omega)^2 \Gamma_\omega$  which results in the form:

$$\alpha = 6\pi\epsilon_0 c^3 \frac{\Gamma/\omega_0^2}{\omega_0^2 - \omega^2 - i(\omega^3/\omega_0^2)\Gamma} \quad (10)$$

We now can plug the real part of this expression in (5) and obtain the very known formula:

$$U_{dip}(\mathbf{r}) = -\frac{3\pi c^2}{2\omega_0^3} \left( \frac{\Gamma}{\omega_0 - \omega} + \frac{\Gamma}{\omega_0 + \omega} \right) I(\mathbf{r}) \quad (11)$$

In this case, the damping parameter  $\Gamma$  corresponds to the linewidth of the optical transition, which numerical value is  $\Gamma = 5.8724$  MHz for the considered D2-Line [3].

#### 1.4.2 Energy-Shift in Perturbation Theory

After this classical treatment, we come back to calculating the same effect quantum-mechanically. For calculating the energy-shift for the first excited state, this is the only way to get a trustworthy result since in contrast to the ground state of Lithium it can not be approximated by a two-level-system with only one transition. Therefore we have to solve the problem more precisely.

The interaction of the atom with laser-light is described by the two additional parts in the original hamiltonian (1.1)  $H_L + H_{AL}$ . The light-hamiltonian  $H_L$  is hereby negligible, because the regarded laser-light of the used dipole-trap is farly detuned from the relevant transition

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resonances. Therefore the only relevant part of this set of terms is the interaction-hamiltonian, which depends on the dipole-operator  $\mu$  and the electric-field-operator  $E$  and has the following form:  $H_{AL} = -\mu E = -erE$ . It can be treated as a small perturbation of the atomic hamiltonian, thus in the relevant second-order perturbation-theory the energy-shift is the following [8]:

$$\Delta W = \sum_{k \neq j} \frac{|\langle j | H_{AL} | k \rangle|^2}{W_k - W_j} \quad (12)$$

Although the hyperfine splitting is highly relevant for the experiment itself, it is sufficient for the calculation of the Stark-Shift to only consider the fine-structure regime. Aspecially at high-strength magnetic fields, the hyperfine Paschen-Back-Effect leads to degeneracy of the different hyperfine states and the total angular momentum  $J$  is a "good quantum-number" again. In the low-field-regime the corrections due to hyperfine-splitting are small, because of the little energy-differences compared to the relevant transitions between the levels in the fine-structure-regime and the considered large detuning of the dipole-trap-light. Hence also there this picture is sufficient. In this case (12) can be expressed in terms of  $J$  and  $m_J$  and with the explicit form of  $H_{AL}$  this becomes[5]:

$$\Delta W_{Jm_j} = -e^2 \sum_{K \neq J} \sum_{m_k} \frac{\langle Jm_J | \mathbf{r}E | Km_K \rangle \langle Km_K | \mathbf{r}E | Jm_J \rangle}{W_k - W_j} \mathbf{r}E \quad (13)$$

The main problem now is to calculate the coupling of different angular momenta. That is why most of the calculation is dedicated to simplify the calculation of all relevant Clebsch-Gordan coefficients.

We will now describe the electric field in terms of irreducible tensor operators:

$$E_{\pm} = \mp \frac{1}{2} \sqrt{2} (E_x \pm iE_y), \quad E_0 = E_z \quad (14)$$

$$r_{\pm} = \mp \frac{1}{2} \sqrt{2} (r_x \pm ir_y), \quad r_0 = r_z \quad (15)$$

$$(16)$$

In this notation we can rewrite (13) in terms of these operators:

$$\Delta W_{Jm_j} = -e^2 \sum_{K \neq J} \sum_{m_k} \sum_{\mu\nu} (-1)^{\mu+\nu} E_{\mu} E_{\nu} \frac{\langle Jm_J | r_{-\mu} | Km_K \rangle \langle Km_K | r_{-\nu} | Jm_J \rangle}{W_k - W_j} \quad (17)$$

With  $\mu = 0, \pm 1$ . Now, we define the following sum, that will be used later on. Note that is a simple shorting for simplification.

$$\mathcal{E}(L, m_L) := \text{sum}_{\mu\nu} \sqrt{2L+1} (-1)^{m_L} \begin{pmatrix} 1 & 1 & L \\ \mu & \nu & -m_L \end{pmatrix} E_{\mu} E_{\nu} \quad (18)$$

