

Calculation of Magic Wavelengths of Calcium⁺ and the Trap Depth of Rydberg States of Calcium

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Abstract

In this semester project we expand an existing atomic properties python library by implementing the calculation of the polarizability and the magic wavelength of atomic states. To test the library, we calculate the polarizability of the $4s\ ^2S_{1/2}$, $4p\ ^2P_{1/2,3/2}$ and $3d\ ^2D_{3/2,5/2}$ states of Ca^+ when exposed to a linearly and circularly polarized laser field. We present the obtained magic wavelengths of the $4s\ ^2S_{1/2} \leftrightarrow 3d\ ^2D_{3/2,5/2}$ transitions and compare them to literature values. The polarizability as a function of the wavelength of the laser field shows the expected behaviour. We find magic wavelengths that closely match the literature values with only small misalignment. This is mainly due to the limited set of atomic transitions available to calculate the polarizability. We use the Alkali-Rydberg-Calculator python library to calculate the trap depth of Ca in $4s\ ns\ ^3S_1$ Rydberg states by adding the ponderomotive potential experienced by the outer electron to the trap depth of the Ca^+ core. We see that this approximation is problematic for states with low principle quantum number n . The trap depth as a function of n shows a discontinuity at $n = 97$, which we can not explain.

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1 Introduction

The development of the optical tweezer has allowed researchers to manipulate and observe single atoms in a controlled environment. The optical trapping technique has essential applications in quantum computing and quantum simulation. Recently, several groups have advanced the neutral Rydberg atoms trapped in optical tweezers as a promising platform for realizing scalable and universal quantum computers [1] as they provide flexible experimental geometries, large system sizes, very good coherence, and strong interactions [2]. Furthermore, optical tweezers provide excellent single-atom control and can produce defect-free atomic arrays [3].

Leveraging the atomic interaction via Rydberg states for quantum computation purposes requires a superposition of two atomic states. It is an essential task to realize a setup that allows one to trap and control the atoms in either state [4]. The optical tweezer can be tuned to a wavelength at which the atomic states have the same polarizability and experience the same trapping potential. This prevents unwanted effects like heating and decoherence[5]. This wavelength is referred to as the *magic wavelength*.

In this semester project, we are interested in testing and expanding an existing python library to reliably calculate the polarizability of atoms in an external laser field. This is a crucial step to finding the magic wavelength of the optical tweezers that can trap the atom both in its ground state and an excited state. The TIQI-group is interested in utilizing Calcium in Rydberg states to conduct quantum information experiments and aims to trap the atoms by controlling the atomic ion core. To that end, the goal is to calculate the magic wavelengths of Ca^+ .

As a next step, we use the 'Alkali-Rydberg-Calculator'[6] python library (ARC) to extract the radial wave function of Rydberg states of Calcium and perform calculations of the trap depth that help analyse which states would be viable candidates for later experiments.

2 Theoretical Background

Trapping techniques like optical tweezers operate with focused laser beams, making use of the effect that dielectric objects are attracted towards the region of highest laser intensity. The potential a trapped atom experiences corresponds to the shift of the energy levels due to the external field, known as the *AC Stark shift*. This potential is called the trap depth.

The following subsections will give a summary of the description of laser fields, the mechanics of a dipole in an electric field and the polarizability of atoms. The concept of the magic wavelength and Rydberg states of atoms will be explained and a short description of Calcium will be given.

2.1 Properties of a Laser Field

In the following, we consider a monochromatic field of the form

$$\mathbf{E}(\mathbf{r}, t) = \hat{\epsilon} E_0^{(+)}(\mathbf{r}) e^{-i\omega t} + \text{c.c.} \quad (1)$$

Here, ω is the angular frequency of the field, **c.c.** stands for the complex conjugate of the preceding term. This term arises from a separation of the field into its positive and negative frequency components[5]. The polarization of the light is expressed in the complex polarization vector $\hat{\epsilon}$. It is a unit vector orthogonal to the wave vector $\mathbf{k}$ and thus orthogonal to the propagation direction of the light

$$\hat{\epsilon}^* \cdot \hat{\epsilon} = 1 \quad \hat{\epsilon} \cdot \mathbf{k} = 0. \quad (2)$$

It follows that

$$\hat{\epsilon}^* \times \hat{\epsilon} = iA\hat{\mathbf{k}}, \quad (3)$$

where $\hat{\mathbf{k}}$ denotes the unit wave vector and A describes the degree of circular polarization[7]. A takes values in the interval $[-1, 1]$, with $A = 0$ describing linearly and $A = +1(-1)$ describing

right(left)-handed circularly polarized light. In the context of an experimental setup the angles θ_k and θ_p are additional properties of the laser beam. θ_k is the angle between the wave vector of the electric field and the defined z-axis, θ_p the angle between polarization vector of the field and the quantization axis.[8]. From geometrical considerations, it follows that

$$\cos^2 \theta_k + \cos^2 \theta_p \leq 1. \quad (4)$$

Optical trapping techniques operate with focused laser beams. For simplicity we assume a Gaussian intensity profile. The intensity of a Gaussian laser beam is given by [9]

$$I(r, z) = I_0 \left(\frac{w_0}{w(z)} \right)^2 \exp \left(\frac{-2 r^2}{w(z)^2} \right), \quad (5)$$

where

$$I_0 := \frac{2 P}{\pi w_0^2} \quad w(z) := w_0 \sqrt{1 + \left(\frac{z}{z_R} \right)^2} \quad z_R := \frac{\pi w_0^2 n}{\lambda}.$$

Here, λ is the wavelength, w_o is the waist, z_R is the Rayleigh length, P is the total power of the laser beam and n the refractive index of the medium ($n = 1$ for vacuum). r is the radial distance from the beam's center axis and z is the distance from its focus point along the beam.

2.2 Polarizability

The polarizability is a property both of atoms and of larger objects that obey the laws of classical mechanics, e.g., glass spheres [10], in an external electric field.

Unless indicated otherwise, this section is based on [5](D. Steck, Quantum and Atom Optics, sections 1.1, 1.4.1, 7.7.1-3).

2.2.1 Classical Introduction to the Polarizability

The separation in Eq. (1) enables us to look at the interaction with an electric field of the form

$$\mathbf{E}^{(+)}(\mathbf{r}, t) = \hat{\mathbf{e}} E_0^{(+)}(\mathbf{r}) e^{-i\omega t} =: \mathbf{E}^{(+)}. \quad (6)$$

Since the positive and negative frequency components of the electric field are complex conjugates we can write the physical field as

$$\mathbf{E}(\mathbf{r}, t) = 2\text{Re} \left[\mathbf{E}^{(+)} \right]. \quad (7)$$

Given the real amplitude of the electric field E_0 and the complex amplitude $E_0^{(+)}$ the intensity is given by

$$I(\mathbf{r}) = \frac{1}{2} c \epsilon_0 |E_0(\mathbf{r})|^2 = 2c\epsilon_0 \left| E_0^{(+)}(\mathbf{r}) \right|^2, \quad (8)$$

where $\mathbf{r}$ denotes the position of the atom, ϵ_0 the vacuum permittivity and c the speed of light.

