Simulation of Chromatic Laser Pulse Amplification

Lukas Kuhn

Bachelors thesis
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Abstract

This thesis proposes a model for a single-pass simulation of an ultra-short laser pulse amplification with a Ho:YAG amplification crystal. First, the reader will be introduced to the general laser principle, underlying equations and both main topics being temperature change of the amplification crystal and a spectral profile of the incident seed pulse. Afterwards, the required formalism consisting of the respective rate equations as well as the general transport equation derived from Frantz and Nordvik are explained. The basis of a computer simulation is shown and some of the challenges one has to face are summarized. Especially the dimensional triplet of time, space and wavelength which one deals with in the topic of this thesis will be addressed here. Since particularly ultra-short pulses are broadened in their spectral bandwidth a simulation solution referring to this will be given. To enlarge the simulation possibilities further, a temperature dependent model for the occurrence of heat emergence while for example the pumping process or the amplification process itself is implemented. Therefor two methods to retrieve temperature dependent cross section values are shown, explained and compared with measured data. Those include a method from M. Eichhorn as well as the McCumber equation. To ensure simplicity in the usage of the simulation model the pumping process is implemented as well to retrieve the initial value for the population inversion. Furthermore, the reader will get an overview on the physical principles required for building up an amplification simulation with the mentioned functionalities. The last section provides an outlook, a comparison of the methods and optimization potential.
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1 Introduction

Many of today’s technological breakthroughs have been enabled by the discovery of laser principles made by Albert Einstein in the beginning of the 20th century. From then on scientists all over the world aspire to optimize and further develop those ground braking principles to create the basis for advanced applications. Most of our daily used mobile devices and industry solutions were only possible through massive research in the field of lasers. The variety of applications and technologies is immensely broad. From the medical usage in for example high precision tissue ablation up to approaches in satellite-satellite communication in outer space. Taking the example of the medical use case of tissue ablation, especially ultra-short pulsed lasers enable doctors to perform high precision surgeries with almost no heat penetration as the tissue is vaporized instantly. Another important feature is that one is able to skim a very thin layer of tissue in for example eye surgeries. The complexity of understanding lasers and their behavior leads to the usage of computer simulations to predetermine optimal parameters for different use cases and to reduce experimental costs. Although there are almost no limitations towards complexity and quantum physical theories given, being able to built up such simulations with the use of very few equations which sufficiently describe the general light-matter interaction is surely one of the most fascinating properties of lasers. In this thesis all simulations are performed on a 2%-doped Ho:YAG (Holmiumions in Yttrium aluminium garnet, \( Ho^{3+} : Y_3Al_5O_{12} \)) amplification crystal which is usually operated at wavelengths around 2 µm. With prospect to the mentioned eye surgery application this is of special importance as the mid-infrared region is considered to be "eye-safe". There are a variety of advanced laser simulation software available on the market including [Dr ] for example. The focus of this thesis is to describe the basis implementation of those main equations needed for building up a computer simulation. Sec. 2 is meant to give an insight into the underlying physical principles and to show some of the challenges one is faced with when describing the light-matter interaction. Sec. 3.1 shows the overall approaches made to solve the challenges presented in Sec. 2 and usage of the main equations. The structure and behavior of a computer simulation are introduced in Sec. 3.2 to provide the reader with a first assistance for the build-up of a computer simulation. Afterwards some suggestions on how to deal with chromaticity of the incident laser beam and temperature change of the laser amplification crystal are given in Sec. 3.3 - 3.4. The results of the implemented methods are discussed in Sec. 4. Sec. 5 gives an outlook about possible options on how to further increase accuracy.

2 Theory

This section provides an overview about the theoretical concepts needed to simulate the laser behavior in an amplification crystal. Those include the laser principle, modifications to the equation set to account for chromaticity and methods to provide a temperature dependent model. Furthermore the pumping process before the actual amplification process is explained.

2.1 General physics

To begin, the physical background and available methods are shown and explained in this section.