We here also use the Wigner 3-j-symbol-notation<sup>2</sup>. Therefore we can write the product in (17) in terms of this sum:

$$E_\mu E_\nu = \sum_{L=0}^2 \sum_{m_L=-L}^L \sqrt{2L+1}(-1)^{m_L} \begin{pmatrix} 1 & 1 & L \\ \mu & \nu & -m_L \end{pmatrix} \mathcal{E}(L, m_L) \quad (22)$$

For later-on simplification, we can calculate (18) explicitly for different combinations of  $L$  and  $m_L$ .

$$\begin{aligned} \mathcal{E}(0, 0) &= -\frac{1}{\sqrt{3}}(E_0^2 - 2E_{-1}E_1) = -\frac{1}{\sqrt{3}}(E_z^2 - 2(-\frac{1}{2}(E_x + iE_y)(E_x + iE_y))) \\ &= -\frac{1}{\sqrt{3}}(E_z^2 + E_x^2 + E_y^2) = -\frac{1}{\sqrt{3}}E^2 \end{aligned}$$

$$\mathcal{E}(1, \pm 1) = 0$$

$$\mathcal{E}(1, 0) = 0$$

$$\mathcal{E}(2, \pm 2) = E_{\pm 1}^2 = \frac{1}{2}(E_x \pm iE_y)^2$$

$$\mathcal{E}(2, \pm 1) = (E_x \pm iE_y)E_z$$

$$\begin{aligned} \mathcal{E}(2, 0) &= \sqrt{\frac{2}{3}}(E_0^2 + E_{-1}E_1) = \sqrt{\frac{2}{3}}(E_z^2 + \frac{1}{2}E_x^2 - \frac{1}{2}E_y^2 - \frac{1}{2}(E_x^2 + E_y^2)) \\ &= \frac{1}{\sqrt{6}}(3E_z^2 - E^2) \end{aligned}$$

After finishing that horrible calculation, the next step is to evaluate the sum in (17), which is even more terrifying, as you can imagine!

The first step is to evaluate the inner part, that is the summation over the respective magnetic quantum numbers  $m_J$ . Thus we give it an own name and define:

$$\mathcal{S}(J, m_J) = \sum_{m_k} \sum_{\mu\nu} (-1)^{\mu+\nu} E_\mu E_\nu \langle Jm_J | r_{-\mu} | Km_K \rangle \langle Km_K | r_{-\nu} | Jm_J \rangle \quad (23)$$

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<sup>2</sup>The Wigner 3-j symbol and 6-j symbol are definded in terms of Clebsch-Gordan-Coefficients:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} := \frac{(-1)^{j_1-j_2-m_3}}{\sqrt{2j_3+1}} \langle j_1 m_1 j_2 m_2 | j_3 - m_3 \rangle \quad (19)$$

$$\left\{ \begin{matrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{matrix} \right\} := \sum_{m_j}^6 (-1)^{\sum_{k=1}^6 (j_k - m_k)} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_5 & j_6 \\ -m_1 & m_5 & m_6 \end{pmatrix} \quad (20)$$

$$\times \begin{pmatrix} j_4 & j_5 & j_3 \\ m_4 & -m_5 & m_3 \end{pmatrix} \begin{pmatrix} j_4 & j_2 & j_6 \\ -m_4 & -m_2 & -m_6 \end{pmatrix} \quad (21)$$

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The matrix elements can be calculated using the Wigner-Eckart theorem<sup>3</sup>.

$$\begin{aligned} \mathcal{S}(J, m_J) = & (-1)^{J-K} |\langle J || r || K \rangle|^2 \times \\ & \sum_L \sqrt{2L+1} \sum_{m_L} \mathcal{E}(L, m_L) \sum_{\mu\nu} (-1)^{\mu+\nu} (-1)^{m_L} \begin{pmatrix} 1 & 1 & L \\ \mu & \nu & -m_L \end{pmatrix} \times \\ & \sum_{m_K} \left[ (-1)^{J-m_J} \begin{pmatrix} J & 1 & K \\ -m_J & -\mu & m_K \end{pmatrix} (-1)^{K-m_K} \begin{pmatrix} K & 1 & J \\ -m_K & -\nu & m_J \end{pmatrix} \right] \quad (26) \end{aligned}$$

