On the Theory of Direct Frequency Comb Spectroscopy

Börge Hemmerling

Physikalisch Technische Bundesanstalt, Braunschweig
boerge.hemmerling@quantummetrology.de

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Contents

1 Introduction

This is a summary on a theoretical description of the interaction of a fs-pulsed laser with a multi-level atom. The basic algorithm described here is adapted from the papers of Daniel Felinto [1, 2]. Furthermore, the implementation of the corresponding Matlab simulations is discussed and first tests and results are presented.

2 Theory

In this chapter a mathematical description of the properties of a fs-pulsed laser field in the time and frequency domain. Later we investigate the interaction of a multi-level atom with such a laser field in the scope of the optical Bloch equations with the density matrix approach.

2.1 Frequency Comb

2.1.1 Time Domain

Let $E_k(t)$ be the electric field of a single pulse

$$E_k(t) \quad = \quad \sigma(t) \cdot \left(e^{i\omega_c t + i\phi_k} + e^{-i\omega_c t - i\phi_k} \right) \tag{1}$$

where $\sigma(t) \in \Re$ is the envelope function[1], ω_c the carrier frequency of the laser and ϕ_k represents the carrier-envelope phase.

A train of p pulses is then given by

$$E_T(t) = \sum_{k=0}^{p} E_k(t - t_k) = \sum_{k=0}^{p} \sigma(t - t_k) \cdot \left(e^{i\omega_c (t - t_k) + i\phi_k} + e^{-i\omega_c (t - t_k) - i\phi_k} \right) \tag{2}$$

where

$$\begin{aligned} t_k &= \frac{k}{\nu_R} & (3) \\ \phi_k &= \phi_0 + k \cdot \delta\phi & (4) \\ \delta\phi &= 2\pi \cdot \frac{\nu_0}{\nu_R} = \omega_0 \tau_R & (5) \end{aligned}$$

We call $\nu_R = \tau_R^{-1}$ the repetition rate, $\omega_0 = 2\pi\nu_0$ the offset frequency, ϕ_0 initial offset phase and $\delta\phi$ the pulse-to-pulse phase shift. The reasons for these designations will become clear in the frequency domain which is considered in the following section.

[1] This function is many times represented by a gaussian or a sech, i.e. $\sigma(t) = e_0 \cdot \mathrm{sech}(t/\sigma)$.

2.1.2 Frequency Domain

We now calculate the fourier spectrum of the train of pulses $E_T(t)$

$$\begin{aligned}
\mathrm{FFT}\left\{E_T(t)\right\} &= \sum_{k=0}^{p} \mathrm{FFT}\left\{E_k(t-t_k)\right\} \tag{6}\\
&= \sum_{k=0}^{p} \mathrm{FFT}\left\{\sigma(t-t_k)\cdot\left(e^{i\omega_c(t-t_k)+i\phi_k}+e^{-i\omega_c(t-t_k)-i\phi_k}\right)\right\} \tag{7}\\
&= \sum_{k=0}^{p} \mathrm{FFT}\left\{\sigma\left(t-t_k\right)\cdot\left(e^{i\omega_c(t-t_k)+i\phi_k}+c.c.\right)\right\} \tag{8}\\
&= \sum_{k=0}^{p} \left\{e^{-i\omega t_k+i\phi_k}\sigma_F\left(\omega-\omega_c\right)+e^{-i\omega t_k-i\phi_k}\sigma_F\left(\omega+\omega_c\right)\right\} \tag{9}\\
& \tag{10}
\end{aligned}$$

$\sigma_F(\omega)$ corresponds to the fourier transform of the envelope function. The second term is left out since it only represents the (symmetric) negative frequencies.

$$\begin{aligned}
\mathrm{FFT}\left\{E_T(t)\right\} &= \sigma_F\left(\omega-\omega_c\right)\cdot\sum_{k=0}^{p} e^{-i\omega t_k+i\phi_k} \tag{11}\\
&= \sigma_F\left(\omega-\omega_c\right)\cdot\sum_{k=0}^{p} e^{-i\omega\frac{k}{\nu_R}+i\phi_0+ik\delta\phi} \tag{12}\\
&= \underbrace{\sigma_F\left(\omega-\omega_c\right)}_{\text{envelope}}\cdot e^{i\phi_0}\cdot\underbrace{\sum_{k=0}^{p} e^{-i(\omega-\omega_0)k\tau_R}}_{\text{comb structure}} \tag{13}
\end{aligned}$$

The sum can be simplified. See Appendix (A.1).

$$\mathrm{FFT}\left\{E_T(t)\right\} = \sigma_F\left(\omega-\omega_c\right)\cdot e^{i\phi_0}\cdot e^{-i(\omega-\omega_0)\frac{p}{2}\tau_R}\cdot\left\{\frac{\sin\left(\frac{1}{2}(\omega-\omega_0)(p+1)\tau_R\right)}{\sin\left(\frac{1}{2}(\omega-\omega_0)\tau_R\right)}\right\} \tag{14}$$

The extrema of this function are found at the condition

$$\begin{aligned}
(\omega-\omega_0)\cdot\tau_R/2=\pi\cdot n \qquad \text{with} \quad n\in\{0,1,2,\ldots\} \tag{15}\\
\tag{16}
\end{aligned}$$

With $\tau_R^{-1}=\omega_R/2/\pi$ we find the following condition for the peaks in the spectrum

$$\boxed{\omega=\omega_0+\omega_R\cdot n \qquad (17)}$$

This periodic structure corresponds to a frequency comb. The offset frequency ω_0 which has been designated in the beginning of this chapter results from the pulse-to-pulse phase shift. The repetition rate of the laser pulses is reflected in the periodic structure of the comb teeth.

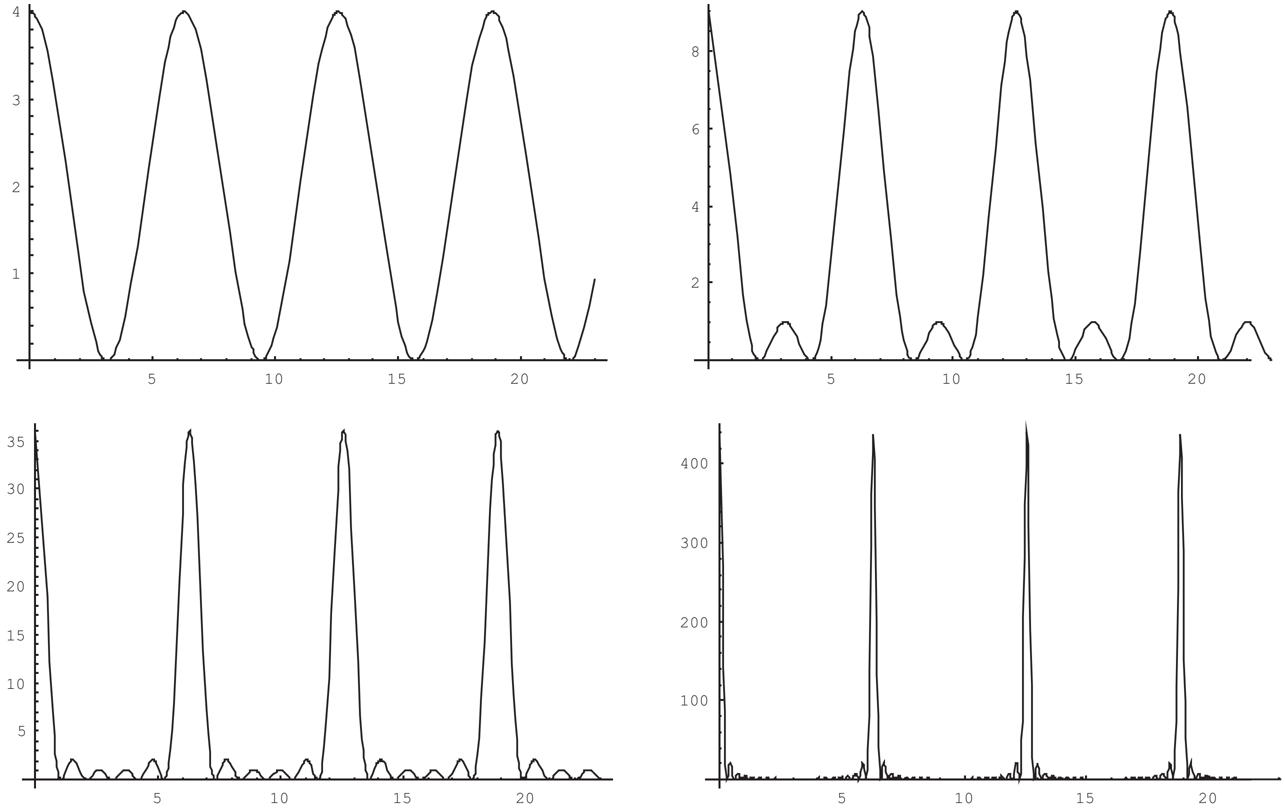

Figure 1: The power comb spectrum excluding the envelope $P(\omega)/|\sigma_F\left(\omega-\omega_c\right)|^2$ is depicted. The difference in the pictures is the number of total pulses (top left: 1, top right: 2, bottom left: 5, bottom right: 20) We clearly see the creation of the comb teeth after the interference of even a small number of pulses.

The power spectrum of the comb is giving by the square of the fourier transform of the electric field

$$P(\omega)=|\mathrm{FFT}\left\{E_T(t)\right\}|^2 \quad = \quad |\sigma_F\left(\omega-\omega_c\right)|^2\cdot\left\{\frac{\cos\left(\left(\omega-\omega_0\right)\cdot(p+1)\cdot\tau_R\right)-1}{\cos\left(\left(\omega-\omega_0\right)\cdot\tau_R\right)-1}\right\} \tag{18}$$

The power value at the position of the comb teeth is by[2]

$$P(\omega_0+\omega_R\cdot n)=|\sigma_F\left(\omega_0+\omega_R\cdot n-\omega_c\right)|^2\cdot(p+1)^2 \tag{19}$$

In Fig. 1 a comb spectrum for a different total number of pulses is shown.

[2] Derived by the rule of L'Hopital.

2.2 Time Evolution of the Atomic System

We describe the interaction of the pulsed laser with a multi-level atom in the scope of the optical Bloch equations. Numerically, the major problem here is the existence of two thoroughly different time scales, i.e. the repetition rate (typically ns) and the pulse width (typically fs). In order to circumvent this problem we derive an algorithm that outputs the state of the atom after the interaction with one pulse. At the same time we loose the information about the detailed time-evolution on the much shorter time scale which is fortunately for our experiment not of any importance. However, the resulting new state of the atoms will then be used as input to the same algorithm, so that one can iteratively get the final density matrix for a certain number of pulses.

2.2.1 Definition of the Atom-Laser-Ion Trap System

The atom is represented by a set of energy states

$$|i\rangle \quad \text{with} \quad i = 1, \ldots, N \tag{20}$$

with energies ϵ'_i where $\epsilon'_1 < \epsilon'_2 < \cdots < \epsilon'_N$.