2.1.1 Laser principle

One of the major principles of quantum physics is the particle-wave-dualism in which a beam of light behaves differently dependent on how the observation is performed [Bal18]. This is especially important when a laser system is described. The incoming laser beam consists of photons propagating in a wavelike shape. The amplification crystal consists of the host material YAG which is doped with \( Ho^{3+} \) impurity ions. To describe the light-matter interaction in an amplification medium one can define the energy states in which the atoms can be found as levels. An atom can change its energy state by for example the stimulation by external photons [Sve10] by for example the photons of the incident laser beam. Without external factors that atom is found at the ground state. To characterize general properties of lasing materials the composition of those levels is of special importance. Therefor the notation of laser levels from zero to four is chosen. The energy levels of Ho:YAG have been measured by [BEZ12] in Fig. 2 by...
performing a laser spectroscopy at 293 K. Reference data can be found in [Ji+17] and [Sko]. From Fig. 2 one can see that that the levels actually consist of many sublevel which makes it difficult to distinguish the notation from zero to four at first. For the case of an Ho:YAG amplification crystal this system can further be described as a quasi-three-level laser system [Eic08]. The upper blue level compose level 2 and 3 according to the notation [Sve10]. The level 0 and 1 form the red levels in Fig. 2 and are separated by a gap which is close to $k_B T$ which is the requirement for a quasi-three-level laser denomination. The positions of the energy manifolds necessary to describe the Ho:YAG laser system are described as $^5J_7$ and $^5J_8$ which are spectroscopic notations [Ter16]. In the steady state of the crystal the atoms are found in the ground energy level. To enable lasing, or stimulated emission of light, of the Ho:YAG amplification crystal a pumping process has to be performed. This takes place before the incoming seed pulse, the pulse which will be amplified, is inserted into the crystal. The pumping process therefor aims to establish a population inversion. The population inversion as the requirement for lasing means that atoms are in an excited energy state. The pumping process therefor inserts for example a pump light into the amplification crystal (Sec. 2.1.5). The energy induced by the photons the pump light is consisting of, will excite the atoms of the amplification crystal. This process is called stimulated absorption. It means that atoms get excited from the ground level to the excited level by consuming a photon. After the pumping process is performed, more atoms are in an excited state. This is a state called population inversion which will roughly persist for 7 ms which is the lifetime of the excited $^5J_7$ energy level if no further energy is supplied to the system [BEZ12]. If this requirement is met the actual amplification of the seed pulse can take place. Therefor a stimulated emission of light is desired. That means that the energy induced by the photons of the seed pulse will deexcite the excited atoms of the amplification crystal eventually. This deexcitation will produce an additional photon which has the same phase, direction and frequency as the stimulating photon [Sve10]. One then has an additional gain to the seed pulse. Exactly this process is the overall desire in the amplification process. As mentioned before the experimental setup states ultra-short pulse amplification so the pulse duration ($ns − fs$ range) is well below the upper state lifetime. That is important for the incident laser beam to gain as much additional energy from the amplification crystal as possible before spontaneous emission can occur. Spontaneous emission occurs when the lifetime of the excited level is exceeded. This will also produce photons but those do (most likely) not have the same phase nor direction which is why they will not increase the gain of the seed pulse. To describe the change of the seed pulse during the propagation through the amplification crystal the equations in this thesis use the assumption of the particle part of the mentioned particle wave dualism. Meaning that one can describe the time dependent parts of the seed pulse by describing its number of photons per time unit. The wave part is used to define the individual photon energies that come with different spectral compositions of the seed pulse. Especially ultra-short seed pulses have no consistent number of photons over the whole duration. That requires a time dependent model which will be further explained in Sec. 3. The change of atoms in the respective energy states of an amplification crystal are described by rate equations which are shown in Sec. 2.1.2. The change of the population of the energy levels is mainly described by the absorption cross section and the emission cross section which are material dependent parameters. Those cross sections usually come from measurements and are explained in Sec. 2.1.3. In this thesis upconversion mechanisms as well as branched fluorescence in which the levels $^5J_5$ and $^5J_6$ are involved are intentionally neglected as the main focus lays on the amplification process [Spr+19].

2.1.2 Rate equation system

To model the behavior of the amplification crystal with prospect to the incoming laser pulse one can use the rate equations for the involved laser level. Those rate equations describe the rate of decay for the respective states [Sve10]. The rate equations for the upper (index $u$) and the ground laser level (index $g$) are:

$$\frac{\delta N_u}{\delta t} = -\frac{N_u}{\tau_u} - \sigma_c cn N_u + \sigma_a cn N_g$$  

$$\frac{\delta N_g}{\delta t} = \frac{N_u}{\tau_u} + \sigma_c cn N_u - \sigma_a cn N_g$$
Where $N_u$ denotes the population of the upper laser level, $N_g$ respectively the one of the ground level [Sve10]. $n$ is the number of photons of the incoming beam. $\sigma_a$ and $\sigma_e$ are the absorption and the emission cross section. Together with the transport equation (Sec. 3.1) necessary to describe the beam propagation through the amplification crystal this equation set is thus sufficiently describing the amplification process. The reader is referred to Sec. 2.1.5 for the procedure for obtaining the initial value for the population inversion. The population inversion is assumed to be homogeneously distributed over the amplification crystal.

### 2.1.3 Cross sections

Two different cross sections exist. These cross sections are parameters describing the transition rate of the stimulated emission or absorption and are a function of the frequency as can be seen in Fig. 1. One can think of it as if a photon enters this cross section it will interact with the atom [Sve10]. The emission cross section $\sigma_e$ describes the section where an incident photon will alter a stimulated emission of light if it enters. The absorption cross section $\sigma_a$ is the exact opposite for stimulated absorption. The cross sections are dependent on temperature, wavelength and material and therefore also the doping concentration.

![NASA Cross sections](image)

Figure 1: Emission and absorption cross section data from the NASA database [Sko]

It is helpful to take a look at the involved energy manifolds $^5I_7$ and $^5I_8$ which consist of many sublevel as can be seen in Fig. 2.

There are 15 sublevel in the $^5I_7$ and 17 sublevel for $^5I_8$ manifold. If one is speaking generally of a laser level 0 for example, usually the lowest sublevel of this manifold is meant. Those sublevel are each separated from each another with different energies assigned (Fig. 2). However, the energy differences between sublevel in one laser level are very small compared to for example the difference between the manifolds itself. For a 2% doped Ho:YAG the difference between the ground (0) and excited level (3) is 5227 eV, the difference within the ground level 154 eV as can be seen in Fig. 2. That is why they can usually be summarized when a laser system is described generally. Especially when temperature changes are under investigation that is no longer sufficient. It is therefore important to take a look at the sublevel as the population distribution between them changes with changes in temperature. This will be further explained in Sec. 2.1.4. An important assumption made on this point is that the lifetime, the duration how long a level is populated until steady state is recovered and spontaneous emission occurs, is well below the lifetime of the whole manifold. This is the requirement for the application of Boltzmann statistics [Sve10]. It is applied to determine the population probability of a sublevel in one energy manifold and is given by Eq. 4. If a single photon interacts with this energy level system it has a specific energy which is given by