Note, that the first part of this term can be written in this way because using the Wigner-Eckert theorem the tensor operator in the matrix element now has become the normal spherical coordinate-operator in the respective reduced matrix element, which of course is hermitian. The sum over  $\mu, \nu$  and  $m_K$  can be evaluated and rewritten in terms of the 6-j symbol.

$$\begin{aligned} & \sum_{\mu\nu} (-1)^{\mu+\nu} (-1)^{m_L} \begin{pmatrix} 1 & 1 & L \\ \mu & \nu & -m_L \end{pmatrix} \times \\ & \sum_{m_K} \left[ (-1)^{J-m_J} \begin{pmatrix} J & 1 & K \\ -m_J & -\mu & m_K \end{pmatrix} (-1)^{K-m_K} \begin{pmatrix} K & 1 & J \\ -m_K & -\nu & m_J \end{pmatrix} \right] \\ & = (-1)^{2J} (-1)^{J-m_J} \begin{pmatrix} J & L & J \\ -m_J & 0 & m_J \end{pmatrix} \left\{ \begin{matrix} J & 1 & K \\ 1 & K & L \end{matrix} \right\} \delta_{m_L, 0} \quad (27) \end{aligned}$$

This, together with the values for  $\mathcal{E}(L, m_L)$ , leads to the fact, that only terms with  $L = 0, 2$  and  $m_L = 0$  remain and the following holds:

$$\begin{aligned} \mathcal{S}(J, m_J) = & (-1)^{J-K} |\langle J || r || K \rangle|^2 \times \\ & \sum_L \mathcal{E}(L, 0) \sqrt{2L+1} (-1)^{J-m_J} \begin{pmatrix} J & L & J \\ -m_J & 0 & m_J \end{pmatrix} \left\{ \begin{matrix} J & 1 & K \\ 1 & K & L \end{matrix} \right\} \quad (28) \end{aligned}$$

Now, we arrive at the point, where we can go back to evaluating (13). The finding in (28) means, that we can decompose  $\Delta W_{Jm_J}$  into a sum over different  $L$ :

$$\Delta W_{Jm_J} = \sum_L \Delta W_{Jm_J}^L \quad (29)$$

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<sup>3</sup>The Wigner-Eckart theorem simplifies the calculation of matrix-elements in a spherical basis and breaks it down to the calculation of few reduced matrix elements. For an irreducible tensor-operator  $T_q^r$  between two angular-momentum eigen-states the following holds [4, p. 17]:

$$\langle j, m_j | T_q^r | k, m_k \rangle = \langle j || T^r || k \rangle C_{rqkm_k}^{jm_j} \quad (24)$$

In this formula  $r$  denotes the rank of the tensor, and  $q$  is simply the respective component of the tensor. Writing this in terms of the 3-j symbols yields:

$$\langle j, m_j | T_q^r | k, m_k \rangle = (-1)^{j-m_j} \begin{pmatrix} j & r & k \\ -m_j & q & m_k \end{pmatrix} \langle j || T^r || k \rangle \quad (25)$$

The resulting reduced matrix elements are independent of the respective component of the operator and the  $m$ -quantum-number. Therefore for every pair of angular-momentum quantum numbers  $j$  and  $k$  only one reduced matrix element has to be calculated to evaluate all elements of eigenstates involving said angular momenta.

in which each of the components can be written, using the form of (28).

$$\begin{aligned}\Delta W_{Jm_J}^L &= -e^2 \sum_{K \neq J} \frac{\langle J||r||K\rangle|^2}{W_K - W_J} \mathcal{E}(L, 0) \sqrt{2L+1} \\ &\quad (-1)^{J+K} (-1)^{J-m_J} \begin{pmatrix} J & L & J \\ -m_J & 0 & m_J \end{pmatrix} \begin{Bmatrix} J & 1 & K \\ 1 & K & L \end{Bmatrix}\end{aligned}\quad (30)$$

For this equation we can analyse the only two different cases, namely for  $L = 0, 2$ . If we evaluate both components and use the values vor  $\mathcal{E}(1, 0)$  and  $\mathcal{E}(1, 0)$ , we get to the both contributions to the energy-shift:

$$\Delta W_{Jm_J}^0 = -e^2 E^2 \frac{1}{3(2J+1)} \sum_{K \neq J} \frac{\langle J||r||K\rangle|^2}{W_K - W_J} \quad (31)$$

$$\begin{aligned}\Delta W_{Jm_J}^2 &= -e^2 (3E_z^2 - E^2) \sqrt{\frac{5J(2J-1)}{6(2J+3)(J+1)(2J+1)}} \times \\ &\quad \frac{3m_J^2 - J(J+1)}{J(2J-1)} \sum_{K \neq J} (-1)^{J+K} \begin{Bmatrix} J & 1 & K \\ 1 & J & 2 \end{Bmatrix} \frac{\langle J||r||K\rangle|^2}{W_K - W_J}\end{aligned}\quad (32)$$