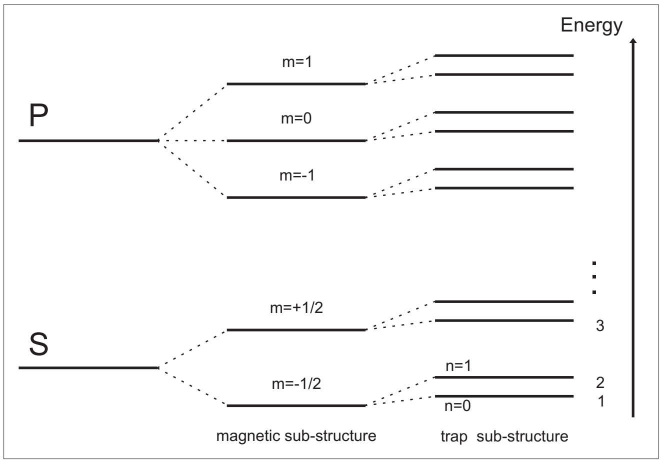

Figure 2: Definition of the atomic system shown at an example of a S-P two-level system and two motional trap levels.

The energy levels of the atom in an ion trap which is subject to a magnetic field is given by

$$\epsilon_i = \epsilon'_i + m^i_{F/J} \cdot g^i_{F/J} \cdot \mu_B \cdot B_z + \hbar\omega_T \cdot \left(n + \frac{1}{2}\right)$$

Here, $m^i_{F/J}$ is the magnetic quantum number, $g^i_{F/J}$ the Lande-factor of the ith level, μ_B the Bohr magneton, $\hbar$ the Planck constant, n the trap excitation quantum number and ω_T the trap frequency. The different indices F or J reflect wether the fine- or the hyperfine structure is taken into account. The magnetic field is pointing in z-direction

$$\vec{B} = \begin{pmatrix} 0 \\ 0 \\ B_z \end{pmatrix}$$

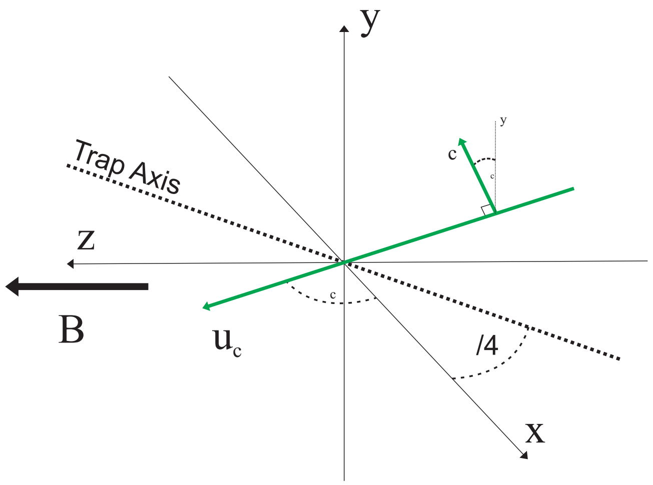

Figure 3: Definition of all axes considering the laser field and the ion trap.

Effects of Polarization on the Matrix Elements. As depicted in Fig.3, we further define the k-vector of the laser field $\vec{u}_c$ and its polarization vector $\vec{\epsilon}_c$

$$\vec{u}_c = \begin{pmatrix} \cos\alpha_c \\ 0 \\ \sin\alpha_c \end{pmatrix} \quad ; \quad \vec{\epsilon}_c = \begin{pmatrix} -\sin\beta_c\cdot\sin\alpha_c \\ \cos\beta_c \\ \sin\beta_c\cdot\cos\alpha_c \end{pmatrix} \tag{21}$$

These quantities are defined to obey the following relations

$$|\vec{u}_c| = 1 \quad ; \quad |\vec{\epsilon}_c| = 1 \quad ; \quad \vec{u}_c \perp \vec{\epsilon}_c \tag{22}$$

However, in order to consider the different kind of atomic transitions $(\vec{\pi}, \vec{\sigma}_{+/-})$ we modify the dipole matrix element by projecting the polarization vector $\vec{\epsilon}_c$ on one of the following vectors

$$\vec{\pi} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad ; \quad \vec{\sigma}_+ = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ i \\ 0 \end{pmatrix} \quad ; \quad \vec{\sigma}_- = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \\ 0 \end{pmatrix} \tag{23}$$

The dipole matrix elements μ_{ij} for the transition from the ith to the jth state is then given by

$$\mu_{ij} = (\vec{\pi}\cdot\vec{\epsilon}_c)\cdot C_{ij}\cdot\sqrt{\frac{3\epsilon_0\hbar A_{ij}\lambda_{ij}^3}{8\pi^2}} \quad \text{(for a π-transition)} \tag{24}$$

where A_{ij} is the Einstein coefficient, C_{ij} the Clebsch-Gordan coefficient and λ_{ij} the wavelength of the corresponding transitions. For a $\sigma_{+/-}$-transition the vector $\vec{\pi}$ has to be replaced by one of the vectors $\vec{\sigma}_{+/-}$.

Einstein Coefficients in an Ion Trap. The Einstein coefficients for the carrier and the blue- and redsideband transitions are given as follows

$$(n\rightarrow n): \qquad A_{ij}^C \quad = A_{ij}\cdot\Big(1-\eta_{ij}^2\cdot(n-1)\Big)^2 \tag{25}$$

$$\begin{aligned}
(n \to n+1): \quad & A_{ij}^{BS} &= A_{ij} \cdot \eta_{ij}^2 \cdot n \qquad (26)\\
(n \to n-1): \quad & A_{ij}^{RS} &= A_{ij} \cdot \eta_{ij}^2 \cdot (n-1) \qquad (27)\\
& & \qquad (28)
\end{aligned}$$

where A_{ij} denotes the pure atomic Einstein coefficient and η the lamb-dicke parameter

$$\eta_{ij} = \frac{\left|e'_i - e'_j\right|}{\hbar c} \cdot \sqrt{\frac{\hbar}{2m\omega_T}} \qquad (29)$$

Definition of the Hamiltonian. With the above designated quantities we can define the Hamiltonian of the atomic system interacting with a train of p laser pulses in the dipole approximation. We find

$$\begin{aligned}
H &= H_0 + H_{int} && (30)\\
H_0 &= \sum_k \epsilon_k \left|k\right\rangle\left\langle k\right| && (31)\\
\hbar\omega_{ij} &= (\epsilon_i - \epsilon_j) \quad ; \quad \omega_{ii} = 0 && (32)\\
H_{int} &= -E_T(t) \sum_{r<k} \mu_{rk} \left(\left|r\right\rangle\left\langle k\right| + \left|k\right\rangle\left\langle r\right|\right) && (33)\\
E_T(t) &= \sum_{k=0}^{p} \sigma(t - k\tau_R) \left(e^{i\omega_c(t-k\tau_R)+i\phi_k} + e^{-i\omega_c(t-k\tau_R)-i\phi_k}\right) && (34)
\end{aligned}$$

The rest of the definitions is the same as in the previous chapter. We note that the only difference of the otherwise periodic Hamiltonian from pulse-to-pulse is the change in the carrier-envelope phase $\phi_k = \phi_0 + k\omega_0\tau_R$. We will make use of this feature in the following algorithm.

2.2.2 Optical Bloch Equations with a Pulsed Laser

We describe the atom-laser system in the density matrix formalism where the time-evolution of the density matrix is given by the the optical Bloch equations including spontaneous emission[3]

$$\dot{\rho}_{ij} = -\frac{i}{\hbar}\left[H, \rho\right]_{ij} - \Gamma_{ij}\rho_{ij} + \delta_{ij} \sum_r \gamma_{ir}\rho_{rr} \qquad (35)$$

Here, Γ_{ij} represents the decay rates (coherence times) of the matrix elements and γ_{ij} the feeding terms, i.e. γ_{ij} is the rate with which the ith level is 'fed' by the jth level. They have the following properties

$$\begin{aligned}
\gamma_{ij} &= C_{ij}^2 \cdot A_{ij} && (36)\\
\Gamma_{jj} &= \sum_i \gamma_{ij} && (37)\\
\Gamma_{ij} &= \frac{1}{2}\left(\Gamma_{ii} + \Gamma_{jj}\right) && (38)
\end{aligned}$$

[3] δ_{ij} is the Kronecker-Delta

We further transform the equations into a rotating frame (R) via the unitary operator[4]

$$U_R(t) = \sum_k e^{-i\delta_k t} \left|k\right\rangle\left\langle k\right| \quad \longrightarrow \quad U_R U_R^\dagger = 1 \tag{39}$$

Here, δ_k represents the shift of the energy level k. Their choice depends on the special atomic system.

However, the density matrix and the Hamiltonian transform in the following way

$$\begin{aligned} \rho^R &= U_R^\dagger \cdot \rho \cdot U_R = e^{-i(\delta_l - \delta_k)\cdot t} \rho_{kl} \left|k\right\rangle\left\langle l\right| & (40) \\ H^R &= U_R^\dagger \cdot H \cdot U_R - i\hbar U_R^\dagger \frac{dU_R}{dt} = e^{-i(\delta_l - \delta_k)\cdot t} H_{kl} \left|k\right\rangle\left\langle l\right| - \hbar\delta_k \left|k\right\rangle\left\langle k\right| & (41) \end{aligned}$$

Since unitary transformations do not change physics the optical Bloch equations in the rotating frame look the same[5]

$$\dot{\rho}_{ij}^R = -\frac{i}{\hbar}\left[H^R, \rho^R\right]_{ij} - \Gamma_{ij}\rho_{ij}^R + \delta_{ij}\sum_r \gamma_{ir}\rho_{rr}^R \tag{42}$$

We define

$$H_0^R = \mathrm{diag}(H^R) = (\epsilon_k - \hbar\delta_k)\left|k\right\rangle\left\langle k\right| \tag{43}$$

and use the following properties to simplify the optical Bloch equations

$$\begin{aligned} \left[H_0^R, \rho^R\right]_{ii} &= 0 & (44) \\ \left[H_0^R, \rho^R\right]_{ij} &= \left(\epsilon_i - \epsilon_j - \hbar\left(\delta_i - \delta_j\right)\right)\rho_{ij}^R & (45) \\ \omega_{ij} &:= \left(\epsilon_j - \epsilon_i\right)/\hbar \geq 0 & (46) \\ \Delta_{ij} &:= \omega_{ij} - \left(\delta_j - \delta_i\right) & (47) \\ \Delta_{ii} &:= 0 & (48) \end{aligned}$$

We find

$$\dot{\rho}_{ij}^R = (i\Delta_{ij} - \Gamma_{ij})\rho_{ij}^R - \frac{i}{\hbar}\left[H_{int}^R, \rho^R\right]_{ij} + \delta_{ij}\sum_r \gamma_{ir}\rho_{rr}^R \tag{49}$$

The rotating frame is now chosen to be the frame of the interaction picture (I), i.e.

$$\delta_i = \epsilon_i/\hbar \quad \longrightarrow \quad \Delta_{ij} = 0 \tag{50}$$

$$\dot{\rho}_{ij}^I = -\frac{i}{\hbar}\left[H_{int}^I, \rho^I\right]_{ij} - \Gamma_{ij}\rho_{ij}^I + \delta_{ij}\sum_r \gamma_{ir}\rho_{rr}^I \tag{51}$$

[4] At the moment this transformation into a general rotating frame is not used in the algorithm. However, we transfer as explained above into the frame of the interaction picture. We just mention this general rotation here for completeness.