$$E = \frac{hc}{\lambda}$$

where $h$ denotes Planck’s constant in eVs, $c$ the speed of light in the amplification crystal in $\frac{m}{s}$ and $\lambda$ the wavelength of the incident photon in $m$. The result is that it is possible to determine the
level this single photon will interact with. In other words, when an incoming photon has an energy equal to the separation between two laser levels of the atom it will induce a absorption or emission process [Ter16] of course based on the assumption that it enters the respective cross section. Those level are populated differently. If one single photon of a specific wavelength with a specific photon energy interacts with the crystal it differs from the probability of another photon with a different wavelength and thus energy will experience. This is because they interact with different sublevel in the energy level. The population distribution of the sublevel in one manifold can be described by the Boltzmann distribution given by

$$f_{g/u,i/j}(T) = \frac{d_{i/j} \exp\left(\frac{-E_{g/u,i/j}}{k_B T}\right)}{\sum d_{i/j} \exp\left(\frac{-E_{g/u,i/j}}{k_B T}\right)}$$  \hspace{1cm} (4)$$

where the index $g$ denotes the index of the $^5I_8$ manifold and $u$ the index of the $^5I_7$ manifold. The index $i$ describes one sublevel starting at the one with the lowest energy within the ground manifold $g$. Index $j$ respectively a sublevel of the upper manifold $^5I_7$. $d$ is the degeneration of the respective sublevel (which is 1 for all sublevel in $^5I_8$ and $^5I_7$ according to the data from [Sko]). The sum is formed over all sublevels in the manifold. The degeneration means that a sublevel consists of of two or more degenerated sublevel itself which are so similar in energy that they count as one. $E$ denotes the energy of the sublevel, $k_B$ the Boltzmann constant and $T$ the temperature.

2.1.4 Temperature

Temperature changes are an important factor in overall laser physics. Those may occur while the pumping process, the amplification process itself or as countermeasure in the crystal cooling process. To grasp the physical background it is helpful to take a look at the energy level of the gain medium in Fig. 2. One reason behind temperature changes in the amplification process itself are relaxation processes. When an interaction process took place, the ion is usually located on one of the sublevel. For absorption that is a sublevel of the laser level $3$. For emission a sublevel of the level 1. Due to the overall desire of atomic systems to relax towards the steady-state, those ions will then further relax to the lowest sublevel of the respective level. That induces an energy
exchange with the host material which results in the production of heat [Ter16]. There are multiple consequences. As mentioned in Sec. 2.1.3 the population probability of the individual sublevel changes with temperature. Which gives therefor one explanation for the temperature dependence of cross sections. With increasing temperature the population of the sublevel will increase for the upper sublevel as can be seen in Fig. 3. At lower temperatures one can expect a lesser population of the upper sublevel.

![Figure 3: Boltzmann laser level occupation probability for $^5I_8$ and $^5I_7$](image)

The Boltzmann distribution gives therefor a simple but still quite accurate explanation. However, there are more processes taking place with temperature changes. One are changed lattice vibrations. Those affect the strength of the crystal field and thus the width of the energy levels. If one takes a look at the specific spectral transition lines those changes then affect the strength, width and position of the lines [DP14]. It is not possible to determine cross section values accurately with just the Boltzmann distribution. A comparison between the calculated values using the McCumber equation and measured data from [Sko] is done in Sec. 4.

### 2.1.5 Pumping process

To start the amplification process a population inversion has to be established by performing a pumping process before. That means that the electrons get excited from the ground level (0) to the excited level (4) by the induced pump light. To quantify this value one has to alter the rate equation set mentioned in Sec. 2.1.2. The pumping process establishes the population inversion by exciting atoms from the ground level 0 to the level 4. The electrons then relax back to the laser level 3 due to the very short lifetime of level 4 almost instantly. To account for the pumping process the pump rate $R_p$ has to be added to the rate equations [Sve10].

\[
\frac{\delta N_u}{\delta t} = R_p N_g - \frac{N_u}{\tau_u} \tag{5}
\]

\[
\frac{\delta N_g}{\delta t} = \frac{N_u}{\tau_u} - R_p N_g \tag{6}
\]

To retrieve the initial population inversion from the applied pump power one has to combine the rate equation set with the following equations.

\[
P_{\text{abs}} = P_{\text{in}} - P_{\text{in,exp}}(\exp(-\alpha L)) \tag{7}
\]

$P_{\text{abs}}$ is the effective pump power where losses are subtracted as can be seen in Eq. 7. Those losses are quantified with the absorption cross section. The losses are higher when the amplification crystal is not long enough to absorb all the incoming photons based on its absorption cross section (Eq. 8).

\[
\alpha = N_{\text{total}}\sigma_a(\lambda = 1908\text{nm}) \tag{8}
\]
The value of the absorption cross section is here determined by the usual pumping wavelength of 1908 nm. This is chosen because Ho:YAG has the highest absorption cross section at this wavelength (Fig. 5). The pumping process is thus most efficient at this wavelength. \( n_{\text{total}} \) is the total number of atoms in the amplification crystal.

\[
E = P_{\text{abs}}t
\]  \( (9) \)

The number of induced photons is given by the pump power over time. To retrieve the initial value for the population inversion one uses the threshold where Eq. 5 to Eq. 9 will converge to over time as can be seen in Fig. 4. The methodology is further explained in Sec. 3.1.

![Figure 4: Convergence of population of the upper laser level over time](image)

Figure 4: Convergence of population of the upper laser level over time

![Figure 5: Absorption cross section measured by [BEZ12] at 295 K](image)

Figure 5: Absorption cross section measured by [BEZ12] at 295 K

3 Methodology

In this section the used methods are displayed and explained. Please note that the following equation set and methodology is limited to the simulation model in this thesis which is an ultra-short Lorentzian-shaped pulse amplification simulation with a Ho:YAG amplification crystal.