We now chose the electric field to be directed along the z-axis:  $\mathbf{E} = E\hat{z}$  so we can say, that  $E_z^2 = E^2$ . Thus follows:

$$\begin{aligned}\Delta W_{Jm_J}^2 &= -\frac{1}{2} e^2 E^2 4C \times \\ &\quad \frac{3m_J^2 - J(J+1)}{J(2J-1)} \sum_{K \neq J} (-1)^{J+K} \begin{Bmatrix} J & 1 & K \\ 1 & J & 2 \end{Bmatrix} \frac{\langle J||r||K\rangle|^2}{W_K - W_J}\end{aligned}\quad (33)$$

We are hereby shortening  $C := \sqrt{5J(2J-1)/6(2J+3)(J+1)(2J+1)}$ . Note, that if the z-direction also defines the quantisation axis in a magnetic field, this means assuming  $\pi$ -polarized laser-light. If the light is then supposed to be  $\sigma$ -polarized, the z-component has to be considered individually and it holds  $E_z^2 = 1/2 E^2$ . We now draw an analogy to the classical calculation and link the total energy-shift to the dipole potential by defining a polarizability, composed of the now defined scalar and tensor polarizability.

$$\alpha := e^2 \left[ \alpha_J^0 + \frac{3m_J^2 - J(J+1)}{J(2J-1)} \alpha_J^2 \right] \quad (34)$$

$$\alpha_J^0 = \frac{2}{3(2J+1)} \sum_{K \neq J} \frac{|\langle J||r||K\rangle|^2}{W_K - W_J} \quad (35)$$

$$\alpha_J^2 = 4C \sum_{K \neq J} (-1)^{J+K} \begin{Bmatrix} J & 1 & K \\ 1 & J & 2 \end{Bmatrix} \frac{|\langle J||r||K\rangle|^2}{W_K - W_J} \quad (36)$$

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An additional factor has to be multiplied in analogy to the classical formula. The electric field is oscillating and the average thus results in a factor of  $1/2$ , because we did not take the time into account, when calculating the polarizability.

$$\begin{aligned} U &= -\frac{1}{2}\alpha E^2 \\ U &= -\frac{1}{4}e^2 \left[ \alpha_J^0 + \frac{2m_J^2 - J(J+1)}{J(2J-1)} \alpha_J^2 \right] E^2 \end{aligned} \quad (37)$$

## 1.5 Dipole Traps

The AC-Stark-Shift, as described above can, as stated in the beginning, be used to trap neutral atoms. We so far have seen, that an electric field induces a dipole moment in the atom that leads to a dipole-potential. The resulting force is proportional to the gradient of the intensity-distribution around the atom, therefore to understand how a dipole trap works exactly, one has to study the properties of the applied laser-beams.

## 2 Calculation of the AC-Stark-Shift

The calculation of the AC-Stark-Shift is done, using the formulas resulting from perturbation theory, as carried out in the previous sections. The first part of this chapter reviews the main results regarding the polarizabilities of the ground and first excited state. This will reveal also whether the excited state can also be trapped in the high intensity region of the lasers and how the trapping compares to that of the ground state. All calculations use the computer algebra system mathematica.

For the measurement, testing the theoretical foundation, that is presented in this thesis, concrete shift calculations are made regarding the big, crossed dipole trap. At the end of this section, values for the small microtrap will be presented, that will suggest, in how far the goal of imaging atoms in small traps and single sites of optical lattices can be managed. The magnetic field, and thus the quantisation axis is defined to be along the z-direction.