[5] One can easily see that by inserting the rotated properties (ρ^R, H^R) and simplify the equation.

It is now convenient to integrate these equations in order to use some approximations regarding the time scales of the system. We seek the density matrix after the interaction of the system with the kth laser pulse, i.e. we integrate the Bloch equations over one repetition rate

$$\begin{aligned} t_1 &= k\tau_R && (52) \\ t_2 &= (k+1)\tau_R && (53) \end{aligned}$$

By using the following trivial relation where $\alpha = -\Gamma_{ij}$

$$\begin{aligned} \dot{\rho}(t) &= \alpha\rho(t) + f(t) \qquad \Big| \cdot \int_{t_1}^{t_2} dt' e^{-\alpha t'} && (54) \\ \Rightarrow \rho(t_2) &= e^{\alpha(t_2-t_1)}\rho(t_1) + e^{\alpha t_2}\int_{t_1}^{t_2} dt' e^{-\alpha t'} f(t') && (55) \\ \rho(t_2) &= e^{\alpha\tau_R}\left(\rho(t_1) + \int_{t_1}^{t_2} dt' e^{\alpha(t_1-t')} f(t')\right) && (56) \end{aligned}$$

we find the final form of the optical Bloch equations to be

$$\boxed{\rho_{ij}^I(t_2) = e^{-\Gamma_{ij}\cdot\tau_R}\left(\rho_{ij}^I(t_1) - \frac{i}{\hbar}\int_{t_1}^{t_2} dt' e^{\Gamma_{ij}\cdot(t'-t_1)}\left[H_{int}^I, \rho^I\right]_{ij} + \delta_{ij}\sum_r \gamma_{ir}\int_{t_1}^{t_2} dt' e^{\Gamma_{ii}\cdot(t'-t_1)}\rho_{rr}^I(t')\right) (57)}$$

$\rho^I(t_2)$ then yields the density matrix after the pulse whereas $\rho^I(t_1)$, as an initial condition to the algorithm, represents the density matrix prior to the kth laser pulse.

We further simplify these equations that govern the dynamics of the system by using the fact that the interaction of the laser pulse with the atom is short compared to all other time scales in the system.

2.2.3 Approximations and Iterative Method

Since the eletric field in the interaction Hamiltonian H_{int}^I is only present for a short time on the order of femtoseconds we can set the exponential term to unity for both diagonal and off-diagonal elements, i.e. $\Gamma_{ij}\cdot(t'-t_1) \approx 0$ for $t' = t_1 + \epsilon$ where $\epsilon \sim 10^{-15}$ and $\Gamma \sim 10^8$. We find

$$\int_{t_1}^{t_2} dt' e^{\Gamma_{ij}\cdot(t'-t_1)}\left[H_{int}^I, \rho^I\right]_{ij} \approx \int_{t_1}^{t_2} dt' \left[H_{int}^I, \rho^I\right]_{ij} \qquad (58)$$

This leads us to the following expressions for the density matrix

$$\begin{aligned} \rho_{ij}^I(t_2) &= e^{-\Gamma_{ij}\cdot\tau_R}\cdot\left(\rho_{ij}^{I,c}(t_2) + \delta_{ij}\sum_r \gamma_{ir}\int_{t_1}^{t_2} dt' e^{\Gamma_{ii}\cdot(t'-t_1)}\rho_{rr}^I\right) && (59) \\ \rho_{ij}^{I,c} &= \rho_{ij}^I(t_1) - \frac{i}{\hbar}\int_{t_1}^{t_2} dt' \left[H_{int}^I, \rho^I\right]_{ij}(t') && (60) \end{aligned}$$

where ρ_{ij}^c is the coherently excited density matrix. It only takes the interaction of the laser with the atom into account.

However, the algorithm to solve for the time-evolution works in the following way[6]

[6] A more detailed description on how it is implemented will be given in the section about the used Matlab program.

- Given some initial condition for the density matrix and the frequency comb, i.e. a certain population distribution and laser parameters, i.e. offset frequency, carrier-envelope phase, ..., we determine the Hamiltonian H^I_{int} and solve for the coherently excited density matrix Eq. (60) - this will be explained in the next section. This gives the time evolution on the short fs time scale where the laser interaction with one pulse is present.
- After the laser pulse excited the system we apply equation Eq. (59) to the density matrix which corresponds to a free evolution of the system since no laser field is present for the rest of the repetition period.
- Jump back to first step while using the resulting density matrix as new initial condition to apply the next pulse to the system. We note one has to adjust the Hamiltonian H^I_{int} for the second pulse because of the pulse-to-pulse change of the carrier-envelope phase.

This algorithm is applied then up to the number of desired pulses. Since the change of the frame does not change the population, i.e. the diagonal elements of the density matrix, it is not necessary to transform into the lab frame after all.

2.2.4 Coherently Excited Density Matrix

The coherently excited density matrix can be calculated using the time propagation formalism (see also Appendix A.2). First we rewrite Eq. (59) as follows

$$\dot{\rho}^{I,c}_{ij} = -\frac{i}{\hbar}\left[H^I_{int}, \rho^I\right]_{ij} = \dot{\rho}^I_{ij} \tag{61}$$

which represents nothing else than the optical Bloch equations in the interaction picture without decay.

The solution of Eq. (61) is then given by

$$\rho^I(t_2) = U_I(t_2, t_1) \cdot \rho^I(t_1) \cdot U^\dagger_I(t_1, t_2) \tag{62}$$

where $U_I(t)$ denotes the time propagation operator. It is determined by the Schrödinger equation

$$i\hbar\dot{U}_I(t) \quad = \quad H^I_{int}(t)U_I(t) \tag{63}$$

In order to get the time propagation operator that yields the time evolution between the consecutive pulses k and $k+1$ we shift the time variable $t = t' + k\tau_R$ and integrate or solve the equation over one repetition time

$$i\hbar\dot{U}_I(t' + k\tau_R) \quad = \quad H^I_{k,int}(t' + k\tau_R)U_I(t' + k\tau_R) \qquad \left| \int_0^{\tau_R} dt' \right. \tag{64}$$

The Hamiltonian in the interaction picture is of the following form

$$\begin{aligned} H^I_{k,int}(t' + k\tau_R) &= -\sigma(t')\sum_{i,j}\mu_{ij}e^{-i\Delta^I_{ij}t' + i\phi_k}\,|i\rangle\langle j| + c.c. && (65)\\ \Delta^I_{ij} &= \omega_{ij} - \omega_c && (66)\\ \phi_k &= k\cdot(\omega_0 - \omega_{ij})\tau_R && (67)\end{aligned}$$

where we applied the rotating-wave approximation[7] for terms $\omega_{ij}+\omega_c$ and left out all other terms (pulses) in the sum which equal zero for the times over which we integrate.

We call the resulting time propagation operator that describes the evolution due to the kth pulse $U_I(\phi_k)$. We note that the operator $U_I(\phi_k)$ is given as a function of the detuning and repetition rate ($\phi_k = k\,(\omega_0-\omega_{ij})\,\tau_R$) which is due to the different carrier-envelope phases of each pulse[8].

However, we can get rid of this dependency by applying a unitary transformation K. So far, this assumption is without proof and works out for up atomic systems with up to sixteen levels that have only dipole transitions included. However, it is strongly supported by the following paper [3].

Applying this transformation we can rewrite the equations as

$$H^I_{int} = K^\dagger(\phi_k)H^I_{k,int}(t'+k\tau_R)K(\phi_k) = -\sigma(t')\sum_{i,j}\mu_{ij}e^{-i\Delta^I_{ij}t'}\,|i\rangle\langle j| + c.c. \tag{68}$$

The time-propagation operator is then given by

$$\begin{aligned} U_I(\phi_k) &= K(\phi_k)U_I(0)K^\dagger(\phi_k) && (69)\\ K(\phi_k)\cdot K^\dagger(\phi_k) &= \mathbb{1} && (70)\end{aligned}$$

It should be emphasized that now it is enough to solve the differential equation Eq. (64) for $\phi = 0$ and apply the unitary transformation K to get the full phase dependence. Some examples and explicit expressions for K are given in the Appendix A.4.

Thus in the following two sections we present methods to determine the time propagation operator neglecting the phase dependence. The first method corresponds to a straight forward brude force direct integration of the equation using Matlab whereas the second uses the Dyson series. However, it turned out that the Dyson method is not always applicable numerically which will be shown in detail.

2.2.5 Direct Integration of the Time Propagation Operator

We currently use the Matlab function `ode45` in order to integrate Eq. (64) directly (only using the rotating wave approximation as approximation). As a numerical check we have a look at the unitarity of the time propagation operator. Taking the analytic phase dependence into account the unitarity is typically given as $U_I\cdot U_I^\dagger - \mathbb{1} \approx 10^{-12\ldots-15}$ independent of the phase[9].

However this method can be used in general and has no crucial restriction regarding the atomic system. In contrast to that the method using the Dyson expansion of the differential equation does not converge always and yields a much rougher approximation, but uses less time to compute the expansion terms, though.

[7] Wether the rotating wave approximation really can be applied here, should be investigated more thoroughly since on the fs timescale only a few oscillations (~ 100) actually take place.

[8] We further note, that the phase shift between the pulses equals $\delta\phi = \omega_0\tau_R$ where as the second term is just an effect of the sampling with the repetition frequency and the rotating frame.

[9] Before we found this possibility we solved equation Eq. (64) for many different phases and interpolated the result a) with a spline and b) with a sin function. Unfortunately, apart from much more computer time you need it turns out that the unitarity condition is only given down to a level of 10^{-8}

2.2.6 Dyson Series

In the Dyson approximation we integrate the differential equation (64) after the application of the unitarity transformation K and insert $U_I(t)$ successively yielding

$$\begin{aligned} & U_I(\tau_R) && (71) \\ = \; & U_I(0) + \left(-\frac{i}{\hbar}\right) \int_0^{\tau_R} dt_1 H^I_{int}(t_1) + \left(-\frac{i}{\hbar}\right)^2 \int_0^{\tau_R} dt_1 \int_0^{t_1} dt_2 H^I_{int}(t_1) H^I_{int}(t_2) + \cdots && (72) \\ = \; & 1 + \sum_{k=1}^{\infty} \left(-\frac{i}{\hbar}\right)^k \int_0^{\tau_R} dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_k} dt_k \prod_{p=1}^{k} H^I_{int}(t_p) && (73) \end{aligned}$$

The different terms of the expansion correspond to multi-photon transition, e.g. the second order term $H^I_{int}(t_1)H^I_{int}(t_2)$ includes the term $\mu_{13}\mu_{32}$ which corresponds to a transition from the first to the second level via the third.