An electron within an atom that is exposed to the electric field $\mathbf{E}^{(+)}$ experiences a displacement from its equilibrium position, resulting in an electric dipole moment $\mathbf{d}^{(+)}$ of the atom. We define the polarizability $\alpha(\omega)$ to describe the degree to which an electric field can induce the dipole moment:

$$\mathbf{d}^{(+)} = \alpha(\omega) \mathbf{E}^{(+)} \quad (9)$$

Taking into account also the complex conjugate term in Eq.(1) the potential energy of the electric dipole is given by

$$V_{\text{Dipole}} = -\frac{1}{2} \mathbf{d} \cdot \mathbf{E} = -\frac{1}{2} (\mathbf{d}^{(+)} + \mathbf{d}^{(-)}) (\mathbf{E}^{(+)} + \mathbf{E}^{(-)}). \quad (10)$$

The terms $\mathbf{d}^{(\pm)} \cdot \mathbf{E}^{(\pm)}$ oscillate with twice the frequency of the field. We can drop these terms by assuming that this frequency is too fast for the atom to respond mechanically. Using Eq.(7), (8) and (9) we can then write the potential as

$$V_{\text{Dipole}} = -\frac{1}{2}\mathbf{d}^{(+)} \cdot \mathbf{E}^{(-)} - \frac{1}{2}\mathbf{d}^{(-)} \cdot \mathbf{E}^{(+)} = -\text{Re}[\alpha(\omega)] \left| \mathbf{E}^{(+)} \right|^2 = -\frac{1}{2c\epsilon_0} \text{Re}[\alpha(\omega)] I(\mathbf{r}). \quad (11)$$

The corresponding force on the dipole is related to the potential gradient, i.e. intensity gradient, meaning the atom will be in equilibrium at the point of maximum intensity

$$\mathbf{F}_{\text{Dipole}} = -\nabla V_{\text{Dipole}} \propto \nabla I(\mathbf{r}). \quad (12)$$

2.2.2 Quantum Mechanical Introduction to the Polarizability

In order to talk about the polarizability of atoms, it is necessary to express the above in quantum mechanical terms. Consider a laser whose electric field component is characterized by Eq. (1) interacting with a two-level-atom with ground state $|\alpha\rangle$, excited state $|\beta\rangle$ and corresponding energies E_α and E_β . The atomic dipole operator is given by

$$\mathbf{d} = -e\mathbf{r}. \quad (13)$$

where $\mathbf{r}$ is the position of the atomic electron. The interaction of the atom with the electric field is given by

$$\mathbf{V} = -\mathbf{E} \cdot \mathbf{d}. \quad (14)$$

We can treat this interaction as a perturbation. The energy shift of state $|\alpha\rangle$, i.e. the AC Stark shift, is first relevant for the second order, since the first order shift vanishes[7]. The second order AC Stark shift is given by

$$\Delta E_\alpha = -\frac{2\omega_{\beta\alpha} |\langle\alpha|\hat{\mathbf{e}} \cdot \mathbf{d}|\beta\rangle|^2 \left| E_0^{(+)}(\mathbf{r}) \right|^2}{\hbar(\omega_{\beta\alpha}^2 - \omega^2)} \quad (15)$$

with

$$\omega_{\beta\alpha} = \frac{(E_\beta - E_\alpha)}{\hbar}.$$

Generalizing from a two level to a multi level system introduces a sum over all other states $|\beta\rangle$.

$$\Delta E_\alpha = -\sum_{\beta} \frac{2\omega_{\beta\alpha} |\langle\alpha|\hat{\mathbf{e}} \cdot \mathbf{d}|\beta\rangle|^2 \left| E_0^{(+)}(\mathbf{r}) \right|^2}{\hbar(\omega_{\beta\alpha}^2 - \omega^2)} \quad (16)$$

Together with Eq. (10), this leads to the Kramers-Heisenberg formula for the real part of the polarizability for state $|\alpha\rangle$:

$$\alpha(\omega) = \sum_{\beta} \frac{2\omega_{\beta\alpha} |\langle\alpha|\hat{\mathbf{e}} \cdot \mathbf{d}|\beta\rangle|^2}{\hbar(\omega_{\beta\alpha}^2 - \omega^2)} \quad (17)$$

We will generalize this treatment to a tensor representation to find an explicit formula for the polarizability with angular momentum degeneracy. The Kramers-Heisenberg polarizability tensor is a rank 2 tensor whose components are expressed as in Eq. (17) with the polarization vector omitted.

$$\alpha_{\mu\nu}(\omega) = \sum_{\beta} \frac{2\omega_{\beta\alpha} \langle\alpha|d_\nu|\beta\rangle \langle\beta|d_\mu|\alpha\rangle}{\hbar(\omega_{\beta\alpha}^2 - \omega^2)} \quad (18)$$

In the case of the fine structure levels $|Jm_J\rangle$ with total angular momentum J and projection m_J this yields

$$\alpha_{\mu\nu}(\omega) = \sum_{J'm_{J'}} \frac{2\omega_{\beta\alpha} \langle Jm_J | d_\nu | J'm_{J'} \rangle \langle J'm_{J'} | d_\mu | Jm_J \rangle}{\hbar(\omega_{\beta\alpha}^2 - \omega^2)} =: \sum_{J'} \frac{2\omega_{\beta\alpha} T_{\mu\nu}}{\hbar(\omega_{\beta\alpha}^2 - \omega^2)} \quad (19)$$

where we have defined the rank 2 dipole-product tensor $T_{\mu\nu}$. This tensor can be decomposed into its irreducible parts of rank 0, 1 and 2:

$$T_{\mu\nu} = \sum_{m_{J'}} \langle Jm_J | d_\mu | J'm_{J'} \rangle \langle J'm_{J'} | d_\nu | Jm_J \rangle = \frac{1}{3} T^{(0)} \delta_{\mu\nu} + \frac{1}{4} T_\sigma^{(1)} \epsilon_{\sigma\mu\nu} + T_{\mu\nu}^{(2)} \quad (20)$$

$$\begin{aligned} T^{(0)} &= T_{\mu\mu} & T_\sigma^{(1)} &= \epsilon_{\sigma\mu\nu} (T_{\mu\nu} - T_{\nu\mu}) & T_{\mu\nu}^{(2)} &= T_{\mu\nu} - \frac{1}{3} T_{\sigma\sigma} \delta_{\mu\nu} \\ \text{(scalar part)} & & \text{(vector part)} & & \text{(tensor part)} \end{aligned} \quad (21)$$

This leads to the decomposition of the polarizability tensor (19). With the definition of the Wigner 6j symbol and the Wigner-Eckart theorem it takes the following form (see Eq.(36) and (35) in the appendix):

$$\alpha^{(0)}(J, \omega) = \sum_{J'} \frac{2\omega_{JJ'} |\langle J || \mathbf{d} || J' \rangle|^2}{3\hbar(\omega_{JJ'}^2 - \omega^2)} \quad \text{(scalar polarizability)} \quad (22)$$

$$\alpha^{(1)}(J, \omega) = \sum_{J'} (-1)^{J+J'+1} \sqrt{\frac{6J(2J+1)}{J+1}} \left\{ \begin{matrix} 1 & 1 & 1 \\ J & J & J' \end{matrix} \right\} \frac{\omega_{JJ'} |\langle J || \mathbf{d} || J' \rangle|^2}{\hbar(\omega_{JJ'}^2 - \omega^2)} \quad \text{(vector polarizability)} \quad (23)$$

$$\alpha^{(2)}(J, \omega) = \sum_{J'} (-1)^{J+J'} \sqrt{\frac{40J(2J+1)}{(J+1)(2J+3)}} \left\{ \begin{matrix} 1 & 1 & 2 \\ J & J & J' \end{matrix} \right\} \frac{\omega_{JJ'} |\langle J || \mathbf{d} || J' \rangle|^2}{\hbar(\omega_{JJ'}^2 - \omega^2)} \quad \text{(tensor polarizability)} \quad (24)$$

Finally, for arbitrarily polarized light, the polarizability $\alpha(\omega)$ is given by [8]:

$$\alpha(\omega) = \alpha^{(0)}(\omega) + A \cos \theta_k \frac{m_J}{2J} \alpha^{(1)}(\omega) + \left(\frac{3 \cos^2 \theta_p - 1}{2} \right) \frac{3m_J^2 - J(J+1)}{J(2J-1)} \alpha^{(2)}(\omega) \quad (25)$$

2.3 Magic Wavelength

The polarizability of atoms in an external laser field depends on the angular frequency ω of the field and consequently on the wavelength λ . For two atomic states, there exists a wavelength at which the polarizability takes the same value. From Eq.(17) the identical polarizability implies an identical shift of the energy levels, which causes the atom to experience the same potential in either state. This wavelength is called the magic wavelength. With a fitting polarization of the laser, it is even possible to find the magic wavelength of more than two atomic states.