### 2.1 Polarizability

For the calculation of the polarizabilities for the respective states, the geometry and power of the used laser-beams are not important, since it only depends on the wavelength of the incoming light and on its polarization, that has a notable role for the tensor-polarizability in the vicinity of a transition resonance and renders unimportant, when using very far detuned trap-light. Before talking about concrete results, we recall the formulas given in the theory-section.

$$\alpha = \left[ \alpha_J^0 + \frac{3m_J^2 - J(J+1)}{J(2J-1)} \alpha_J^2 \right] \quad (38)$$

$$\begin{aligned} \alpha_J^0 &= \frac{2}{3(2J+1)} \sum_{K \neq J} \frac{|\langle J|r||K\rangle|^2}{W_K - W_J} \\ \alpha_J^2 &= 4C \sum_{K \neq J} (-1)^{J+K} \begin{Bmatrix} J & 1 & K \\ 1 & J & 2 \end{Bmatrix} \frac{|\langle J|r||K\rangle|^2}{W_K - W_J} \end{aligned}$$

Following [6], the polarizability is calculated using atomic units (a.u.). For the calculation transitions up to  $n = 7$  were considered. The respective dipole-transition matrix elements are listed below, together with the energy-differences between the levels.

Transition	Matrix-element [ a.u.]	Resonance [ nm]
$2s_{1/2} - 2p_{1/2}$	3.3169	670.791
$2s_{1/2} - 2p_{3/2}$	4.6909	670.776
$2s_{1/2} - 3p_{1/2}$	0.183	323.2657
$2s_{1/2} - 3p_{3/2}$	0.259	323.2657
$2s_{1/2} - 4p_{1/2}$	0.160	274.1203
$2s_{1/2} - 4p_{3/2}$	0.226	274.1203
$2s_{1/2} - 5p_{1/2}$	0.1198	256.2312
$2s_{1/2} - 5p_{3/2}$	0.169	256.2312
$2s_{1/2} - 6p_{1/2}$	0.0925	247.5061
$2s_{1/2} - 6p_{3/2}$	0.131	247.5061
$2s_{1/2} - 7p_{1/2}$	0.0737	242.5426
$2s_{1/2} - 7p_{3/2}$	0.1042	242.5426
$2p_{1/2} - 3s_{1/2}$	3.4403	812.645
$2p_{1/2} - 4s_{1/2}$	0.9167	497.175
$2p_{1/2} - 5s_{1/2}$	0.4929	427.313
$2p_{1/2} - 6s_{1/2}$	0.3268	398.554
$2p_{1/2} - 7s_{1/2}$	0.2397	383.564
$2p_{1/2} - 3d_{3/2}$	2.2658	610.366
$2p_{1/2} - 3d_{5/2}$	6.7975	670.776
$2p_{1/2} - 4d_{3/2}$	0.8627	460.283
$2p_{1/2} - 4d_{5/2}$	2.5882	460.289
$2p_{1/2} - 5d_{3/2}$	0.5015	413.262
$2p_{1/2} - 5d_{5/2}$	1.5045	413.262
$2p_{1/2} - 6d_{3/2}$	0.3435	391.535
$2p_{1/2} - 6d_{5/2}$	1.0306	391.535
$2p_{1/2} - 7d_{3/2}$	0.2565	379.507
$2p_{1/2} - 7d_{5/2}$	0.7696	379.507

Figure 2.1: Reduced Dipole-Transition-Matrix-Elements [6] in a.u. and the respective detuning [1], i.e. the resonance-energy for the relevant levels:  $1s_2 2s_{1/2}$  and  $1s_2 2p_{3/2}$

Figure 2.2 shows how the polarizability behaves for different levels and different wavelength of the incoming laser-light. In this case,  $\pi$ -polarized light is assumed. The qualitative behaviour does not change due to different polarizations, only the magnitude of the tensor polarizability. The differences in the practical case of our experiment will be discussed later on.