It should be noted that we did not manage to get a good unitarity for the time propagation operator using this approximation for simulating the Ca$^+$ level system. This is due to the different order of magnetitude of the dipole-matrix elements of the D to P transition compared to the quadrupole transitions S to D[10].

First of all we consider the product of the Hamiltonians (so far up to fourth order in the program, for simplicity here we show the calculations up to second order only). The Hamiltonian is given in the interaction picture as

$$H^I_{int}(t) = U_0^\dagger(t) H_{int}(t) U_0(t) \qquad (74)$$

Inserting all the terms yields

$$\begin{aligned} H^I_{int}(t_1) &= -E(t_1) \sum_{r<k} \mu_{rk} e^{i\omega_{rk}\cdot t_1} |r\rangle\langle k| + \mu_{rk} e^{-i\omega_{rk}\cdot t_1} |k\rangle\langle r| && (75) \\ &= -\Sigma(t_1)\left(e^{i\omega_c t_1 + i\phi_k} + e^{-i\omega_c t_1 - i\phi_k}\right) \sum_{r<k} \mu_{rk} e^{i\omega_{rk}\cdot t_1} |r\rangle\langle k| + \mu_{rk} e^{-i\omega_{rk}\cdot t_1} |k\rangle\langle r| && (76) \end{aligned}$$

We again use the rotating wave approximation where we leave out fast oscillating (!) terms as $\exp(\pm i(\omega_{rk} + \omega_c)\cdot t)$ in the Hamiltonian.

With these approximations we end up with the following integrand for the single photon processes

$$H^I_{int}(t_1) = -\Sigma(t_1) \sum_{r<k} \mu_{rk} e^{-i\Delta_{rk}\cdot t_1 - i\phi_k} |r\rangle\langle k| + \mu_{rk} e^{i\Delta_{rk}\cdot t_1 + i\phi_k} |k\rangle\langle r| \qquad (77)$$

The two photon processes are described by the following Hamiltonian

$$\begin{aligned} & H^I_{int}(t_2) H^I_{int}(t_1) && (78) \\ = \; & \left(-\Sigma(t_2) \sum_{l<m} \mu_{lm} e^{-i\Delta_{lm}\cdot t_2 - i\phi_k} |l\rangle\langle m| + \mu_{lm} e^{i\Delta_{lm}\cdot t_2 + i\phi_k} |m\rangle\langle l|\right) && (79) \end{aligned}$$

[10] This effect can be more easily understood if one tries to reconstruct the analytic solution for a two-level system with a cw laser for high power with the Dyson series: the resulting sinusoidal behaviour of the operator can hardly be approximated if the argument of the sin function is large.

$$\cdot \left(-\Sigma(t_1)\sum_{r<k}\mu_{rk}e^{-i\Delta_{rk}\cdot t_1-i\phi_k}\,|r\rangle\langle k| + \mu_{rk}e^{i\Delta_{rk}\cdot t_1+i\phi_k}\,|k\rangle\langle r|\right) \tag{80}$$

$$= \left(\Sigma(t_2)\Sigma(t_1)\sum_{l<m<k}\mu_{lm}e^{-i\Delta_{lm}\cdot t_2}\mu_{mk}e^{-i\Delta_{mk}\cdot t_1}\,|l\rangle\langle k|\right)\cdot e^{-i2\phi_k} \tag{81}$$

$$+ \left(\Sigma(t_2)\Sigma(t_2)\sum_{\substack{l<m\\r<m}}\mu_{lm}e^{-i\Delta_{lm}\cdot t_2}\mu_{rm}e^{i\Delta_{rm}\cdot t_1}\,|l\rangle\langle r|\right) \tag{82}$$

$$+ \left(\Sigma(t_2)\Sigma(t_2)\sum_{\substack{l<m\\l<k}}\mu_{lm}e^{i\Delta_{lm}\cdot t_2}\mu_{lk}e^{-i\Delta_{lk}\cdot t_1}\,|m\rangle\langle k|\right) \tag{83}$$

$$+ \left(\Sigma(t_2)\Sigma(t_1)\sum_{r<l<m}\mu_{lm}e^{-i\Delta_{lm}\cdot t_2}\mu_{rl}e^{-i\Delta_{rl}\cdot t_1}\,|m\rangle\langle r|\right)\cdot e^{i2\phi_k} \tag{84}$$

We define the following matrix

$$M_{ij}(t) = -\mu_{ij}e^{-i\Delta_{ij}\cdot t}\Sigma(t) \tag{85}$$

and rewrite the Hamiltonian for the one photon processes

$$H^I_{int}(t_1,\phi_k) = M^\dagger(t_1)\cdot e^{i\phi_k} + M(t_1)\cdot e^{-i\phi_k} \tag{86}$$

and the two photon processes

$$H^I_{int}(t_2,\phi_k)H^I_{int,\phi_k}(t_1) \tag{87}$$

$$= M^\dagger(t_2)\cdot M^\dagger(t_1)\cdot e^{i2\phi_k} + M(t_2)\cdot M^\dagger(t_1) + M^\dagger(t_2)\cdot M(t_1) + M(t_2)\cdot M(t_1)\cdot e^{-i2\phi_k} \tag{88}$$

The terms of higher order are calculated in the same way. The unitary transformation to cancel out the phase dependence is not necessary since the phase is directly given in the resulting terms for the multi-photon processes. The only thing remaining is the integration of the actual integrals in Eq. (71). For this we used a nested multi-dimensional Clenshaw-Curtis algorithm [4]. A source code that can be adapted can be found in this reference [5]. Furthermore, there is a multi-dimensional source code for Clenshaw-Curtis available in the internet by John Burkardt [6] but we haven't had a look at that yet. Maybe that one is a bit faster!

2.3 Feeding Terms

The last thing we have to consider in order to get the desired time evolution of the system are the feeding terms for the diagonal elements (see Eq. (59)). Since only the diagonal elements of Γ and ρ^c contribute we use the convention that $\Gamma_{ii} = \Gamma_i$ and $\rho^c_{ii} = \rho^c_i$.

We re-write the time dependence of the diagonal elements in the integral of Eq. (59) as follows

$$\begin{aligned}
\rho^I_{a_1}(t) &= e^{-\Gamma_{a_1}\cdot(t-k\tau_R)}\cdot\left(\rho^{I,c}_{a_1}(t) + \sum_{a_2}\gamma_{a_1a_2}\int_{t_1}^{t}dt' e^{\Gamma_{a_1}\cdot(t'-t_1)}\rho^I_{a_2}(t')\right)\\
&= e^{-\Gamma_{a_1}\cdot(t-k\tau_R)}\cdot\left(\rho^{I,c}_{a_1}(t) + \sum_{a_2}\gamma_{a_1a_2}\int_{0}^{t-k\tau_R}dt' e^{\Gamma_{a_1}\cdot t'}\rho^I_{a_2}(t'+k\tau_R)\right)\\
t_1 &= k\tau_R \quad ; \quad t_1 \le t \le t_1+\tau_R
\end{aligned}$$

After inserting the relation for the density matrix elements recursively we find for the feeding terms

$$\begin{aligned}
& \sum_{a_2} \gamma_{a_1 a_2} \int_0^{t-k\tau_R} dt_2 e^{\Gamma_{a_1} t_2} \rho_{a_2}(t_2 + k\tau_R) \\
= & \sum_{a_2} \gamma_{a_1 a_2} \rho^c_{a_2} \int_0^{t-k\tau_R} dt_2 e^{\left(\Gamma_{a_1} - \Gamma_{a_2}\right) \cdot t_2} \\
+ & \sum_{a_2,a_3} \gamma_{a_1 a_2} \gamma_{a_2 a_3} \rho^c_{a_3} \int_0^{t-k\tau_R} dt_2 \int_0^{t_2} dt_3 e^{\left(\Gamma_{a_1} - \Gamma_{a_2}\right) \cdot t_2 + \Gamma_{a_2} \cdot t_3} \rho_{a_3}(t_3 + k\tau_R) \\
= & \sum_{k=2}^{N} \sum_{a_2,\ldots,a_k} \left(\prod_{j=1}^{k-1} \gamma_{a_j a_{j+1}} \right) \rho^c_{a_k} \int_0^{t-k\tau_R} dt_2 \cdots \int_0^{t_{k-1}} dt_k \exp \left(\sum_{l=1}^{k-1} \left(\Gamma_{a_l} - \Gamma_{a_{l+1}} \right) \cdot t_{l+1} \right)
\end{aligned}$$

Here we used the fact that there is a highest level N and the recursion stops at that point

$$\rho_N(t) = e^{-\Gamma_N \cdot (t-k\tau_R)} \rho^c_N \tag{89}$$

So far we have no general solution for this integral since the solution strongly depends on the given atomic system. Thus, in the real implementation these feeding terms are integrated symbolically for the system of interest using the symbolic toolbox and the matlab `int` function.

For the program it is easier to use the following recursion for the diagonal elements[11]

$$\begin{aligned}
\rho_N(t) &= e^{-\Gamma_N \cdot (t-k\tau_R)} \rho^c_N \\
\rho_{N-1}(t) &= e^{-\Gamma_{N-1} \cdot (t-k\tau_R)} \Big(\rho^c_{N-1} + \gamma_{N-1,N} \int_0^{t-k\tau_R} dt' e^{\Gamma_{N-1} \cdot t'} \rho_N(t' + k\tau_R) \Big) \\
\rho_{N-2}(t) &= e^{-\Gamma_{N-2} \cdot (t-k\tau_R)} \Big(\rho^c_{N-2} + \gamma_{N-2,N-1} \int_0^{t-k\tau_R} dt' e^{\Gamma_{N-2} \cdot t'} \rho_{N-1}(t' + k\tau_R) \\
&\qquad + \gamma_{N-2,N} \int_0^{t-k\tau_R} dt' e^{\Gamma_{N-2} \cdot t'} \rho_N(t' + k\tau_R) \Big)
\end{aligned}$$

[11] Note that we do not have to sum over all levels since only higher levels decay into lower ones.