2.4 Rydberg Atoms and the Ponderomotive Potential

Rydberg atoms are characterized by having their valence electrons in highly excited states. When exposed to an external laser field, an outer electron experiences the ponderomotive potential [11]

$$U_{nl}(\mathbf{R}) = \frac{e^2}{2\epsilon_0 c m_e \omega^2} \int |\Psi_{nl}(\mathbf{r})|^2 I(\mathbf{r} + \mathbf{R}) d^3\mathbf{r}. \quad (26)$$

Here, e is the elementary charge, m_e the electron mass, ω the laser frequency and $I(\mathbf{r})$ the laser intensity as in Eq.(5). $\Psi_{nl}(\mathbf{r})$ is the wave function of the valence electron in the nl state, n denoting the principle quantum number and l the orbital angular momentum quantum number. The coordinate $\mathbf{r}$ refers to the electron position relative to the nucleus, and $\mathbf{R}$ is the position of the nucleus relative to the focus point of the laser beam. Recent studies have demonstrated the possibility to trap Rydberg atoms by trapping the ion core. The ponderomotive potential will be important to study, since it can cause a repulsion from the intensity maximum of the applied laser[11].

2.5 Calcium - Properties and Notation

Calcium is an alkaline earth metal with atomic number $Z = 20$. The electron configuration in the ground state is $[\text{Ar}]4s^2$, where $[\text{Ar}]$ denotes the configuration of Argon. Calcium has two valence electrons occupying the state with $n = 4$, $l = 0$, and in the ground state the electron spins are oriented such that they oppose each other with a total angular momentum of zero. In the following, the atomic states will be referred to by their term symbols:

$$(2S+1)L_J$$

S is the total spin, L the total orbital angular momentum and J the total angular momentum quantum number. Rydberg states of Ca with one excited electron will have the configuration $[\text{Ar}]4s\ nl$, with n large. The total spin can then take the values 0 and 1.

3 Method

3.1 Structure and Features of the Atom-phys Python Library

In this semester project we expanded an existing python library called atom-phys. It is a practical tool for accessing physical properties of the elements. It operates by automatically fetching atomic data from the National Institute of Standards and Technology Atomic Spectra Database (NIST ASD)[12]. This includes the atomic states, energy levels, transitions, transition wavelengths and transition rates. Additionally, there is the possibility to input atomic data in JSON format. This is useful in the case that there is additional data to an element that is not provided by NIST ASD. From the atomic data, atom-phys can then calculate various properties of the atoms. The user can create an object of the class **Atom**. This class can then access the classes **State** and **Transition**. The atomic properties are calculated in the suitable class, e.g. the transition rate Γ is a member of the **Transition** class and the total angular momentum quantum number J is a property of the **State** class. The user would access the data with the following commands:

```
>>> atom = atomphys.Atom('Ca+')
>>> atom('2S1/2')
State(4s 2S1/2: 0 E_h)
>>> atom('2S1/2').to('4p 2P1/2')
Transition(4s 2S1/2 <---> 4p 2P1/2*,  $\lambda=397$  nm,  $\Gamma=2\pi\times 22.28$  MHz)
>>> print(atom('2S1/2').to('4p 2P1/2'). $\Gamma$ )
3.3864380572199533 $\times 10^{-9}$  E_h/ $\hbar$ 
```

Consequently, the polarizability should be a member of the **State** class and the magic wavelength a member of **Transition**, since a **Transition** object holds information about both the upper and lower state. To be able to calculate the polarizability of atoms, the scalar part (22) was already implemented in **State** and the calculation for the vector and tensor part was implemented outside of the class.

3.2 Added Features

The calculation of the polarizability and the ponderomotive potential depends on the parameters describing an external laser field. As a compact solution, we added a class **Laser** to the library that has the wavelength λ , the degree of circular polarization A and the angles θ_k and θ_p as properties.

To calculate the total polarizability with Eq.(25) we added the scalar and vector polarizability to complete the calculation in **State**. The total polarizability function takes the total angular momentum projection m_J as an input, since it is not a property of **State**. In this process we consult the calculations in [8] and [5].

To find the magic wavelength of two states we need to find the wavelength at which the difference between the polarizabilities vanish. We implement this with a root finding algorithm in **Transition**.

4 Polarizability and Magic Wavelengths of Ca^+

4.1 Calculation

To preclude mistakes due to limited data on Ca^+ provided by NIST ASD, we generated a JSON file with data on additional transitions calculated by Kaur et al. [13]. To check whether our calculations are correct, we compared results for the polarizabilities of the $4s\ ^2S_{1/2}$, $4p\ ^2P_{1/2,3/2}$, $3d\ ^2D_{3/2,5/2}$ states of Ca^+ including the possible orientations of angular momentum with $m_J = -J, -J+1, \dots, J$ to the results by Kaur et al.[4] and Jiang et al.[8]. Here, $4s$, $4p$ and $3d$ indicate the state of the valence electron. Kaur et al. use linearly polarized light ($A=0$) with $\theta_k = \pi/2$, $\theta_p = 0$, thus dropping the vector polarizability in Eq.(25). For $A \neq 0$ we compared our results to Jiang et al., who use circularly polarized light ($A=\pm 1$) with $\theta_k = 0$ and $\theta_p = \pi/2$.

We then calculated the magic wavelengths of the $4s\ ^2S_{1/2}$ ground state and the excited states. The $3d\ ^2D_{5/2}$ state is the most relevant to applications in quantum computing and simulation because of its relatively long lifetime of 1.1s[14]. For the three $3d\ ^2D_{5/2}$ states with $m_J = 1/2, 3/2, 5/2$ we found a common magic wavelength by choosing a polarization of the laser that causes the vector and tensor polarizability to vanish.

4.2 Results

Fig.1 shows the polarizability of the $4s\ ^2S_{1/2}$ $m_J=1/2$ and $3d\ ^2D_{5/2}$ $m_J = \pm 1/2, \pm 3/2, \pm 5/2$ states, calculated using the transitions from NIST ASD (1a) and the transitions from Kaur et al.(2b)[13] for linearly polarized light as a function of the wavelength. The points at which magic wavelengths with the $4s\ ^2S_{1/2}$ state were found are indicated with black. Tab.1 lists the calculated magic wavelengths $\lambda_{\text{magic}}^{\text{NIST}}$ and $\lambda_{\text{magic}}^{\text{Kaur}}$ and allows to compare them to the literature values $\lambda_{\text{magic}}^{\text{exp}}$ as reported by Kaur et al.[4]. The polarizability of the $4p\ ^2P_{1/2,3/2}$ and $3d\ ^2D_{3/2}$ states with indicated magic wavelengths are shown in Fig.5 and 6.

Comparing Fig.1 and the corresponding magic wavelengths to the literature values, we see that we achieve better matching results using the transitions by Kaur et al.. From this point on we only use this method to calculate the polarizability.

Fig.2 shows the polarizability of the $4s\ ^2S_{1/2}$ $m_J = -1/2$ and $3d\ ^2D_{3/2,5/2}$ $m_J = \pm 1/2, \pm 3/2, \pm 5/2$ states for circularly polarized light with $A = 1$ (2a) and $A = -1$ (2b) as a function of the wavelength. The points at which magic wavelengths with the $4s\ ^2S_{1/2}$ state were found are indicated with black. Tab.2 lists the calculated magic wavelengths $\lambda_{\text{magic}}^{\text{Kaur}}$ and allows to compare them to the literature values $\lambda_{\text{magic}}^{\text{exp}}$ as reported by Jiang et al.[8]. The uncertainty of the literature values is given in parentheses. The polarizability of the $4p\ ^2P_{1/2,3/2}$ and $3d\ ^2D_{3/2}$ states with indicated magic wavelengths are shown in Fig.7 and 8 for right handed circularly polarized light ($A=1$).

4.3 Discussion

In the above, the results were given without uncertainties. Possible errors arising from our calculation mainly come from the limited set of transitions available for the calculation of the polarizability.