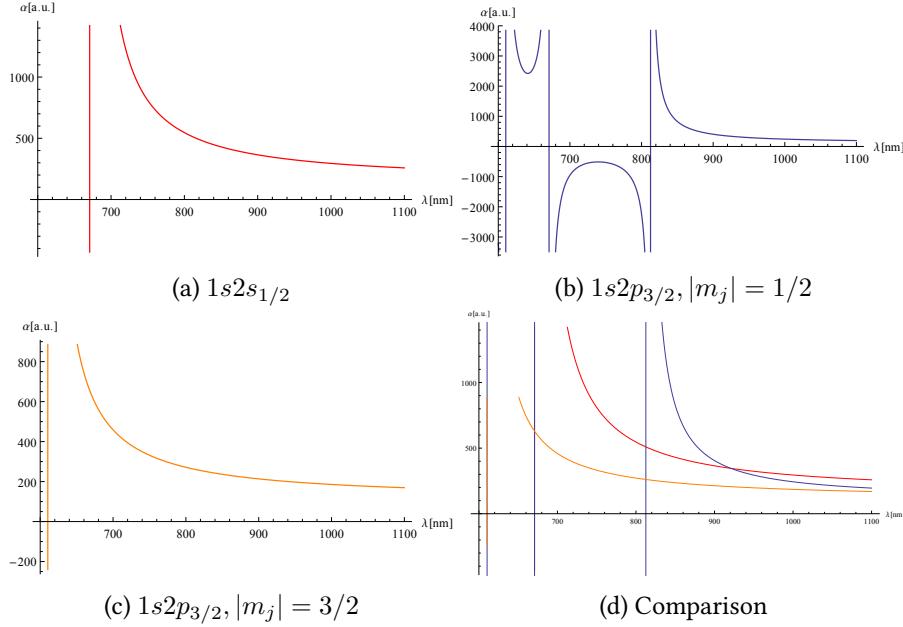


Figure 2.2: Polarizability  $\alpha$  for the states  $1s2s_{1/2}$  (red),  $1s2p_{3/2}, |m_j| = 1/2$  (blue) and  $1s2p_{3/2}, |m_j| = 3/2$  (orange)

What can be seen in the plots are some interesting properties. The first important result is, that, considering a far detuned light-source, the ground state, as well as the excited state show positive polarizabilities. This fundamentally contradicts the picture of a two-level system, for example described in [2]. In this model, the excited state will be shifted in opposition to the ground state, i.e. the relative sign in the polarizability flips. This reflects the fact, that in a real atom, especially in the excited states of Lithium, the structure is much more complicated, than what results from the two-level approximation, because many different levels are roughly in the same energy-range and no single transition dominates. Practically this results in the fact, that both the ground-state and the first excited states can be trapped in the same type of dipole-trap, because the positive polarizability results in a negative potential. Therefore the atoms are attracted to the highest intensity of the laser-beam. The difference lies in the exact values. For farly detuned light, i.e. above around 1000 nm of wavelength, the ground state shows a higher polarizability, than both excited states, which means, that the potential is deeper for the ground state. From figure can be seen, how the different excited states behave relative to the ground state for the both relevant laser-wavelength for the big and the small dipole-trap in the experiment. As one could expect the difference in the regime of farly detuned light is negligible.

The picture looks different, when cosidering higher frequencies. There, the picture looks different, especially when comparing the two excited states with different magnetic quantum number. Below around 900 nm and  $m_j = 3/2$  the absolute value of the polarizability is much higher than for both other states. Mathematically this can easiest be seen, when looking at the formula for the total polarizability. The tensor-part of this formula is multiplied by a factor, that is -1 or +1, depending on whether  $|m_j| = 1/2$  or  $|m_j| = 3/2$ . This means, that it decides

## 2 Calculation of the AC-Stark-Shift

State	$\alpha$ at 1070 nm [ $\alpha_{\text{ground}}$ ]	$\alpha$ at 1064 nm [ $\alpha_{\text{ground}}$ ]
$2p_{3/2},  m_j  = 1/2$	0.7694	0.7726
$2p_{3/2},  m_j  = 3/2$	0.6487	0.6472

Figure 2.3: Polarizabilities of the excited states for the relevant laser-wavelengths, in relation to the ground state polarizability.

whether the tensor part is added or subtracted, when calculating the total value. If it is subtracted, in case of  $|m_j| = 3/2$ , in the vicinity of many resonances, the diverging terms will cancel each other out and instead of a singularity a finite value is the result.

This does not mean, that one state can be trapped easier. When using laser-light, that is not far detuned from the respective resonances absorbtion effects cause the light to transfer momentum onto the atoms, that thus will heat up and the overall force field is no longer conservative. However using this effects in special settings can also result in effective trapping and cooling techniques. An optical molasse for example uses a standing wave of circular polarized laser-beams, so that the electric field and thus the polarizability and the respective light-shift are spacially dependent. Using the fact, that for different  $m_J$ -levels the light shift is different, one can tune the different beams such that after an absorbtion cycle the atoms decay into lower  $m_J$ -states and thus lose energy and cool down. In an optical dipole trap however, absorbtion is an unwanted heating-effect and therefore it is most efficient, when using laser-light farly detuned from the resonances. In this regime, all magnetic sublevels strive towards the same vale of polarizability, only depending on the scalar part, that is isotropic and does not depend on the light-polarization.