2.4 Formula Summary

$$H = H_0 + H_{int} \tag{90}$$

$$H_0 = \sum_k \epsilon_k \left|k\right\rangle\left\langle k\right| \quad ; \quad \hbar\omega_{ij} = (\epsilon_i - \epsilon_j) \quad ; \quad \omega_{ii} = 0 \tag{91}$$

$$H_{int} = -E(t) \sum_{r<k} \mu_{rk} \left(\left|r\right\rangle\left\langle k\right| + \left|k\right\rangle\left\langle r\right|\right) \tag{92}$$

$$E_k(t) = \Sigma(t) \left(e^{i\omega_c t + i\phi_k} + e^{-i\omega_c t - i\phi_k}\right) \tag{93}$$

$$\dot{\rho}_{ij} = -\frac{i}{\hbar} \left[H, \rho\right]_{ij} - \Gamma_{ij}\rho_{ij} + \delta_{ij} \sum_r \gamma_{ir}\rho_{rr} \tag{94}$$

$$\rho^I_{ij}(t) = e^{-\Gamma_{ij}\cdot t} \left(\rho^{I,c}_{ij} + \delta_{ij} \sum_r \gamma_{ir} \int_0^t dt' e^{\Gamma_{ij}\cdot t'} \rho^I_{rr}\right) \tag{95}$$

$$\rho^{I,c}(t) = U_I(t,\phi_k) \cdot \rho^{I,c}(0) \cdot U_I^\dagger(t,\phi_k) \tag{96}$$

$$U_I(t,\phi_k) = K(\phi_k) \cdot U_I(t) \cdot K^\dagger(\phi_k) \tag{97}$$

$$K(\phi_k) \cdot K^\dagger(\phi_k) = \mathbb{1} \tag{98}$$

$$\sum_{a_2} \gamma_{a_1 a_2} \int_0^t dt_2 e^{\Gamma_{a_1} t_2} \rho_{a_2}(t_2) \tag{99}$$

$$= \sum_{k=2}^{N} \sum_{a_2,\ldots,a_k} \left(\prod_{j=1}^{k-1} \gamma_{a_j a_{j+1}}\right) \rho^c_{a_k} \int_0^t dt_2 \cdots \int_0^{t_{k-1}} dt_k \exp\left(\sum_{l=1}^{k-1} \left(\Gamma_{a_l} - \Gamma_{a_{l+1}}\right) \cdot t_{l+1}\right) \tag{100}$$

3 Analytical Results on the Two-Level System

3.1 Pulsed Laser

We compare analytical expressions given in the paper [7] for the interaction of the comb with a two-level system with our simulations.

The population in the excited state induced by a train of N pulses that are of the form

$$\sigma(t) = e_0 \cdot \operatorname{sech}\left(1.763 \cdot \frac{t}{t_p}\right) \tag{101}$$

is given by

$$P_2^{(N)} \quad = \quad P_2^{(1)} \cdot \left(\frac{\sin N\theta}{\sin\theta}\right)^2 \tag{102}$$

Here the following definitions have been used

$$\begin{aligned}
P_2^{(1)} &= \operatorname{sech}\left(\frac{1}{2}\cdot\pi\cdot\delta\right)^2 \cdot \sin\left(\frac{1}{2}\cdot A\right)^2 && (103)\\
\varphi &= \frac{1}{2}\cdot\omega_a\cdot\tau && (104)\\
\xi &= \arg\left(\frac{\Gamma\left(\frac{1}{2}+\frac{1}{2}i\delta\right)}{\Gamma\left(\frac{1}{2}+\frac{1}{2}\cdot\frac{A}{\pi}+\frac{1}{2}i\delta\right)+\Gamma\left(\frac{1}{2}-\frac{1}{2}\cdot\frac{A}{\pi}+\frac{1}{2}i\delta\right)}\right)+\varphi && (105)\\
a1 &= \sqrt{1-P_2^{(1)}}\cdot\cos\xi && (106)\\
\theta &= \arccos a1 && (107)\\
\delta &= \Delta\tau && (108)
\end{aligned}$$

This quantities are related to the definitions given in this script by

$$\begin{aligned}
\tau &= t_p/1.763 && (109)\\
\delta &= \tau\cdot\Delta_{12}^I && (110)\\
A &= 2\pi\cdot e_0\mu_{12}\tau && (111)
\end{aligned}$$

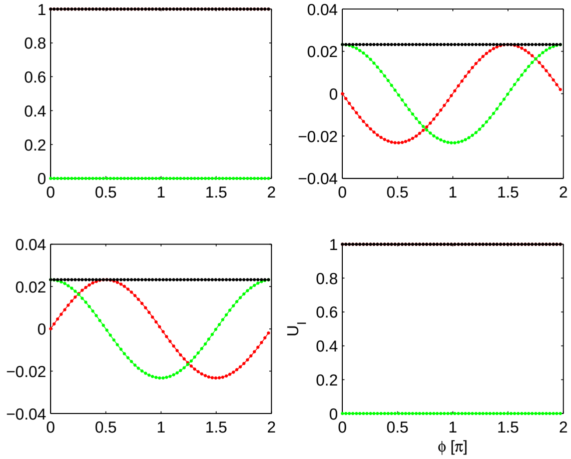

Figure 4:

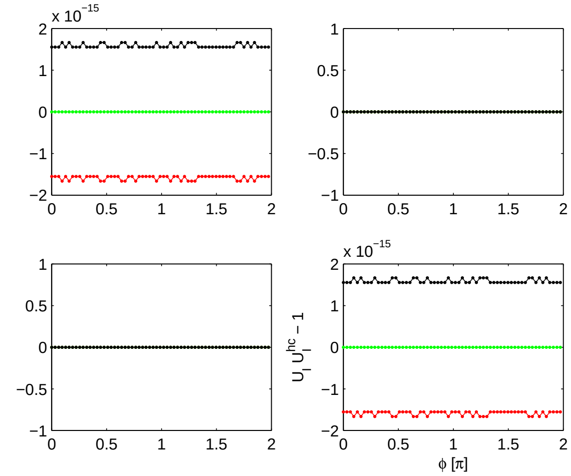

Figure 5:

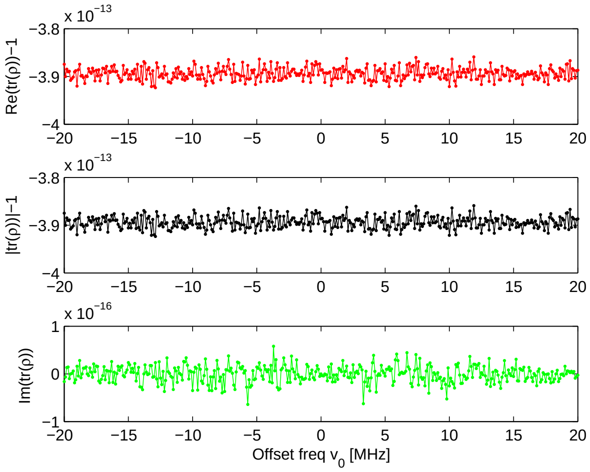

Figure 6:

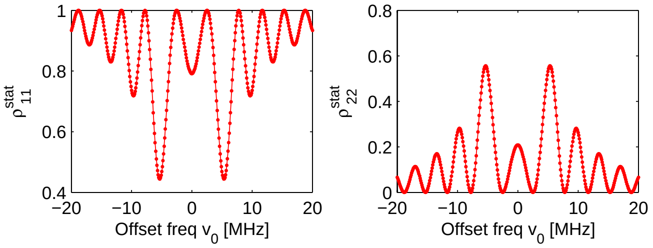

Figure 7:

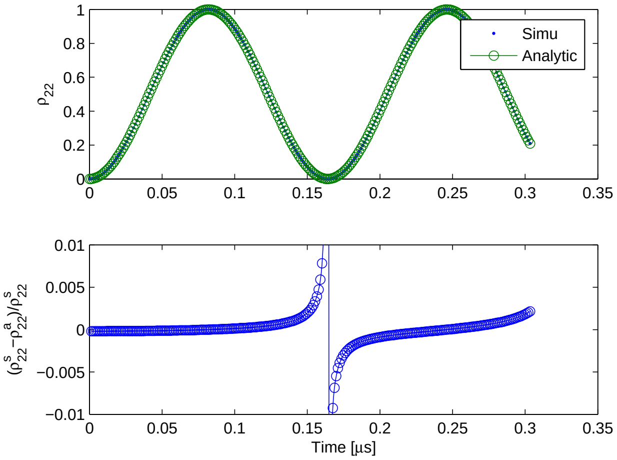

Figure 8:

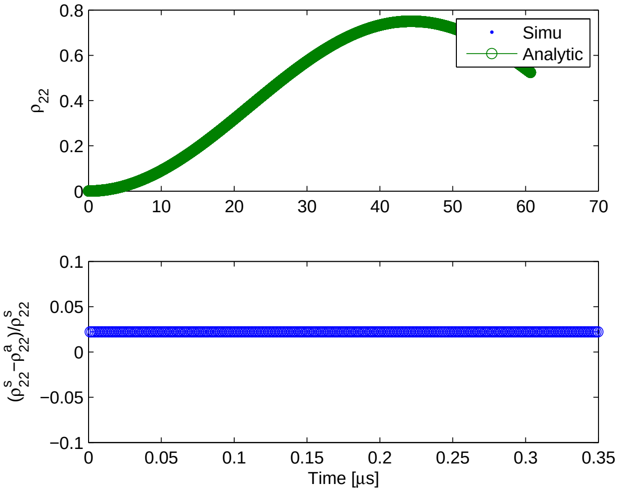

Figure 9:

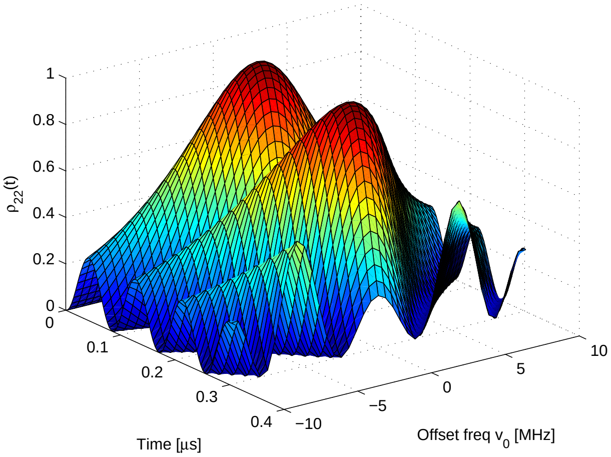

Figure 10:

4 Simulations

In the following section the structure of the implemented algorithm und its realization on the GRID is explained.

4.1 Matlab Modules for the GRID

The main idea of the algorithm is the following

- Define the atomic system and the laser parameters.
- Define the parameter ranges for the comb tuning, e.g. a certain interval for the offset frequency.
- Split the interval in order to distribute it on several computers, i.e. the GRID.
- Run the simulation on the GRID and collect the resulting data.

On overview of the actual implementation is shown in Fig. 11. The structure of main five steps of the program is as follows (more details about input and output parameters will be given in the following section)

- **init_simu (Matlab)** The main experimental parameters of the atomic system and the laser are defined and prepared for proceeding in the following programs.
- **init_scan (Matlab)** The scannning parameters are defined and the number of computers on which the simulation should be distributed.
- **do_compile (Perl/Bash)** The programs are compiled on the GRID machines[12] sending them as a job to the corresponding job manager with a job decription file (here: compile_job).
- **do_calc_u (Perl/Bash)** After the compilation of the programs the time propagation operator is calculated, again as a job on the GRID.
- **do_grid_scan (Perl/Bash)** The interval of the parameter scan (e.g. the comb offset frequency) is split up and the calculation of the time evolution of the density matrix is then distributed on a GRID cluster.

[12] That turned out to be necessary since the Matlab architecture on every machine is different.