Looking at Fig.1, we see that the overall dependence of the polarizability on the wavelength of the external laser field aligns with the findings by Kaur et al.[4]. The polarizability for $A = 0$ only depends on m_J^2 (see Eq.25). Thus it is the same for either sign of m_J . The polarizability of the $4s\ ^2S_{1/2}$ ground state shows a divergence at $\sim 400\text{nm}$, for the $3d\ ^2D_{5/2}$ $m_J = \pm 1/2, \pm 3/2$ it shows a divergence at $\sim 900\text{nm}$. These wavelengths characterize atomic transitions, leading to a divergence due to the definition in Eq.17. In agreement with Kaur et al., we find two magic wavelengths with the ground state for each m_J sub level. The polarizability for the $3d\ ^2D_{5/2}$ $m_J = \pm 5/2$ state stays close to constant and we find one magic wavelength. Looking at Tab.1 we see that the calculated magic wavelengths are closer to the literature values $\lambda_{\text{magic}}^{\text{exp}}$ if they are closer to a divergence. Here, deviations of the polarizabilities have smaller impact on the position of an intersection, where magic wavelengths are found. For instance for $m_J = \pm 3/2$, $\lambda_{\text{magic}}^{\text{exp}} = 1052.26\text{ nm}$ and we find $\lambda_{\text{magic}}^{\text{Kaur}} = 1050.45\text{ nm}$ whereas for $\lambda_{\text{magic}}^{\text{exp}} = 395.79\text{ nm}$ we find a matching magic wavelength.

Looking at Fig.2 and comparing to the findings by Jiang et al.[8] we observe similar phenomena for circularly polarized light. For right handed circularly polarized light ($A = 1$) we see characteristic divergences of the polarizability of the $3d\ ^2D_{5/2}$ $m_J = \pm 1/2, -3/2, -5/2$ states at $\sim 850\text{ nm}$. For the $4s\ ^2S_{1/2}$ $m_J = -1/2$ ground state we see a divergence at $\sim 400\text{ nm}$. The $m_J = 3/2, 5/2$ sub levels show an approximately constant polarizability. We find the same number of magic wavelengths as Jiang et al.. Tab 2 shows that our results match better to Jiang et al. at shorter wavelengths, e.g. $\lambda_{\text{magic}}^{\text{exp}} = 394.6339(1)\text{ nm}$. Again this is due to the proximity to a divergence at $\sim 400\text{ nm}$. For left handed circularly polarized light ($A = -1$) the behaviour of the polarizability differs systematically. Here, we see characteristic divergences of the polarizability of the $3d\ ^2D_{5/2}$ $m_J = \pm 1/2, 3/2, 5/2$ states at $\sim 850\text{ nm}$. For the $4s\ ^2S_{1/2}$ $m_J = -1/2$ ground state we see a divergence at $\sim 400\text{ nm}$. The $m_J = -5/2, -3/2$ sub levels show an approximately constant polarizability. Comparing Fig.2a and 2b we see that a state with m_J shows the behaviour of $-m_J$ with the opposite polarization of light. Also for $A = -1$ we find the same amount of magic wavelengths as Jiang et al..

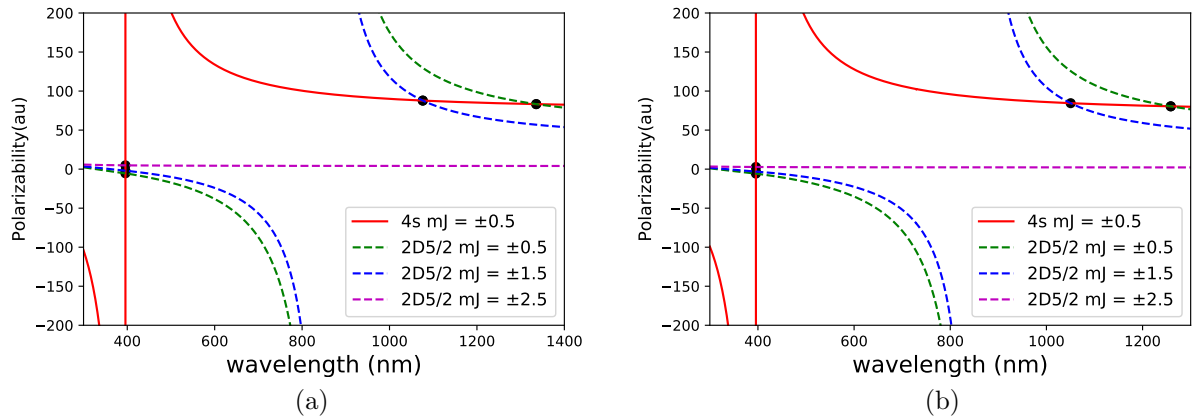


Figure 1: Polarizability of the $4s\ ^2S_{1/2}$ $m_J=1/2$ and $3d\ ^2D_{5/2}$ $m_J = \pm 1/2, \pm 3/2, \pm 5/2$ states of Ca^+ calculated using transitions from NIST ASD (a) and the transitions found by Kaur et al.(b) [13] for linearly polarized light as a function of its wavelength ($A=0$). The points at which magic wavelengths with the $4s\ ^2S_{1/2}$ state were found are indicated with black and the values are listed in Tab.1.

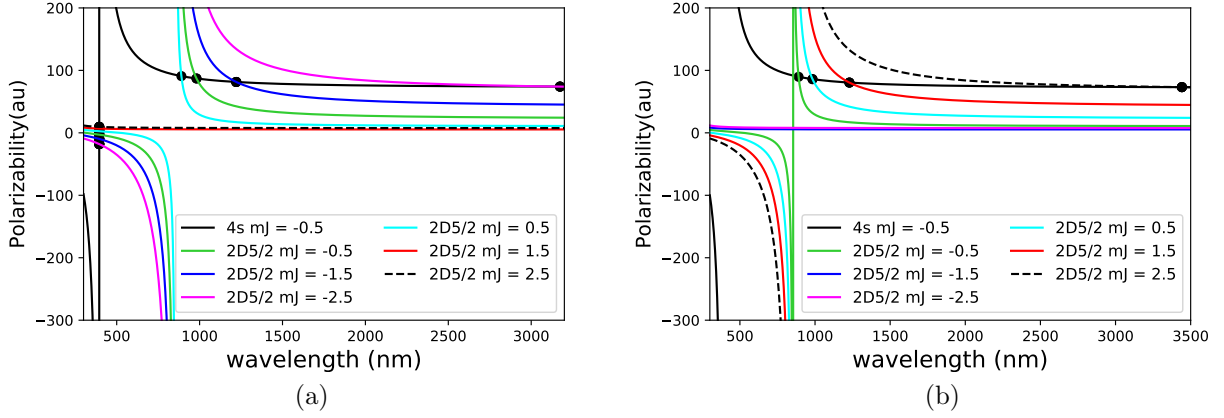


Figure 2: Polarizability of the $4s\ ^2S_{1/2}\ m_J = -1/2$ and $3d\ ^2D_{3/2,5/2}\ m_J = \pm 1/2, \pm 3/2, \pm 5/2$ of Ca^+ for circularly polarized light with $A=1$ (a) and $A=-1$ (b) as a function of its wavelength. The polarizability was calculated using transitions found by Kaur et al.[13]. The points at which magic wavelengths with the $4s\ ^2S_{1/2}$ state were found are indicated with black and the values are listed in Tab 2.

$4s^2S_{1/2} - 3d^2D_{5/2}$	m_J	$\lambda_{\text{magic}}^{\text{NIST}}$ [nm]	$\lambda_{\text{magic}}^{\text{Kaur}}$ [nm]	$\lambda_{\text{magic}}^{\text{exp}}$ [nm]
A = 0	$\pm 1/2$	395.81	395.79	395.79
	$\pm 3/2$	1335.61	1258.67	1271.92
	$\pm 5/2$	395.81	395.79	395.79
		1076.09	1050.45	1052.26

Table 1: Results for the calculated magic wavelength $\lambda_{\text{magic}}^{\text{NIST}}$ and $\lambda_{\text{magic}}^{\text{Kaur}}$ of the $4s\ ^2S_{1/2}\ m_J = 1/2 \longleftrightarrow 3d\ ^2D_{5/2}\ m_J = \pm 1/2, \pm 5/2, \pm 3/2$ transitions of Ca^+ . $\lambda_{\text{magic}}^{\text{NIST}}$ was calculated using transitions from NIST ASD[12], $\lambda_{\text{magic}}^{\text{Kaur}}$ was calculated using transitions from Kaur et al.[13]. We compare our values to the expected magic wavelengths $\lambda_{\text{magic}}^{\text{exp}}$ found by Kaur et al.[4].