3.1 Numerical method

The numerical discretization of the original Frantz-Nodvik equations has been previously presented and discussed in [Spr+18] and [Spr+19]. In the following section those equations are displayed and
explained. The transport equation to account for the photon propagation for a Lorentzian-shaped pulse is derived from Frantz and Nodvik [FN63].

\[
\frac{\delta n}{\delta t} + c \frac{\delta n}{\delta x} = \sigma_e c n \Delta 
\]  

(10)

\(n\) denotes the number of photons, \(\Delta\) the population inversion in \(\text{cm}^{-3}\) and \(c\) the speed of light in the amplification crystal in \(\text{m/s}\). It is thus the main equation needed to express the laser beam change within the laser crystal. With an implicit Euler discretization according to [Spr+19] Eq. 10 derives to:

\[
n_{i+1}^{k+1} = n_i^k (1 + \sigma_e h \Delta_i^k) 
\]  

(11)

While the equations are not so complex in structure one has to pay special attention to the indices used. The index \(k\) denotes time, index \(i\) space according to Fig. 6. To describe the population inversion change [Spr+18] uses the following equation presented by [Sve10].

\[
\Delta = N_u - \frac{\sigma_a}{\sigma_e} N_g 
\]  

(12)

The discretization of Eq. 1 and 2 leads to:

\[
N_{u}^{t+1} = N_{u}^{t} + \Delta_t (-\sigma_e c n_{u}^{t+1} N_{u}^{t} + \sigma_a c n_{u}^{t+1} N_{g}^{t}) 
\]  

(13)

\[
N_{g}^{t+1} = N_{g}^{t} + \Delta_t (-\sigma_e c n_{u}^{t+1} N_{u}^{t} - \sigma_a c n_{u}^{t+1} N_{g}^{t}) 
\]  

(14)

where \(\Delta_t\) denotes the time step for the chosen grid.

The same method is applied to the rate equations for the pumping process. One can therefor write:

\[
N_{u}^{t+1} = N_{u}^{t} + \left( R_p - \frac{N_{u}^{t}}{\tau_u} \right) \Delta t 
\]  

(15)

\[
N_{g}^{t+1} = N_{g}^{t} - \left( R_p - \frac{N_{u}^{t}}{\tau_u} \right) \Delta t 
\]  

(16)

In order to simulate a beam propagation trough a gain medium one has to discretize the rate equations as shown above. In this thesis a numerical solution of those differential equations is applied. The accuracy of this method was previously proven by for example [Spr+19] and will thus be no subject here. The convergence test was passed successfully. To describe the amplification process two different sets of equations are necessary. One, to describe the behavior of the crystal where change of population inversion is important. The other one is used to describe the change of the incoming laser pulse, which can be described mainly by the amount of photons per time unit. To get those two sets together its necessary to differentiate between space-, for the crystal, and time-dependency, for the beam. As previously described by [Spr+19] one can therefor use the grid in Fig. 6.

![Figure 6: Simulation grid from [Spr+19]](image)
Here, the two dimensions are represented by two overlapping grids. To differ between time and space the denomination of point and cell data is used. The cell data represents the population inversion of one crystal slice which changes after each beam slice has passed. The point data represents the number of photons of one beam slice which changes after each crystal slice has been passed. One can then simulate the propagation (Fig. 12).

### 3.2 Implementation

There are various different approaches when building up a computer simulation for a laser amplification. The one presented here intents to display an object based structure which is meant for easy implementation and trial and error purposes.

#### 3.2.1 Code structure

The object based approach with Python (3) leads to a simulation program with the three classes shown in Fig. 7. The main functions and variables are explained in this section.

1. Simulation class
   (a) Functions
      i. run(): Executes the simulation and stores values in the results array. Special attention is required for the correct propagation of the laser beam through the amplification crystal over all three dimensions according to Fig. 6 and the methodology in Sec. 3.3. The algorithm is shown in Alg. 1.
      ii. population_inversion_update(): Contains Eq. 12.
      iii. rate_equation_nX_update(): Contains Eq. 1 or Eq. 2.
      iv. photon_density_update(): Contains Eq. 11.
      v. pump_process(): Calculates the initial value for the population inversion according to Sec. 3.1 and Sec. 2.1.5.
   (b) Variables
      i. grid_points: Global parameter defining the slices both the pulse and crystal are cut into. According to Fig. 6 having the same sizes for both dimensions simplifies the overall implementation.
      ii. pump_energy: Defines the amount of inserted pump energy in Watt to calculate the initial population inversion.
      iii. results: Four dimensional array to store all data over the three dimensions (time, space, wavelength). The last one defines the saved parameter, for example [0] = population inversion, [1] = density and so forth. The storage of all values at each dimension in one array enables detailed information about the evolution within the amplification crystal and simplifies data analysis and plotting.

2. Pulse class
   (a) Functions
      i. construct_lorentzian_pulse(): Applies a Lorentzian distribution of the total number of photons the pulse is consisting of and returns an array containing the number of photons for each pulse slice according to chosen grid size in the Simulation class.
      ii. construct_lorentzian_spectrum(): Takes the array returned by the pulse construction and applies a Lorentzian distribution for the number of photons over the specified wavelengths in spectral_range and returns an array for the usage in the Simulation class.
   (b) Variables
      i. pulse_profile: A string defining the pulse shape over time. In this thesis this is limited to ‘Lorentzian’ due to Eq. 11.
      ii. fwhm, total_number_of_photons_per_unit_area, duration: Parameters defining the Lorentzian function for construct_lorentzian_pulse().
iii. spectral_profile: A string defining the spectral shape over the wavelengths.