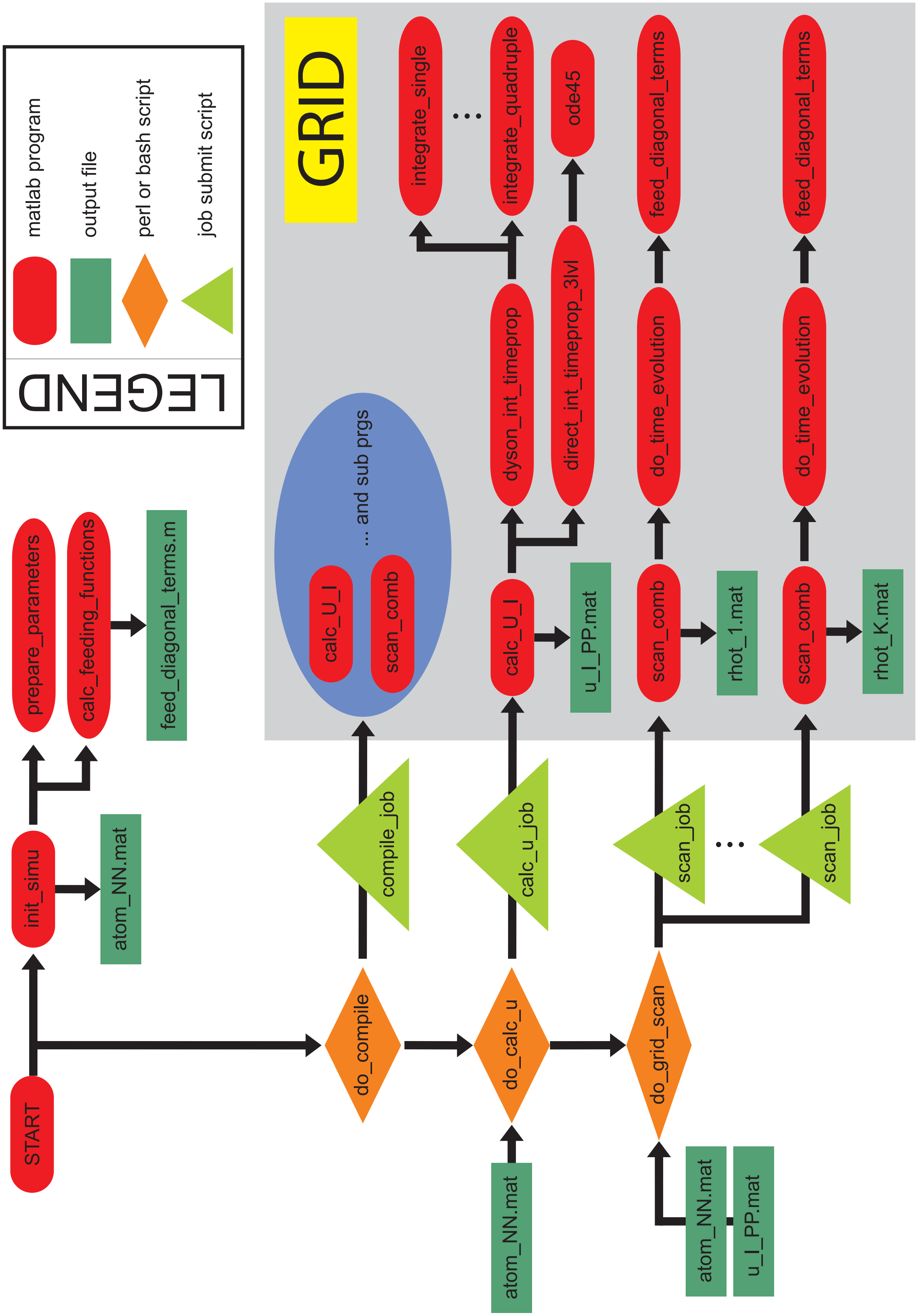

Figure 11: Flow-chart of the program

4.1.1 init_simu

function	init_simu()
input	-
output	atom_NN.mat

Initializes the simulational parameters, i.e. the atomic system and the laser system. Furthermore it calculates with these parameters the feeding functions which of course depend on the decay rates of the atom.

4.1.2 prepare_parameters

function	[result U_Decay detunings_I] = prepare_parameters(exppar, laserpar)
input	Atomic and laser parameters
output	Experimental parameters, decay rates, detunings

Prepares the atomic parameters for the following programs and calculates the off-diagonal elements of the decay matrix, the detunings in the interaction picture and the corresponding wavelengths of the transitions.

4.1.3 calc_feeding_functions

function	[feeding_command, feeding_func] = calc_feeding_functions(atomparameters)
input	Atomic parameters
output	feed_diagonal_terms.m

Calculates the feeding functions and writes it in a matlab file. This is done since the feeding functions change from one atomic system to another. This is done in this way because of the problems with using the feval function and saving anonymous functions while using the compiler in Matlab at the same time. However, the feeding functions themselves are determined using the symbolic toolbox.

4.1.4 init_scan

function	init_scan()
input	-
output	scan_grid_NN.mat

Initializes the scanning parameters and defines the number of intervals, i.e. the number of computers, over which the calculations should be distributed on the GRID.

4.1.5 calc_U_I

function	calc_U_I(atomfingerprint, ufingerprint)
input	atom_NN.mat
output	u_i_PP.mat

Calculates the time propagation operator by either directly integrating the optical Bloch equations using the ode45 function or using the Dyson method.

4.1.6 direct_integration_3lvl

function	U_I_0 = direct_int_timeprop_3lvl(atomparameters, laserparameters, detunings_I)
input	Atom and laser parameters
output	Time propagation operator

Implementation of the direct integration of the optical Bloch equations of a three level system using ode45. This function has to be adapted for systems with more levels.

4.1.7 scan_comb

function	scan_comb(scan_data_basefilename, scan_ind_no, atomfingerprint, uifingerprint, save_simudata_file, no_of_pulses, save_complete_timeevolution)
input	Atom, laser and scan parameters
output	rhot_N.mat

Simulates the scan of the comb over a certain frequency interval for a certain number of pulses.

4.1.8 do_time_evolution

function	help_rho = do_time_evolution(atomparameters, laserparameters, laserscanparameters , propagation_operators, nu_0, nu_R)
input	Atomic, laser and scan parameters and propagation operators
output	time evolution of the density matrix

Simulates the time evolution in the time propagator scope for certain comb parameters and returns the density matrix for every time step.

4.1.9 feed_diagonal_terms

function	new_drhoc = feed_diagonal_terms(d_rhoc, tau)
input	rho_c, repetition rate
output	new_rho_c

Calculates the feeding of the lower levels resulting from the spontaneous decay.

4.2 Data structures

In this section the data structures that are used are explained and examples are given.

4.2.1 atom_nn.mat

This file contains all information about the atomic system and the main laser parameters.

atomparameters.	
N	number of levels
Gamma_decay	NxN matrix, decay rates
gamma_feed	NxN matrix, feeding rates
energies	N vector, energy levels in Joule
mu	NxN matrix, dipole matrix elements
rho0	NxN matrix, initial condition $\rho(0)$
omega	NxN matrix, transition frequencies
wavelengths	NxN matrix, transition wavelengths
detunings_I	NxN matrix, detunings (int. pic.)
flags	direct integration or Dyson method
laserparameters.	
v_group	group velocity [m/s]
v_phase	phase velocity [m/s]
tp	pulse width [s]
e0	electric field amplitude
omega_L	laser carrier frequency
phi0	initial offset cep phase
tau	repetition time [s]
right_integration_limit	limit time prop. int. [s]
shift_pulse	time shift of pulse for time prop. int. [s]
RelTol	relative tolerance parameter for ode45
AbsTol	absolute tolerance parameter for ode45
propagation_operators.	
U_I_phi_coeff	NxN matrix, unitary phase transformation
U_decay	decay matrix

4.2.2 u_i_nn.mat

This file contains the time propagation operators.

propagation_operators.	
U_I_phi_coeff	NxN matrix, unitary phase transformation
U_decay	decay matrix
U_I_0	NxN matrix, numerically calculated U_I at $t = 0$

4.2.3 scan_grid_nn

This file contains the number of pulses in the first line. The following lines contain the (offset) frequencies for the comb at which the time evolution is simulated.

4.2.4 rho_t.mat

This file contains the resulting density matrices (optionally including the full time evolution for every offset frequenc), the scanning parameters and all the parameters that were used for the simulation.

atomparameters	(see above)
detunings_I	(see above)
laserparameters	(see above)
propagation_operators	(see above)
laserscanparameters.	
dnu0_interval	1xm Vector, simulated offset frequencies
Niterations	number of pulses p
simulation_results.	
rho_t	m cell vector of NxN matrix, each cell contains the time evolution at each offset frequency
rho_stat	Nx(mxN) matrix, stationary state for each offset frequency
scan_dnu0_interval	(same as dnu0_interval)
timeinterval	1xp vector, real time scale for all iterations [s]

4.3 About the GRID

In the following sections a possibility is described how to do calculations using the Austrian GRID (see http://www.austriangrid.at/). We furthermore discuss about the use of the hc-cluster which is also available in Innsbruck. A general documentation about GRID computing can e.g. be found here [8, 9].

4.3.1 Some definitions and explanation regarding the GRID

- **Certificates**. A certificate is a key which you need to access any GRID resource in order to identifiy you for obvious security reasons. Considering the Austrian GRID this key is provided by the AustrianGrid Certification Authority (http://www.austriangridca.at/).

- **Virtual Organisations**. This concept is used in GRID computing to grant/restrict access to certain clusters. You have to be member of one or more VOs. Which one you choose depends on what cluster you want to use. You can find an overview about the VOs on this page http://agrid.uibk.ac.at/AustrianGrid/guvw.php.

- **Ganglia**. Which resources are currently available on the Austrian GRID you can see with the GANGLIA monitoring software on this webpage http://agrid.uibk.ac.at/ganglia_gen/index.php.

- **GLOBUS Toolkit**. This toolkit provides you with an interface from the master machine with which you access the GRID to the GRID itself. It allows for transfering data or running programs on the GRID (see also http://www.globus.org/toolkit/).

4.3.2 Preparations to use the GRID in Innsbruck (the full story)

Here are the steps I did to have access to the Austrian GRID

- Request a certificate and install it
  (see http://www.uibk.ac.at/austriangrid/manuals/certificate.sdbk).

- Become member of one or more virtual organisations
  (see http://www.uibk.ac.at/austriangrid/manuals/vo.sdbk).

- Get an account on agrid1.uibk.ac.at (ask the ZID). From there you can access the GRID.

- Copy the certifacte and your private key on agrid1 in the directory $HOME/.globus/.

- Add this line to the `.bashrc` in your home directory on agrid1
  ```
  . /usr/site/grid/etc/profile.d/gt4.sh
  ```
  The call of this script when logging in sets some paths and enables you to use globus commands and some other necessary programs.

4.3.3 How to submit jobs

- Before you can access the GRID you need to create a proxy (e.g. for 24 hours)
  ```
  grid-proxy-init -hours 24
  ```

- With the command `grid-proxy-info` you can see how long the proxy still lasts.