$4s\ ^2S_{1/2 m_J=-1/2} - 3d^2D_{5/2}$	m_J	$\lambda_{\text{magic}}^{\text{Kaur}} \text{ [nm]}$	$\lambda_{\text{magic}}^{\text{exp}} \text{ [nm]}$
$A = 1$	1/2	394.63 890.06	394.6339(1) 894.50(4.03)
	-1/2	394.63 981.17	394.6357(1) 986.63(14.76)
	3/2	394.63	394.6324(2)
	-3/2	394.63 1220.95	394.6377(2) 1185.07(46.46)
	5/2	394.63	394.6311(3)
	-5/2	394.63 3173.85	394.6400(4) 1726.68(198.7)
$4s\ ^2S_{1/2 m_J=-1/2} - 3d^2D_{5/2}$	m_J	$\lambda_{\text{magic}}^{\text{Kaur}} \text{ [nm]}$	$\lambda_{\text{magic}}^{\text{exp}} \text{ [nm]}$
$A = -1$	1/2	983.13	987.60(14.87)
	-1/2	890.55	894.81(4.06)
	3/2	1228.73	1187.42(46.79)
	5/2	3441.59	1732.77(200.04)

Table 2: Results for the magic wavelength $\lambda_{\text{magic}}^{\text{Kaur}}$ of the $4s\ ^2S_{1/2 m_J=-1/2} \longleftrightarrow 3d\ ^2D_{5/2}$ $m_J = \pm 1/2, \pm 3/2, \pm 5/2$, transitions of Ca^+ calculated using the transitions from Kaur et al. [13]. These are compared to the literature values $\lambda_{\text{magic}}^{\text{exp}}$ found by Jiang et al. [8] for circularly polarized light with $A = \pm 1$. The uncertainties are given in parentheses.

4.4 Triple Magic Wavelength

We want to find a common magic wavelength of the $3d\ ^2D_{5/2 m_J=1/2,3/2,5/2}$ states with the $4s\ ^2S_{1/2}$ ground state of Ca^+ by choosing a fitting polarization of the external laser field. Fig.3 shows the magic wavelengths of the $4s\ ^2S_{1/2 m_J=1/2}$ and $3d\ ^2D_{5/2 m_J=1/2,3/2,5/2}$ states for linearly polarized light as a function of $|\cos(\theta_p)|^2$. θ_p is the angle between the polarization vector and the quantization axis. As expected from Eq.25 we find a common magic wavelength $\lambda_{\text{magic}} = 1069.96$ nm at $|\cos \theta_p|^2 = 1/3$ where the tensor polarizability vanishes (see Eq.(25)). The polarizability of the three $3d\ ^2D_{5/2}$ states does not depend on m_J anymore.

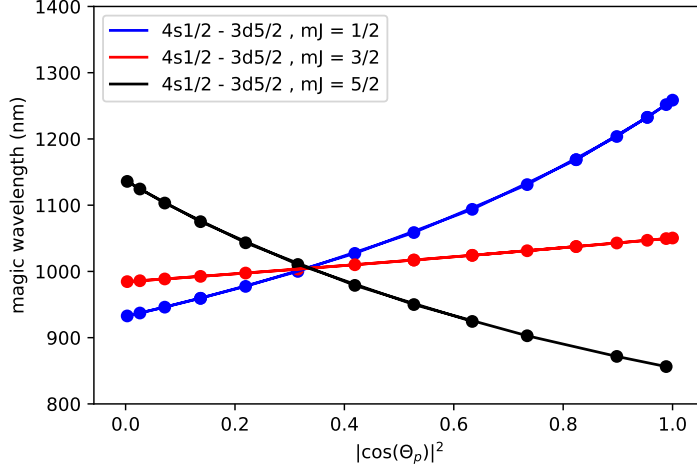


Figure 3: Magic wavelengths of the $4s\ ^2S_{1/2}\ m_J=1/2 \longleftrightarrow 3d\ ^2D_{5/2}\ m_J=1/2, 3/2, 5/2$ transitions of Ca^+ for linearly polarized light with $A = 0$ as a function of $|\cos(\theta_p)|^2$. θ_p is the angle between polarization vector of the electric field and the quantization axis.

5 Ponderomotive Potential and Trap Depth for Ca

5.1 Calculation

We calculated the ponderomotive potential (26) experienced by the outer electron of the $4s\ ns\ ^3S_1$ Rydberg states of Ca in an external laser field. To calculate the electron wave function for the state nl and orbital angular momentum quantum number projection m_l in spherical coordinates

$$\Psi_{nlm_l}(r, \theta, \phi) = R_{nl}(r) Y_l^{m_l}(\theta, \phi)$$

we used the radial wave functions $R_{nl}(r)$ of the Rydberg states from the ARC using the built in method `radialWavefunction`[15]. $Y_l^{m_l}(\theta, \phi)$ are the spherical harmonics which are provided by the python SciPy library[16]. Similar to atom-phys, we can access data from the ARC by creating objects of the classes that hold data on the atom we are interested in, e.g., by using the following commands:

```
>>> atom = arc.Calcium40()
>>> atom.Z
20
```

`radialWavefunction` is implemented for the alkali atoms only. To deal with this problem we create a new class `Calcium` with the atomic number $Z = 20$ and atomic mass of Ca that inherits all properties from the alkali atom class `AlkaliAtom` [17] from the ARC. Thus a `Calcium` object has the `radialWavefunction` method while holding data on an alkline earth atom. Note that ARC does not distinguish between the possible values of the total spin when calculating the radial wave functions.

We calculated the intensity of the laser beam from Eq.(5) assuming a total power $P = 1\text{mW}$ and wavelength $\lambda = 532\text{nm}$. For simplicity, we assume that the ionic core of the Rydberg atom is at the focus of the beam, thus $\mathbf{R} = \vec{0}$.

We calculate the trap depth U_{S_1} of the 3S_1 States of Ca relative to the trap depth U_{S_0} of the 1S_0 ground state by calculating the ratio of the trapping potentials. To calculate U_{S_1} we add the

ponderomotive potential $U_{ns}(\vec{0})$ of the outer electron and the trap depth U_{Ca^+} of Ca^+ in the $^2S_{1/2}$ ground state, effectively neglecting interactions between the outer electron and the Ca^+ ion core.

$$\frac{U_{S_1}}{U_{S_0}} = \frac{U_{Ca^+} + U_{ns}(\vec{0})}{U_{S_0}} \quad (27)$$

We calculate U_{Ca^+} and U_{S_0} from the polarizability provided by atom-physics and the laser intensity using Eq.(5) and (10).

5.2 Results

Fig.4 shows the trap depth for $4s\ ns\ ^3S_1$ Rydberg states, normalized to the 1S_0 ground state as a function of the principle quantum number n of the outer electron. For the trap depth of Ca^+ we find $U_{Ca^+} \simeq -1.82 \cdot 10^{-8}$ eV. For the 1S_0 ground state of Ca we find $U_{S_0} \simeq -4.46 \cdot 10^{-8}$ eV. As the distance between the electron and the nucleus increases, i.e. n increases, the trap depth of the 3S_1 states converges towards the trap depth of the Ca^+ ion core. Hence the ponderomotive potential of the outer electron becomes smaller with increasing n . We see a discontinuity at $n = 97$ where the calculated ponderomotive potential jumps from $U_{96s} \simeq 2.02 \cdot 10^{-8}$ eV to an approximately constant value of order $\sim 10^{-10}$ eV, which is very small compared to the magnitude of U_{Ca^+} . The reason for this discontinuity is not clear.