3. Crystal class

(a) Functions

i. eichhorn_cross_section_approximation()

A. curve_fitting_for_ref_data(): Applies Lorentzian curve fitting over given reference cross section data. A polynomial approximation is recommended before. To save development time the reader is referred to the scipy.optimize.curve_fit library when using Python. As mentioned in Sec. 3.4.1 the locations of the Lorentzian functions are chosen manually. Each of those sections is then fitted to the Lorentzian functions which together compose the spectral range of cross sections for the reference data.

B. lorentzian_approximation(): With the functions gR(), fR(), lambdaIJ(), omegaIJ() it is then possible to simulate the temperature defined in Crystal.temperature according to Sec. 3.4.1.

(b) Variables

i. energy_levels: Contains all the energies of the respective amplification crystal according to Fig. 2.

ii. n2_lifetime: Lifetime of the upper laser level 2.

---

3.2.2 Code process

The overall simulation behavior can be summarized to three major steps. First a pulse object is created, then a crystal object, which then both are assigned to a simulation object where the simulation is executed. The pulse class has to account for the following tasks. The first step after initializing all required parameters is that the pulse can be created on the time dimension (the
number of photons per unit time) according to the specified profile (Lorentzian, Super-Gaussian, etc.). That also includes the division to the desired slice number or grid size. It is important to have in mind, that the grid size has to be a global parameter. The number of slices for the pulse equals the number of slices for the crystal in the proposed model in Fig. 6. Afterwards, the assignment of spectral profiles to each pulse slice takes place where the number of photons per unit time gets split upon the wavelengths. The main element of the pulse object is an array containing all amounts of photons for both the time and wavelength dimension. The crystal class contains all material specific parameters. To implement the temperature dependence the crystal class does the cross section approximation according to the specified crystal temperature. This is done according to the Eichhorn method described in Sec. 3.4.1 and the McCumber method from Sec. 3.4.2. With the existing reference cross sections for at least two temperatures one can divide those curves into sections and then approximate the Lorentzian functions and calculate the temperature parameters. After the assignment of a pulse and laser object the simulation object creates the output array according to the model in Fig. 6. The simulation class calculates the initial population inversion dependent on the specified pumping power and crystal temperature and length for the sake of simplicity. The execution is then started according to Alg. 1. This is the iteration of all pulse slices through the crystal slices for all wavelengths.
Algorithm 1: run() execution algorithm of simulation class

for time = 0 to grid_points * 2 do
    if time == 0 then
        for step = 0 to 2 do
            if step == 0 then
                foreach wavelength do
                    /* fill array with initial values which is here just the number of photons per time unit per wavelength since step==0 is still outside of crystal */
                if step == 1 then
                    foreach wavelength do
                        photon_density_update(population inversion (initial); total number of photons (time; step-1))
                else if time < grid_points then
                    for step == 0 to grid_points + 1 do
                        /* first step of array is the representation of pulse and thus not included in the grid_points value */
                        if step == 0 then
                            foreach wavelength do
                                /* fill array with initial values which is here just the number of photons per time unit per wavelength since step==0 is still outside of crystal */
                            else if step == 1 then
                                foreach wavelength do
                                    rate_equation_update(population inversion (time-1; step))
                                    photon_density_update(population inversion (time; step); total number of photons (time; step-1))
                        else if time == step - 1 then
                            foreach wavelength do
                                photon_density_update(population inversion (initial); total number of photons (time-1; step-1))
                        else
                            foreach wavelength do
                                rate_equation_update(population inversion (time-1; step-1))
                            foreach wavelength do
                                photon_density_update(population inversion (time; step); total number of photons (time-1; step-1))
            else
                foreach wavelength do
                    rate_equation_update(population inversion (time-1; step-1))
                if time - step != grid_points - 1 then
                    /* propagate pulse only if there are still slices in crystal */
                    photon_density_update(population inversion (time; step); total number of photons (time-1; step-1))
else if grid_points <= time then
    /* total number of photons = 0 (pulse duration exceeded) */
    for step = 1 to grid_points + 1 do
        foreach wavelength do
            rate_equation_update(population inversion (time-1; step-1))
            if time - step == grid_points - 1 then
                /* propagate pulse only if there are still slices in crystal */
                photon_density_update(population inversion (time; step); total number of photons (time-1; step-1))
3.3 Chromatic spectrum

The spectral components of the incoming pulse can be simulated by cutting the pulse number of photons per time unit into slices. Each of those slices has a specific amount of photons which of course depends on the time dimension and consequently on the number of slices. One can then assign a specific spectral profile to each of the pulse slices as can be seen in Fig. 8. This is in this case a Lorentzian shaped distribution where the integral matches the number of photons per time unit of the respective time slice. Each of the wavelengths in that spectral profile has then a certain amount of photons.

![Figure 8: Schema of the assignment of spectral components](image)

To account for each wavelength influence on both the pulse number of photons per unit time and population inversion the simulation will calculate Eq. 1, 2 and the transport equation Eq. 11 for each wavelength. That enables the usage of the wavelength related cross section. With that the spectral composition of the pulse is simulated. An especially difficult decision is how to divide the population inversion upon the different wavelengths. Or on a even lower level how to divide the population between $N_g$ in Eq. 1 and $N_u$ in Eq. 2 and consequently all the sublevel. This is a requirement for the proposed calculation method itself. By applying the rate equations to each individual wavelength one has to start with an initial parameter set for the population of both upper and lower laser level. More accurately an initial value set for $N_g$ and $N_u$ is needed. As per definition the Boltzmann distribution of photons for the sublevel is a probability (Eq. 4). One could therefore attempt to split the number of photons based on the Boltzmann distribution upon the respective sublevel. That would mean that one is able to define the population of each sublevel after the pumping process. As the physical support for that is highly spongy the proposed model in this thesis splits the initial values for the population of both upper and lower laser level evenly upon the respective sublevel. This still enables a chromatic approach and increased accuracy by using the rate equations with the associated wavelength dependent cross section.