### 2.1.1 Convergence for the calculation

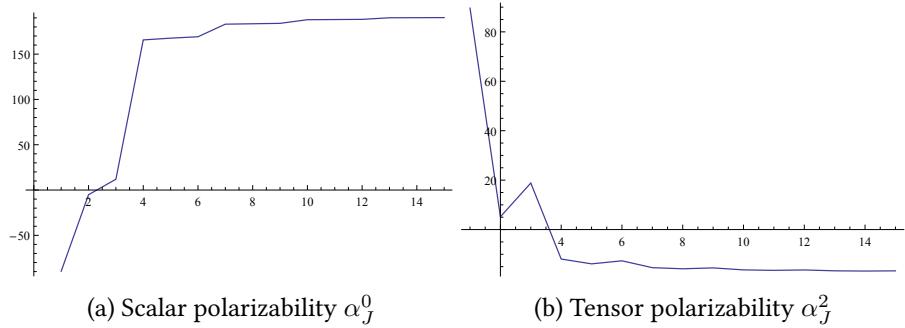


Figure 2.4: Convergence of the polarizability value for the excited state  $1s2p_{3/2}, |m_j| = 3/2$  at 1070 nm.

Another interesing question is, how far one has to go in calculating the energy shift in this

perturbation framework to get a good approximation of the actual value. The maximum accuracy, as written above, was considering levels up to  $n = 7$ . Figure (2.4) shows how the value of  $\alpha$  changes when considering higher levels. The x-coordinate is simply the index of the states, counted from low to high detuning. That means, that the most fundamental changes happen when considering states up to  $n = 3$ . Taking the states above into account

## 2.2 Trap Depth

We shall now calculate the trap depth and the differential light shift, that can be measured in the experiment. Since the ground state and the first excited states have different polarizabilities, also the light shift is varying. That means, that the energy-difference between the two states changes in case of incoming trap-light and as a result the resonance-frequency of the transition shifts, which can be much easier measured than the actual depth of the trap. Although the crossed dipole-trap is not a single beam, the beam profile in the middle, where the intensity is at its maximum, is gaussian. That means, that like for a normal gaussian beam, the trap is characterized by its beam-power and its waist. The power in this case is two times the power leaving the laser, since it gets reflected and forms the second beam as well. The waist in this case is  $40 \mu\text{m}$ , with an error estimated to be around 5%. The experiment will later be performed at multiple powers, that have a much higher accuracy with an error, being roughly 0.1%.

### 2.2.1 Magnetic Field

As stated in the theory-section, the magnetic field shifts the different levels, depending on their respective angular momentum and magnetic quantum numbers. This results in different values for the detuning, that determines the polarizability. However, at 527 G, that is a high field in the framework of the experiment, the shifts due to the Zeeman-effect are very small and the overall change in the resonance is orders of magnitude below the error in predicting the differential light shift altogether. This is an important result, thus it tells us, that in cold atom experiments, where different values of magnetic field from weak to strong are used to tune the respective interaction strength, the trapping efficiency is nearly independent from such tunings.

## 2.3 Using the measurement to calculate trap depth

The trap depth is a parameter, that is not easy to measure exactly but can be a quantity, that is important to know. If the measurement of the differential light shift through some sort of imaging is possible one can use this to estimate the overall depth of the trap for the respective ground and excited states.

## 2.4 Comparison to the classical formula

Since the classical formula in (11) is widely used to calculate depths for optical dipole traps it is interesting to see, in how far it differs from the quantum-mechanical approach. For the excited state, for allready stated reasons, it is not possible to calculate a good value using this approach,

## *2 Calculation of the AC-Stark-Shift*

but the ground state, for that the coupling to other states is dominated by the transition to the first excited state, the formula gives values, that differ only 3.99 % when calculating the shift considering transitions up to  $n = 7$  and using 1070 nm light. When only considering the D-Line transition, both values are the same in range of about 0.01 %. That shows, that using the approach of a harmonic oscillator to model the dipole-trap potential gives good results, when dealing with a system that can be approximated to only consist of two states. In the case of the Lithium-6 ground state, where for infrared light and higher excited states the transitions are very farly detuned, the model gives a good estimate, that is less complicated to calculate than the approach of perturbation theory.

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