5.3 Discussion

Since we neglected the interaction between the outer electron and the ion core, our calculations of the trap depth of Ca in Rydberg states are an approximation. Especially for low n our results are most likely not exact. Using this approximation we find a trap depth of $-3.52 \cdot 10^{-9}$ eV for the 1S_0 ground state. This is one order of magnitude smaller than the trap depth U_{S_0} calculated from the polarizability provided by atom-physics using Eq.(10). An additional error can come from the calculation of the radial wave functions, since we use the `radialWavefunction` method that was not originally built for the Calcium class of the ARC[15]. This includes that `radialWavefunction` does not depend on the total spin of the Rydberg state.

Looking at Fig.4, we conclude that for later experiments using Ca Rydberg states in optical tweezers, the states with $50 < n < 70$ are viable candidates. In this regime the ponderomotive potential is smallest while still allowing for enough control of the Rydberg state.

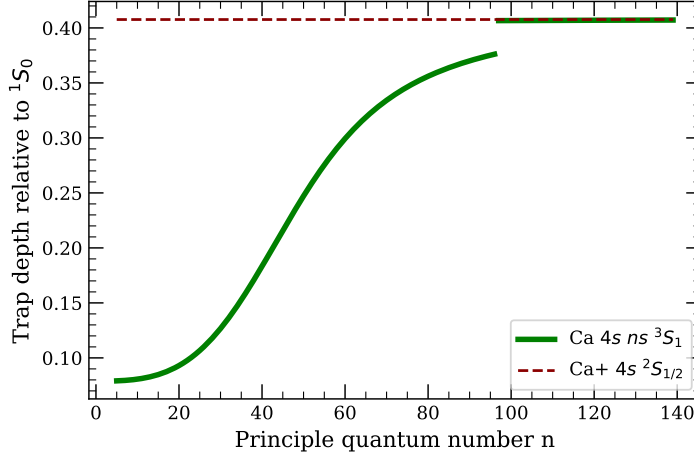


Figure 4: Calculated trap depth for $4s\ ns\ ^3S_1$ Rydberg states of Ca, normalized to the 1S_0 ground state for a Gaussian laser beam of total power $P=1$ mW and wavelength $\lambda=532$ nm. The relative trap depth of the $4s\ ^2S_{1/2}$ Ca^+ core is shown in red for comparison.

6 Conclusion

In this semester project we successfully expanded the python library atom-phys to calculate the polarizability and magic wavelengths of atoms in an external, arbitrarily polarized laser field. We calculated the polarizability and the magic wavelengths of the $4s\ ^2S_{1/2}$ and $3d\ ^2D_{3/2,5/2}$ states of Ca^+ including all possible orientations of angular momentum with $m_J = -J, -J+1, \dots, J$. Comparing our results to the findings by Kaur et al.[4] and Jiang et al.[8] for linearly and circularly polarized laser light respectively, we conclude that our calculations are correct. Misalignment with expected magic wavelengths can be due to our limited set of atomic transitions, which are needed for the calculation of the polarizability. We see that this leads to errors especially when using data provided by the NIST ASD. We find the same number of magic wavelength as Kaur and Jiang et al. that can differ from the literature value slightly depending on their proximity to a divergence of the polarizability.

As expected, for linearly polarized light with $|\cos(\theta_p)|^2 = 1/3$ we find a common magic wavelength of the $3d\ ^2D_{5/2}\ m_J=1/2, 3/2, 5/2$ states of Ca^+ with the $4s\ ^2S_{1/2}$ ground state at $\lambda_{\text{magic}} = 1069.96$ nm.

We implemented a calculation of the ponderomotive potential experienced by the valence electron of Ca in $4s\ ns\ ^3S_1$ Rydberg states. Using this we calculated the trap depth of the 3S_1 states and normalized to the trap depth of the 1S_0 ground state. This lead to the conclusion that the Rydberg states with $50 < n < 70$ are viable candidates for later experiments. As expected we see that for increasing n , the trap depth of the 3S_1 states converges towards the trap depth of the ion core. Concerning our calculation, there are multiple sources of errors. Especially for the states with low n , the approximation that the valence electron does not interact with the ion core leads to errors. Using the ARC to fetch the radial wave functions of Ca leads to uncertainties coming from the fact that the `radialWavefunction` method from the ARC is not implemented for alkali earth atoms and does not depend on the total spin. We see a discontinuity of the ponderomotive potential at $n = 97$ that we can not explain.

For further development of the atom-phys library it might be helpful to implement a fetching of atomic data from a source other than the NIST ASD. This could lead to more exact calculations of the polarizability and the magic wavelengths of atoms. Additionally, to implement a calculation

of the radial wave function of alkali earth atoms would help eliminate that source of error in the calculation of the trap depth of Ca in Rydberg states.

7 Appendix

For a more detailed derivation of the results presented below, see [5] (D.Steck, Quantum and Atom Optics, section 7.1.4 and 7.3.4)

7.1 Addition of Angular Momenta and Wigner 6j Symbol

The Hilbert space of a quantum mechanical system can be described using different bases. If we want to add two or three angular momenta of the system, we can find a basis of simultaneous eigenstates. Consider the angular momentum operators $\mathbf{J}_1$, $\mathbf{J}_2$ and $\mathbf{J}_{12} = \mathbf{J}_1 + \mathbf{J}_2$. Since these commute, we can find a basis of simultaneous eigenstates $|j_1 m_1; j_2 m_2\rangle := |j_1 m_1\rangle |j_2 m_2\rangle$ of $\mathbf{J}_1^2$, $\mathbf{J}_{1z}$, $\mathbf{J}_2^2$ and $\mathbf{J}_{2z}$. The operators $\mathbf{J}_1^2$ and $\mathbf{J}_2^2$ also commute with $\mathbf{J}_{12}^2$ and $\mathbf{J}_{12z}$, consequently we can find a basis of simultaneous eigenstates labeled $|j_1, j_2; j_{12} m_{12}\rangle$. As a transformation rule between the bases we have the following

$$|j_1 m_1; j_2 m_2\rangle = \sum_{\substack{j_{12} m_{12} \\ m_1 + m_2 = m_{12}}} |j_1, j_2; j_{12} m_{12}\rangle \langle j_1, j_2; j_{12} m_{12} | j_1 m_1; j_2 m_2 \rangle \quad (28)$$

$$= \sum_{\substack{j_{12} m_{12} \\ m_1 + m_2 = m_{12}}} |j_{12} m_{12}\rangle \langle j_{12} m_{12} | j_1 m_1; j_2 m_2 \rangle. \quad (29)$$

When adding three angular momenta, the order of this operation becomes relevant. Consider $\mathbf{J}_{12}$, $\mathbf{J}_3$ and $\mathbf{J} = \mathbf{J}_{12} + \mathbf{J}_3$. We can then similarly find a basis of simultaneous eigenstates $|j_{12} m_{12}; j_3 m_3\rangle$ as well as a basis of simultaneous eigenstates $|j_{12}, j_3; j m\rangle$. On the other hand, we can first form the sum $\mathbf{J}_{23} := \mathbf{J}_2 + \mathbf{J}_3$. Then $\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_{23}$ and we find the basis of simultaneous eigenstates $|j_1 m_1; j_{23} m_{23}\rangle$ and $|j_1, j_{23}; j m\rangle$. A compact transformation rule between these bases is given by

$$|j_{12}, j_3; j m\rangle = \sum_{j_{23}} |j_1, j_{23}; j m\rangle (-1)^{j_1 + j_2 + j_3 + j} \sqrt{(2j_{12} + 1)(2j_{23} + 1)} \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j & j_{23} \end{Bmatrix}, \quad (30)$$

where the **Wigner 6j-symbol** is defined as

$$\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j & j_{23} \end{Bmatrix} := \frac{(-1)^{j_1 + j_2 + j_3 + j} \langle j_1, j_{23}; j m | j_{12}, j_3; j m \rangle}{\sqrt{(2j_{12} + 1)(2j_{23} + 1)}}. \quad (31)$$

7.2 Spherical Tensor Operators and the Wigner-Eckart Theorem

An irreducible tensor operator of rank k denoted as $\mathbf{T}^{(k)}$ is a set of $2k + 1$ operators, i.e. a rank k tensor for which each component is taken as an operator.