3.4 Gain medium and temperature change

To simulate a temperature change of the amplification medium the presented formalism will use temperature dependent cross sections. The temperature is assumed to be homogeneously distributed over the amplification crystal.

3.4.1 Eichhorn

To obtain temperature dependent cross sections the simulation model in this thesis uses the model presented in [Eic+08] and [Eic08]. The implementation and used equations will be explained in this section. As the proposed method is based on measured data one has to obtain data about the cross sections for at least two different reference temperatures. From that data one can calculate the temperature dependent parameters (Eq. 17 - Eq. 20) used for the method. As mentioned in Sec. 2.1.3 the Boltzmann distribution is not the only contribution factor in temperature change. It is therefore necessary to also quantify the respective shift and the width of the transition line where the model of [Eic08] uses the following two equations. For the line shift one has to calculate the respective value of Eq. 17 for the existing reference temperatures.
\[
f_R(T) = \left( \frac{T}{\Theta_S} \right)^7 \int_0^{\Theta_S} \frac{x^6 \exp(x)}{(\exp(x) - 1)^2} dx
\]  
(17)

Then the line shift for the transition line is given by:

\[
\frac{1}{\lambda_{ij,0}(T)} = \frac{1}{\lambda_{ij,0}} + \left( \frac{1}{\lambda_{ij}(T_0)} - \frac{1}{\lambda_{ij,0}} \right) \frac{g_R(T)}{g_R(T_0)}
\]  
(18)

For the line width respectively:

\[
g_R(T) = \left( \frac{T}{\Theta_S} \right)^4 \int_0^{\Theta_S} \frac{x^3}{\exp(x) - 1} dx
\]  
(19)

with:

\[
\omega_{ij}(T) = \omega_{ij,0} + \left( \omega_{ij}(T_0) - \omega_{ij,0} \right) \frac{f_R(T)}{f_R(T_0)}
\]  
(20)

Here \( \Theta_S \) denotes the spectroscopic Debye temperature in K, \( \lambda_{ij,0} \) is the transition center and \( \omega_{ij,0} \) the full width at half maximum. It is further important that the approximated Lorentzian functions do not change their integrals when simulating different temperatures as can be seen in Eq. 22. The next step is to determine the transitions which are then approximated with Lorentzian functions. In this thesis this is done manually. However, one could also determine those by directly analyzing the reference data of the cross sections. After a polynomial regression over the measured data it is easy to determine the maxima. It is then possible to set the minima between a maximum as borders and run a curve fitting based on a Lorentzian shape. For further explanation of the implementation the reader is referenced to Sec. 3.2. After the desired spectral range for at least two reference temperatures is approximated with Lorentzian functions those are then coupled with Eq. 17-20. For that the underlying Lorentzian approximation function for in this case the absorption cross section is:

\[
\sigma_{a,ij}(\lambda, T) = \sum_{ij} f_{g,i}(T) \sigma_{a,ij}(\lambda - \lambda_{ij}^a(T), \omega_{ij}^a(T), A_{ij}^a(T_0))
\]  
(22)

One has to mention here, that the functions are not added to another. The combination of the functions will deliver the absorption cross section range by taking the maxima over all functions at each wavelength. The physical background for the Lorentzian shaped approximation is based on the mechanisms contributing to the line broadening of the optical transition. For the case of an crystalline host material, which is here yttrium aluminium garnet, the predominant mechanism is homogeneous broadening. Therefore the Lorentzian shape describes the optical transition line shape according to [Ter16] and [Sve10].

### 3.4.2 McCumber

Derived from the Einstein relations connecting absorption and emission rates of atoms in free space, McCumber extended those relations to solids [McC64]. Sometimes his method is also referred to as generalized Einstein relationship. With the Boltzmann distribution the derived equations put the absorption cross section \( \sigma_a \) and emission cross section \( \sigma_e \) in direct relation and allow the calculation of absolute values. The underlying requirement for this formalism to be applied is that the lifetime of the laser level is greater than the time needed to establish a thermal equilibrium within that manifold [Ter16],

20
\[
\sigma_a(\nu) = \sigma_e(\nu) \exp \left( \frac{h\nu - E_0}{k_B T} \right)
\] (23)

Where \( \nu \) denotes the frequency and \( E_0 \) the energy difference between the lowest sublevel of the both laser level manifolds. With this equation it is then possible to calculate one cross section from the other. In the research performed during this thesis other methods such as the Füchtbauer-Ladenburg and Judd-Ofelt theories have been studied. Those have not been implemented for complexity reasons which would have extended the scope of this thesis.

3.4.3 Combination of methods

To obtain a method which delivers temperature dependent cross sections and thus enables a temperature dependent simulation model it is necessary to combine the two previously described methods. As mentioned in Sec. 3.4.1 the Eichhorn model approximates temperature dependency of cross sections based on reference data. The McCumber method (Sec. 3.4.2) is then able to calculate the corresponding counter part, in this case the emission cross section. With the chromatic approach from Sec. 3.3 one obtains then a chromatic temperature dependent laser amplification model.
4 Results

This section gives the reader an overview about the accuracy and applicability of the previously mentioned methods. A comparison with other possible methods is found in Sec. 4.1. Furthermore some ideas for a more advanced simulation program are given.

4.1 Comparison of methods

The McCumber theory provides a useful instrument to calculate the absolute values of one cross section from another one for a given temperature. In this thesis the aim is to provide cross section data for all operating temperatures without gap. The McCumber methods delivers just a partial solution therefor. This partial solution is chosen to provide emission cross section values because of insufficient available emission cross section data for Ho:YAG crystals. As one can see from Fig. 9 the usage of the McCumber method for a Ho:YAG amplification crystal returns values which underestimate the measured data by $\approx 40\%$. Here, the McCumber method is applied on the approximated absorption cross section data retrieved from the Eichhorn method.