- Copy the necessary files to the GRID cluster computer, e.g.
  ```
  globus-url-copy file:<directory>/scan_comb.m gsiftp://agrid1.uibk.ac.at/<directory>
  ```

- Submit the job with the `qsub` script, i.e. execute the qsub on the cluster machine as follows
  ```
  globus-job-run $server <qsub_directory>/qsub
     ${direc}/compile_job -v arg1=<directory>,arg2=calc_U_I.m
  ```

- Another possibility is to directly login to the GRID machine
  ```
  glogin <server>
  ```
  and call the `qsub` script directly. However, this is not optimal if you want to automatize your calculations.

- The qsub command puts the job into a queue specified in the job description file (here: compile_job, see Appendix).

- In order to copy the files from the GRID machine back to the master machine do
  ```
  globus-url-copy gsiftp://<server>/~/<directory+files> file:<local directory>
  ```

4.4 Used Clusters

This section should give a more detailed overview about certain specialities and experience with the clusters we are currently using.

4.4.1 Agrid1

4.4.2 HC-Cluster

The HC-cluster can be accessed without a GRID certificate which makes life a it easier. One just needs an account on the `hc-ma.uibk.ac.at` machine which can be activated by the ZID. A very good documentation can be found here http://unix-docu.uibk.ac.at/zid/systeme/unix-hosts/hc-cluster/. However, the availability of the cluster can also be checked with the GANGLIA toolkit (http://agrid.uibk.ac.at/ganglia_gen/index.php) under the term HPC-GRID.

In order to use Matlab on has to add the following line to the .bashrc

```
module load matlab/64/R2007a
```

The compilation of the programs and the job submission can be directly done using the `qsub` script again (see Appendix for details on the source code). Here, the steps taken to do the simulations

- Initialize the files with init_simu and init_scan

- Copy the files to the hc-ma

- Compile the calc_u_i and the scan_comb matlab files
  ```
  do_compile_hc
  ```

- Calculate the time propagation operator with the atom_05.mat input file `do_calc_u_hc 05 01`

- Simulate the scan of the comb with the atomic, timepropagtion, scan and output parameter files `perl do_grid_scan_hc.pl 08 05 05 /scratch/c704290/rhot_newtest 1`

- The resulting data can then be found in the directory /scratch/c704290/ (the scratch directory is used to store vast amounts of data).

5 Simulational Tests

5.1 Two-Level System

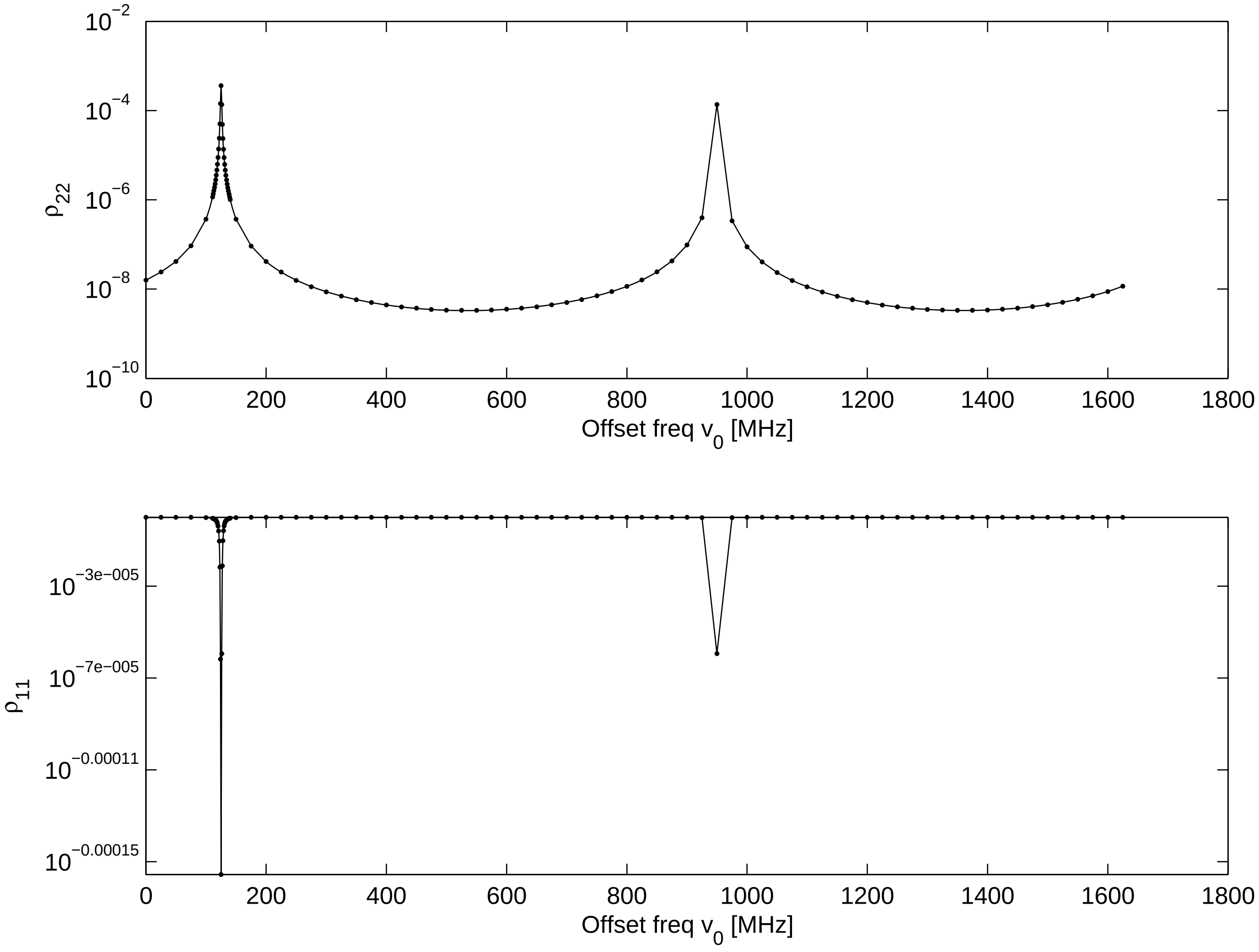

Figure 12: Two Levelsystem

```
atomparameters.N = [                 2   ]

atomparameters.no_of_trap_levels = [                 1   ]

atomparameters.atomic_transition_Gamma = [
                 0          10000000
                 0                 0
]

atomparameters.atomic_clebsch_gordan = [
                 1                 1
                 1                 1
]

atomparameters.atomic_allowed_transitions = [
                 x                pi
                 x                 x
]

atomparameters.atomic_rho0 = [                 1                 0   ]

atomparameters.atomic_energies = [                 0    2.7115355e-019   ]
atomparameters.m_factors = [                 0                 0   ]

atomparameters.trap_density = [                 1                 0   ]

atomparameters.omega_trap = [         6283185.3   ]

atomparameters.mass = [    6.6421551e-026   ]

atomparameters.energy_shift_factors = [                 0   ]

atomparameters.do_montecarlo = [                 0   ]

atomparameters.montecarlo_timestep = [    6.0679612e-010   ]

atomparameters.rho0 = [
                 1                 0
                 0                 0
]

atomparameters.energies = [     3.313034e-028    2.7115355e-019   ]

atomparameters.omega = [
                 0    2.5712202e+015
                 0                 0
]

atomparameters.wavelengths = [
                 0    7.3259054e-007
                 0                 0
]

atomparameters.lamb_dicke = [
                 0       0.096404462
                 0                 0
]

atomparameters.transition_Gamma = [
                 0          10000000
                 0                 0
]

atomparameters.allowed_Gamma = [
                 0                 0
                 0                 0
]

atomparameters.allowed_transitions = [
                 x                pi
                 x                 x
]

atomparameters.clebsch_gordan = [
                 1                 1
                 1                 1
]

atomparameters.Gamma_decay = [
                 0           5000000
           5000000          10000000
]

atomparameters.gamma_feed = [
                 0          10000000
                 0                 0
]

atomparameters.mu = [
                 0         111993.82
                 0                 0
]

laserparameters.alpha_comb = [                 0   ]

laserparameters.beta_pol_comb = [         1.5707963   ]

laserparameters.Bfield = [                 0   ]

laserparameters.v_group = [                 1   ]

laserparameters.v_phase = [                 1   ]

laserparameters.tp = [            5e-014   ]

laserparameters.e0 = [       1.5108e+008   ]

laserparameters.omega_L = [    2.3545645e+015   ]

laserparameters.tau = [    1.2135922e-009   ]

laserparameters.right_integration_limit = [            1e-012   ]

laserparameters.shift_pulse = [          2.5e-013   ]
laserparameters.RelTol = [           3e-014   ]

laserparameters.AbsTol = [           3e-014   ]

propagation_operators.U_I_phi_coeff = [
                 0                  1
                 0                  0
]

laserscanparameters.Niterations = [             1000   ]

laserscanparameters.timeevolution_save_cut = [               10   ]

laserscanparameters.save_time_evolution = [                1   ]
```