We consider the angular momentum state $|\gamma' J' m'_J\rangle$, where γ' represents quantum numbers necessary to describe the state that are without angular dependence. We call these radial quantum numbers. The action of a tensor operator on an angular momentum state is like the mixing of two angular momenta. For a tensor-operator component q we have the relation (compare to Eq.(29))

$$T_q^{(k)} |\gamma' J' m'_J\rangle = \sum_{k' q'} |\tilde{\gamma} k' q'\rangle \langle k' q' | J' m'_J; k q \rangle. \quad (32)$$

$\tilde{\gamma}$ describes the transformed radial quantum numbers. We can then calculate the matrix element

$$\langle \gamma J m_J | T_q^{(k)} | \gamma' J' m'_J \rangle = \sum_{k' q'} \langle \gamma J m_J | \tilde{\gamma} k' q' \rangle \langle k' q' | J' m'_J; k q \rangle = \langle \gamma | \tilde{\gamma} \rangle \langle J m_J | J' m'_J; k q \rangle \quad (33)$$

where in the last equality we used the orthogonality of the angular momentum states. We define the **reduced matrix element** as:

$$\langle \gamma J || \mathbf{T}^{(k)} || \gamma' J' \rangle := (-1)^{2k} \langle \gamma | \tilde{\gamma} \rangle \quad (34)$$

which is as notation suggests independent of m_J and depends on J , J' and $\mathbf{T}^{(k)}$ via the way γ' transforms into $\tilde{\gamma}$.

We arrive at the **Wigner Eckart Theorem**

$$\langle \gamma J m_J | T_q^{(k)} | \gamma' J' m_J' \rangle = (-1)^{2k} \langle \gamma J || \mathbf{T}^{(k)} || \gamma' J' \rangle \langle J m_J | J' m_J'; k q \rangle \quad (35)$$

7.3 Additional Results

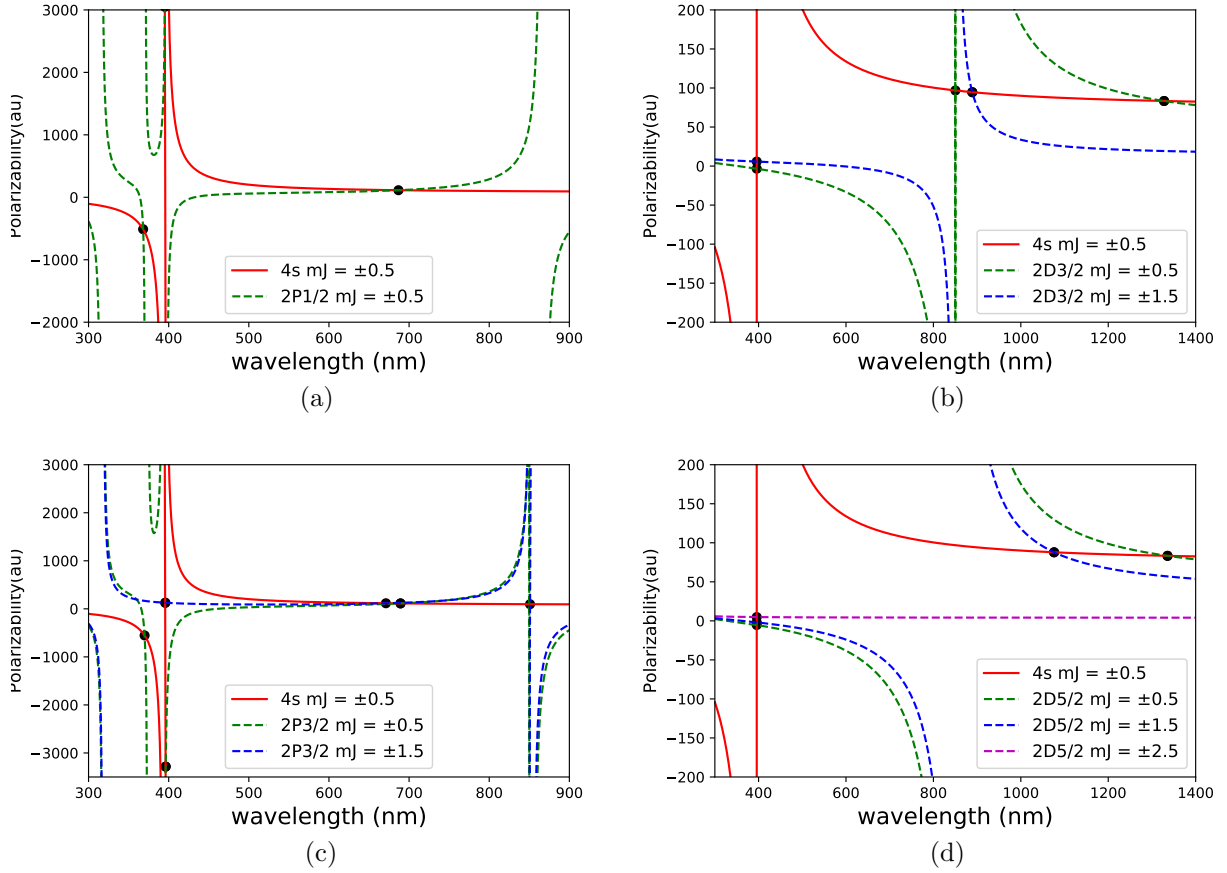


Figure 5: Polarizability of the $4s$ $^2S_{1/2}$, $4p$ $^2P_{1/2,3/2}$ and $3d$ $^2D_{3/2,5/2}$ states of Ca^+ calculated using transitions from NIST ASD and linearly polarized light ($A = 0$) as a function of its wavelength. The points at which magic wavelengths were found with the $4s$ $^2S_{1/2}$ state are indicated with black.