![Figure 9: Comparison of cross sections obtained from the Eichhorn and McCumber methods with NASA data](image)

The deviation of the McCumber method to the measured data can be explained by the considered factors. The main assumption made by the McCumber method is that the population of the sublevel of one manifold is according to the Boltzmann distribution (Eq. 4). Another assumption is that $k_B T$ is small compared to the width of the individual Stark level [Qui02]. That is only partially true for Ho:YAG. At lower, lets assume cryogenic temperatures $k_B T (T = 4 K) \approx 5 \, cm^{-1}$ for room temperatures the value rises to $k_B T (T = 298 K) \approx 372 \, cm^{-1}$. From Fig. 2 one can obtain the average value of energy separation for the upper and lower manifold. That is $\Delta E_l \approx 33 \, cm^{-1}$ for the lower and $\Delta E_u \approx 10 \, cm^{-1}$ for the upper manifold. Especially at rising temperatures where $k_B T$ is increasing the second applicability assumption is not fulfilled. Another explanation is the high energy gap between the $8^{th}$ and $9^{th}$ sublevel of the lower manifold which is comparable high with $\Delta E_{8,9} \approx 236 \, cm^{-1}$. Since the McCumber equation calculates absolute values via the multiplication of a factor there is no account taken for any shift. That becomes clear if one takes a look at the measured cross sections in Fig. 1 at for example the absorption cross sections at 2094 nm and 2097 nm. The minimum and maximum are shifted to the left for the emission cross sections. Exactly that shift is not realizable with just a factor multiplication. The overall result for the applicability of the McCumber method in the scope of this thesis is therefor not very satisfying and is implemented because of the initially mentioned lack of measured data and complexity of other methods. The information about the ratio of absorption cross section to emission cross section is lost with this approach. As can be seen in Fig. 10 the ratio of the turquoise line which shows the measured data at 298 K is changing over the shown spectral range. At the peaks of the emission cross section, for example 2089 nm and 2097 nm, the ratio is lower than in the valleys at 2082 nm.
or 2094 \text{ nm}. Exactly this information is lost when one calculates the emission cross sections with the McCumber method over the whole spectrum. That leads to an underestimated gain and an overestimated loss of the seed pulse in the amplification process. Still, the trend is shown correctly by the McCumber method. One can observe that the decreasing trend of the blue, green and red lines follows the average of the measured data quite well. The averaged decreasing trend is therefore well approximated.

Figure 10: Ratio of emission and absorption cross section data at different temperatures

As explained in Sec. 3.4.1 the Eichhorn method can be generally described as a temperature dependent interpolation of measured data. Together with the equations 17 - 20 it is possible to determine the temperature dependency more accurately than for example the McCumber method does by including more assumptions than just the temperature dependent Boltzmann distribution. Also the approximation with a Lorentzian shaped line appears to be suitable and delivers a high degree of precision as can be seen in Fig. 11 for the yellow and red colored lines and follows [Ter16] and [Sve10]. Especially the temperature dependent overall values but also the shift for the respective transition lines are under investigation in this thesis since those cannot be simulated with for example the McCumber method. That is observable for example at the transition line between 2087 nm – 2094 nm where the peak shifts slightly to the left and the overall function compresses with decreasing temperature. However, the absolute values of the respective approximations do not deliver the expected accuracy as can be seen when one compares the approximated and measured values for 83 K and 175 K. There are various different reasons for that where two are explained here. The first being that the application of the Eichhorn method was performed on a large spectral shape or in other words a low spectral resolution. That means that all cross sections for example in the range 2087 nm – 2094 nm are approximated with one Lorentzian function. One can observe that there are a lot more transition lines which one can all approximate and describe by unique Lorentzian functions which might result in a decreased accuracy from the measured data in Fig. 11. However, that would require a high degree of well resolved transition lines for the measured data and the determination of affiliated lines. According to [Ter16] the resolution of the individual Stark levels gets especially for triply ionized rare-earth ions higher at cryogenic temperatures. The data from [BEZ12] in Fig. 2 is obtained at 293 K. The same issue arises with the spectroscopic Debye temperature which is different to the usual Debye temperature as stated by [Eic08]. Data was only available for the host material YAG and is thus insufficiently accurate. One can therefore expect some improvement potential for both McCumber and Eichhorn method by using data obtained from a spectroscopy performed at lower temperatures. Such data is not yet available to the best of the authors knowledge. If one takes a look again at the measured data in Fig. 11 it is apparent that that this determination is possible for single peaks at for example the one at 2092 nm for all given
temperatures. For the spectral range between 2080 nm - 2085 nm however that imposes a more difficult task. Therefore one needs to determine the underlying involved sublevels from the obtained cross section data in order to be able to identify togetherness of transition lines and to describe their change with temperature. The second reason might be that the approximation with Lorentzian line shapes follows the assumption of solely homogeneous broadening of the Ho:YAG amplification crystal [Sve10] [Ter16]. According to [Sve10] [Ter16] it is the predominant broadening mechanism and it is thus possible to use Lorentzian shaped transition lines. In turn it is not possible to neglect inhomogeneous broadening mechanism completely since the crystal quality can not be assumed to be perfect. The overall trend that laser operation of Ho:YAG at lower temperatures delivers a higher emission cross section and a lower absorption cross section and therefore a higher gain potential is shown by both the Eichhorn method and the measured data by [DrB]. This outlines the importance of the cooling setup while operating Ho:YAG amplifiers. The sharp bends in the absorption cross section lines obtained from the Lorentzian approximation are not conform with the measured data as one can see in Fig. 9. Those are a result of the low spectral resolution used in this implementation which was mentioned before. The described enhancement in resolution, meaning the approximation with more Lorentzian functions, is expected to offer an improvement potential therefor. One has to keep in mind that the heat distribution in an amplification crystal in reality is not homogeneously distributed. The described model here is dividing the crystal into same sized slices. Although the present model does assume a homogeneous heat distribution it is implementable to assign a specific temperature to each of the crystal slices. This is meant to further increase accuracy. To account for the punctual heat generation while for example the pumping process or due to the incident seed pulse the model has to be altered towards a three dimensional approach. The present model is in the described structure thus a simplified two dimensional approach. Two other methods have been under consideration as substitution for the McCumber method. The Judd-Ofelt theory delivers a prediction of emission cross section data based on known transitions. It is then possible to obtain the transition rates as well as lifetimes from general parameters of the transition such as initial and final state combined with parameters obtained from measurements of the oscillator strength [Ter16]. As already mentioned in Sec. 3.4.2 this theory exceeds the scope of this thesis and is not implemented. However, [Ter16] implies an accuracy of 10-15% for rare-earth ions which excels the accuracy of the McCumber method applied in this thesis. The Füchtbauer-Ladenburg theory provides a method to obtain the emission cross section from the radiative lifetime [Ter16] as well. This method was also not implemented in this thesis as the McCumber method showed promising results.