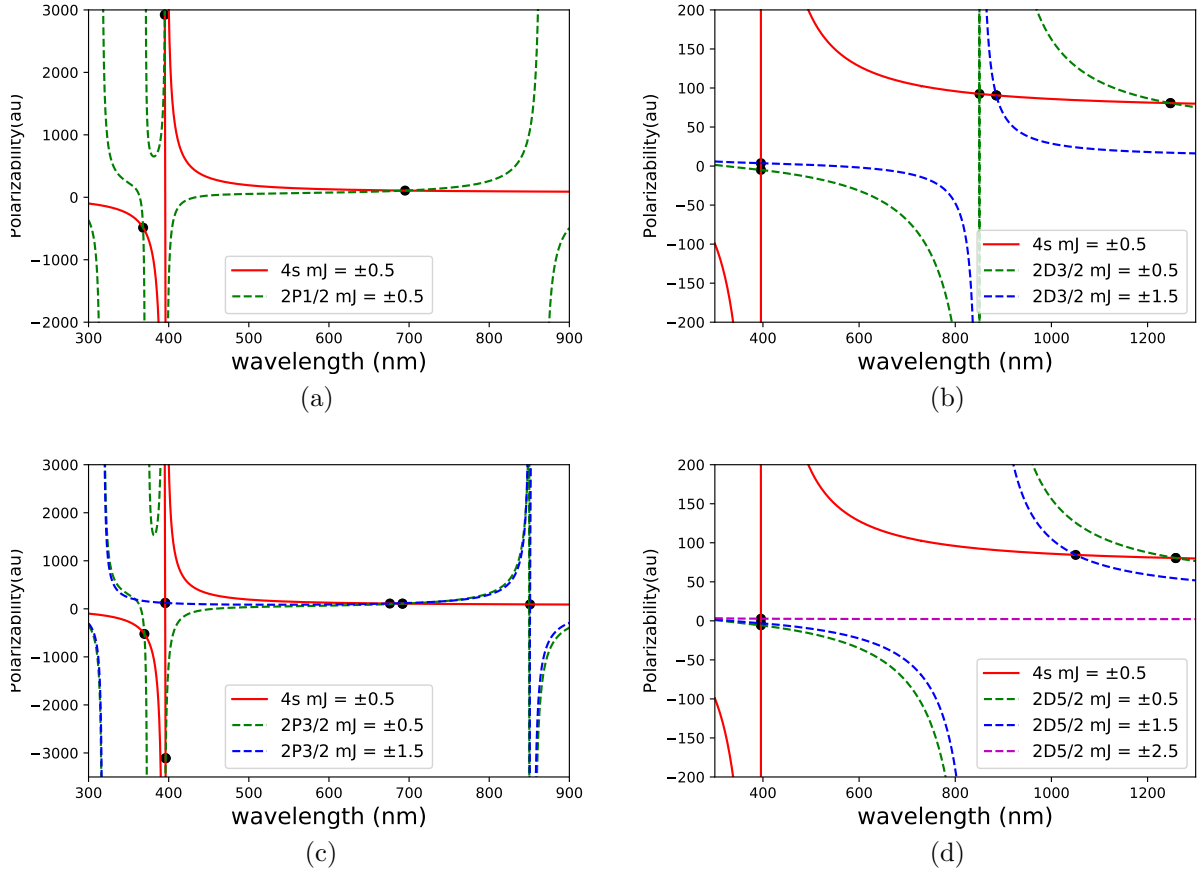


Figure 6: Polarizability of the $4s$ $^2S_{1/2}$, $4p$ $^2P_{1/2,3/2}$ and $3d$ $^2D_{3/2,5/2}$ states of Ca^+ calculated using transitions found by Kaur et al.[13] and linearly polarized light with $A = 0$ as a function of its wavelength. The points at which magic wavelengths were found with the $4s$ $^2S_{1/2}$ state are indicated with black.

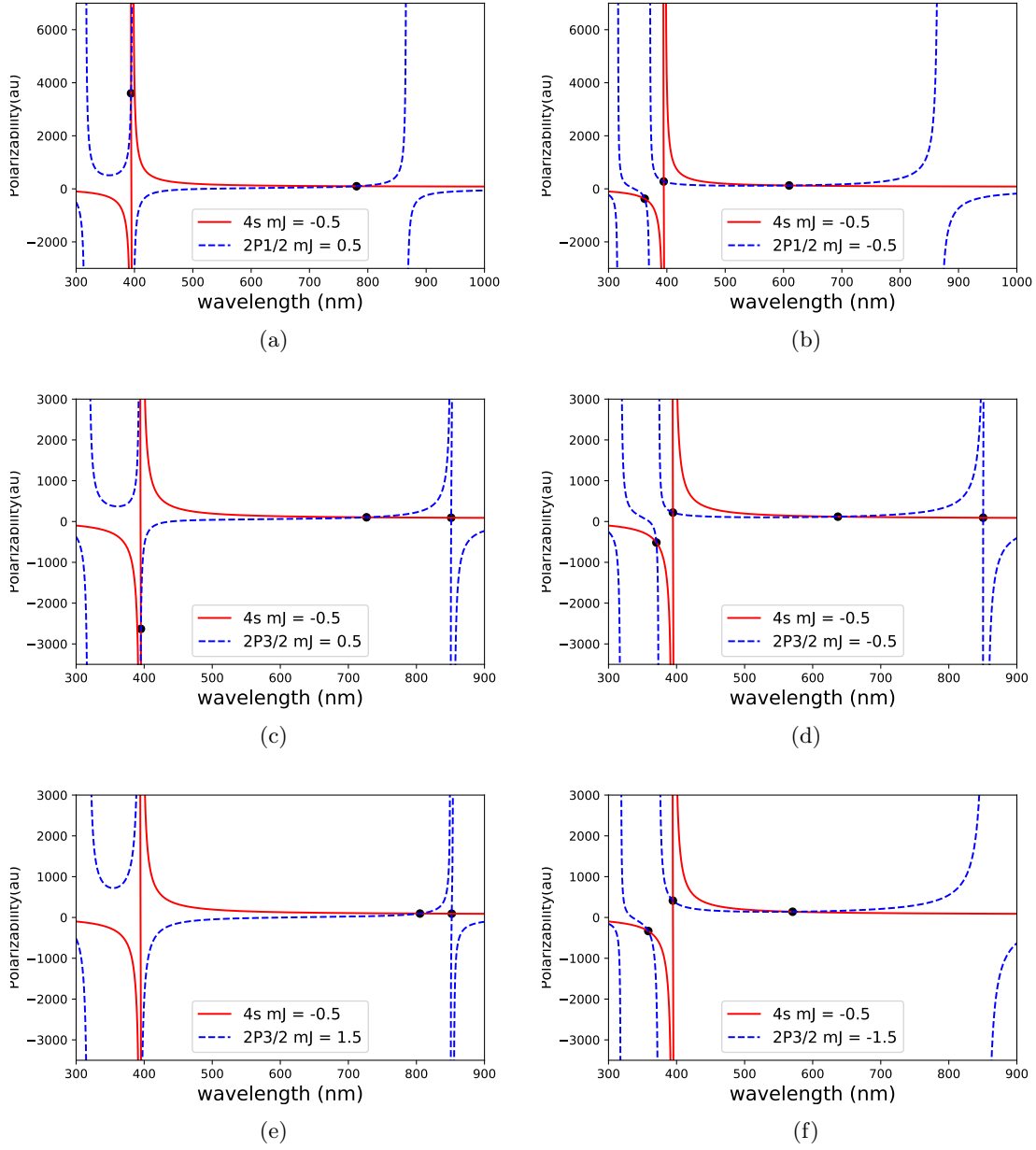


Figure 7: Polarizability of the $4s\ ^2S_{1/2}$, $m_j = -1/2$, $4p\ ^2P_{1/2,3/2}$ $m_j = -3/2, -1/2, 1/2, 3/2$ states of Ca^+ calculated using transitions found by Kaur et al.[13] and circularly polarized light with $A = 1$ as a function of its wavelength. The points at which magic wavelengths with the $4s\ ^2S_{1/2}$ state were found are indicated with black.

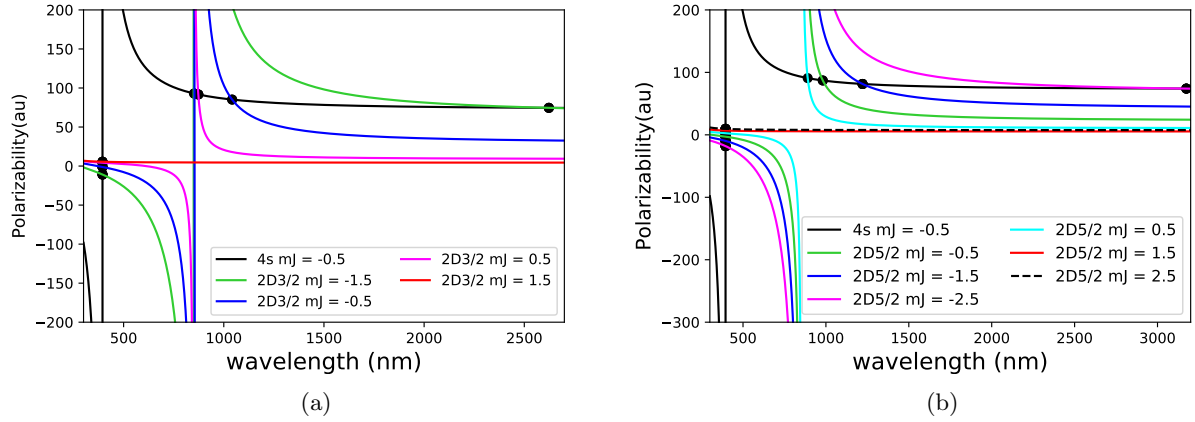


Figure 8: Polarizability of the $4s\ ^2S_{1/2}\ m_J = -1/2$, $3d\ ^2D_{3/2,5/2}$ with $m_J = -3/2, -1/2, 1/2, 3/2, -5/2, 5/2$ of Ca^+ calculated using transitions found by Kaur et al.[13] and circularly polarized light with $A = 1$ as a function of its wavelength. The points at which magic wavelengths with the $4s\ ^2S_{1/2}$ state were found are indicated with black.

(36)

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