Figure 11: Comparison of the absorption cross sections obtained from the Eichhorn method with the measured data from NASA
This strong object based approach enables an easy to use simulation program while being able to easily vary different parameters and run multiple simulations parallel. Changes in code behavior or structure are faster to implement and less error-prone. The downside of a high computing time which also comes with Python is in this case acceptable. Fig. 12 shows an example of the pulse propagation according to the methodology described in Sec. 3.

![Propagation of pulse through Ho:YAG amplification crystal](image)

Figure 12: Propagation of pulse trough amplification crystal according to grid from [Spr+19]

The overall change of population inversion due to a different composition of the seed pulse can be observed best in Fig. 13. The population inversion (Eq. 12) is decreasing most at wavelengths where the emission cross section peaks are. Accordingly, the spectral component gets amplified more.

![Population inversion behavior in amplification process](image)

Figure 13: Population inversion for spectral range of 2080 nm to 2110 nm before and after amplification process

Due to the rate equations the population over the respective laser levels changes differently with a different spectral composition of the seed pulse. That can be observed in Fig. 13. The upper lines show the population inversion before the amplification process. As mentioned in Sec. 3.3 the initial values are assumed to be equally distributed over the whole spectrum. The idea to account for a chromatic spectrum of the seed pulse is best seen when one compares the lines in Fig. 13 before and after the amplification process. A wavelength dependent population inversion can be observed after the seed pulse has passed the amplification crystal. The shape is defined by the cross sections in Fig. 9 which were obtained by the Eichhorn and McCumber method. With consideration of Eq. 12
the gain of the seed pulse leads to a lower population inversion in the amplification crystal. One can say that the population inversion for a wavelength decreases more if this wavelength experiences a high gain. With relation to the cross sections this wavelength will enter the respective cross section more likely since its value is higher and thus interact more likely with the amplification crystal. Especially for the valleys in Fig. 13 this means that those wavelengths get amplified most for the shown spectral range. Dependent on the spectral composition of the seed pulse the amplification is thus more or less efficient.

5 Conclusion

A laser amplification model with an object based Python approach has been presented. This thesis is meant to provide a first assistance in the field of laser amplification simulations. Therefor the needed equations are displayed and explained. The implementation of the simulation grid shown in Fig. 6 by [Spr+19] has been explained with the structure in Sec. 3.2. Additionally the determination of the initial population inversion with a given pumping power can be simulated according to Sec. 2.1.5. Several methods have been under investigation during the research performed for this thesis. The physical background of these has been explained. The two most promising methods being the McCumber and Eichhorn methods were implemented. The comparison with measured data for both methods were not able to deliver results fulfilling the initial expectations. However, some improvement options were given which are estimated to provide more accurate values. The mentioned assumptions and the underlying physical processes can be extended and taken into account. Since the available data on cross section for Ho:YAG is insufficient especially for the reference data based Eichhorn method one can expect a better potential with increasing research done with this type of amplification crystal. To get a better basis for the usage of all the mentioned methods the spectroscopic analysis of the energy levels of a Ho:YAG crystal at cryogenic temperatures seems indispensable. The usage of Python to build up a simulation program was a perfect fit especially since many different methods have been implemented and investigated. Also the object based code structure helps with this trial and error purpose. Changing different components like the crystal or the pulse becomes an isolated task which can be altered without affecting for example the pulse propagation routine. Also experimenting with different simulation parameters such as temperature or spectral composition becomes a handy task with the possibility to swap pulse or crystal objects between different simulations parallel. [Eic08] applied his method for Ho:YAG at the transition line at $2121 \text{ nm}$. The continuous decrease of the absorption cross sections for decreasing temperatures has been shown. This trend is also observable in Fig. 9. However the desired accuracy shown for example for $\text{Er}^{3+}:YAG$ at $1532 \text{ nm}$ could not be reproduced for the case of Ho:YAG in this thesis. That being said and with prospect to the available methods to obtain temperature dependent cross section this attempt still appears to be the most promising one. As explained before the method presented by [Eic08] considers a plurality of physical processes. It is therefore recommended to use the Eichhorn method as well for the emission cross section if the required data is available.
## Parameters

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<tr>
<th>Description</th>
<th>Symbol</th>
<th>Unit</th>
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</tr>
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References