5.2 Two Level System with 3-lvl Trap

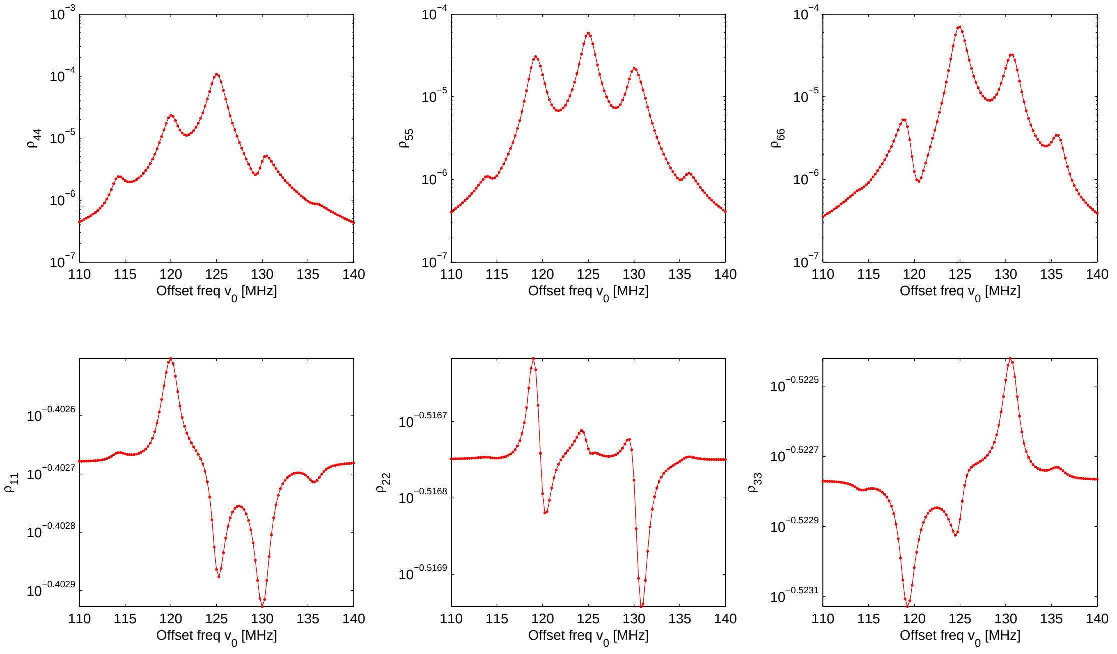

Figure 13: Two Level system with three trap levels

```
atomparameters.N = [                 2   ]

atomparameters.no_of_trap_levels = [                 3   ]

atomparameters.atomic_transition_Gamma = [
                 0           10000000
                 0                  0
]

atomparameters.atomic_clebsch_gordan = [
                 1                  1
                 1                  1
]

atomparameters.atomic_allowed_transitions = [
                 x                 pi
                 x                  x
]

atomparameters.atomic_rho0 = [                 1                  0   ]

atomparameters.atomic_energies = [                 0    2.7115355e-019   ]
atomparameters.m_factors = [                 0                 0   ]

atomparameters.trap_density = [               0.4               0.3               0.3   ]

atomparameters.omega_trap = [          31415927   ]

atomparameters.mass = [    3.3210776e-026   ]

atomparameters.energy_shift_factors = [                 0   ]

atomparameters.do_montecarlo = [                 0   ]

atomparameters.montecarlo_timestep = [    6.0679612e-010   ]

atomparameters.rho0 = [
               0.4                 0                 0                 0                 0                 0
                 0               0.3                 0                 0                 0                 0
                 0                 0               0.3                 0                 0                 0
                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0
]

atomparameters.energies = [     1.656517e-027     4.969551e-027     8.282585e-027    2.7115355e-019    2.7115355e-019    2.7115355e-019   ]

atomparameters.omega = [
                 0          31415927          62831853    2.5712202e+015    2.5712202e+015    2.5712202e+015
                 0                 0          31415927    2.5712201e+015    2.5712202e+015    2.5712202e+015
                 0                 0                 0    2.5712201e+015    2.5712201e+015    2.5712202e+015
                 0                 0                 0                 0          31415926          62831853
                 0                 0                 0                 0                 0          31415926
                 0                 0                 0                 0                 0                 0
]

atomparameters.wavelengths = [
                 0         59.958492         29.979246    7.3259054e-007    7.3259053e-007    7.3259052e-007
                 0                 0         59.958492    7.3259054e-007    7.3259054e-007    7.3259053e-007
                 0                 0                 0    7.3259055e-007    7.3259054e-007    7.3259054e-007
                 0                 0                 0                 0         59.958492         29.979246
                 0                 0                 0                 0                 0         59.958492
                 0                 0                 0                 0                 0                 0
]

atomparameters.lamb_dicke = [
                 0       0.060971535
                 0                 0
]

atomparameters.transition_Gamma = [
                 0                 0                 0          10000000         37175.281                 0
                 0                 0                 0         37175.281         9925787.6         74350.562
                 0                 0                 0                 0         74350.562         9851851.7
                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0
]

atomparameters.allowed_Gamma = [
                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0
]

atomparameters.allowed_transitions = [
                 x                 x                 x                pi                pi                 x
                 x                 x                 x                pi                pi                pi
                 x                 x                 x                 x                pi                pi
                 x                 x                 x                 x                 x                 x
                 x                 x                 x                 x                 x                 x
                 x                 x                 x                 x                 x                 x
]

atomparameters.clebsch_gordan = [
                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1
]

atomparameters.Gamma_decay = [
                 0                 0                 0         5018587.6         5018656.7         4963101.1
                 0                 0                 0         5018587.6         5018656.7         4963101.1
                 0                 0                 0         5018587.6         5018656.7         4963101.1
         5018587.6         5018587.6         5018587.6          10037175          10037244         9981688.8
         5018656.7         5018656.7         5018656.7          10037244          10037313         9981757.9
         4963101.1         4963101.1         4963101.1         9981688.8         9981757.9         9926202.2
]

atomparameters.gamma_feed = [
                 0                 0                 0          10000000         37175.281                 0
                 0                 0                 0         37175.281         9925787.6         74350.562
                 0                 0                 0                 0         74350.562         9851851.7
                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0
]

atomparameters.mu = [
                 0                 0                 0         111993.82         6828.4352                 0
                 0                 0                 0         6828.4355         111577.48         9656.8657
                 0                 0                 0                 0         9656.8661         111161.14
                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0
]

laserparameters.alpha_comb = [                0   ]

laserparameters.beta_pol_comb = [         1.5707963   ]

laserparameters.Bfield = [                0   ]

laserparameters.v_group = [                1   ]

laserparameters.v_phase = [                1   ]

laserparameters.tp = [           5e-014   ]

laserparameters.e0 = [      1.5108e+008   ]

laserparameters.omega_L = [    2.3545645e+015   ]

laserparameters.tau = [    1.2135922e-009   ]

laserparameters.right_integration_limit = [           1e-012   ]

laserparameters.shift_pulse = [          2.5e-013   ]

laserparameters.RelTol = [           3e-014   ]

laserparameters.AbsTol = [           3e-014   ]

propagation_operators.U_I_phi_coeff = [
                 0                 0                 0                 1                 1                 1
                 0                 0                 0                 1                 1                 1
                 0                 0                 0                 1                 1                 1
                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0
]

laserscanparameters.Niterations = [             1000   ]

laserscanparameters.timeevolution_save_cut = [               10   ]

laserscanparameters.save_time_evolution = [                1   ]
```

5.3 Ca 780nm Comb

```
atomparameters.N = [                5   ]

atomparameters.no_of_trap_levels = [                1   ]

atomparameters.atomic_transition_Gamma = [
                 0               1.3               1.3                 0                 0
                 0                 0                 0          10600000           1110000
                 0                 0                 0                 0           9900000
                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0
]

atomparameters.atomic_clebsch_gordan = [
                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1
]

atomparameters.atomic_allowed_transitions = [
                 x                pi                pi                 x                 x
                 x                 x                 x                pi                pi
                 x                 x                 x                 x                pi
                 x                 x                 x                 x                 x
                 x                 x                 x                 x                 x
```

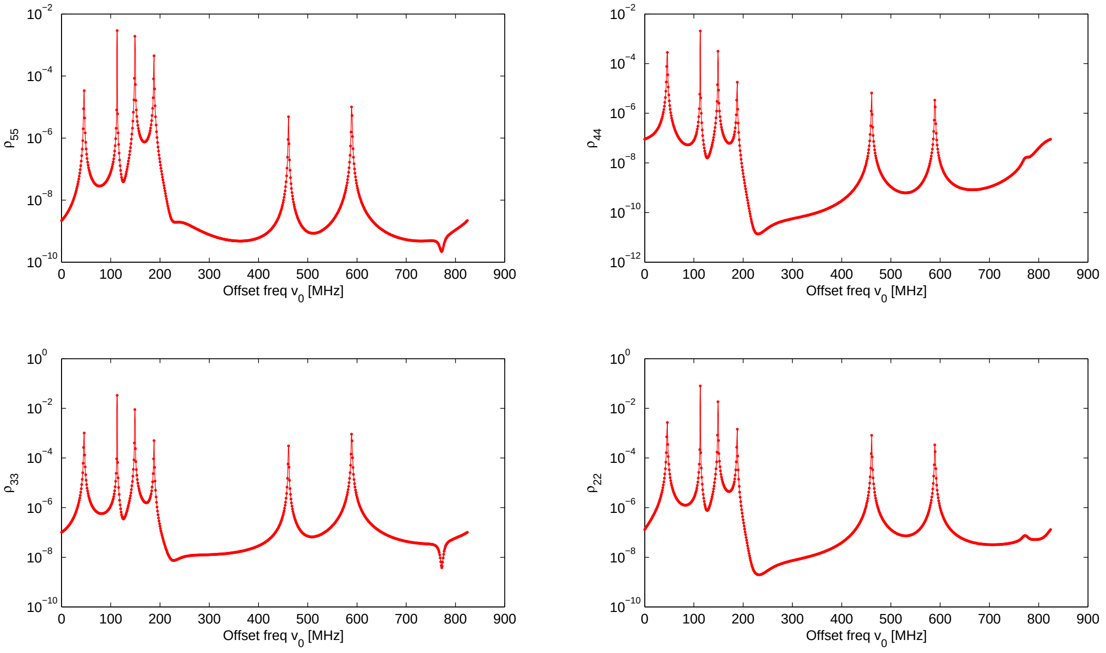

Figure 14: Ca system

```
]

atomparameters.atomic_rho0 = [                 1                 0                 0                 0                 0   ]

atomparameters.atomic_energies = [                 0    2.7115355e-019    2.7235912e-019    5.0041554e-019    5.0484313e-019   ]

atomparameters.m_factors = [                 0                 0                 0                 0                 0   ]

atomparameters.trap_density = [                 1                 0                 0                 0                 0   ]

atomparameters.omega_trap = [         6283185.3   ]

atomparameters.mass = [    6.6421551e-026   ]

atomparameters.energy_shift_factors = [                 0   ]

atomparameters.do_montecarlo = [                 0   ]

atomparameters.montecarlo_timestep = [    6.0679612e-010   ]

atomparameters.rho0 = [
                 1                 0                 0                 0                 0
                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0
]

atomparameters.energies = [     3.313034e-028    2.7115355e-019    2.7235912e-019    5.0041554e-019    5.0484313e-019   ]

atomparameters.omega = [
                 0    2.5712202e+015    2.5826521e+015    4.7452027e+015    4.7871874e+015
                 0                 0    1.1431881e+013    2.1739826e+015    2.2159673e+015
                 0                 0                 0    2.1625507e+015    2.2045354e+015
                 0                 0                 0                 0     4.198471e+013
                 0                 0                 0                 0                 0
]

atomparameters.wavelengths = [
                 0    7.3259054e-007    7.2934779e-007    3.9695913e-007    3.9347771e-007
                 0                 0     0.00016477179    8.6645202e-007    8.5003583e-007
                 0                 0                 0    8.7103234e-007    8.5444379e-007
                 0                 0                 0                 0     4.486518e-005
                 0                 0                 0                 0                 0
]
```

```
atomparameters.lamb_dicke = [
                 0       0.096404462       0.096833085                 0                 0
                 0                 0                 0       0.081510568       0.083084729
                 0                 0                 0                 0       0.082656106
                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0
]

atomparameters.transition_Gamma = [
                 0               1.3               1.3                 0                 0
                 0                 0                 0          10600000           1110000
                 0                 0                 0                 0           9900000
                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0
]

atomparameters.allowed_Gamma = [
                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0
]

atomparameters.allowed_transitions = [
                 x                pi                pi                 x                 x
                 x                 x                 x                pi                pi
                 x                 x                 x                 x                pi
                 x                 x                 x                 x                 x
                 x                 x                 x                 x                 x
]

atomparameters.clebsch_gordan = [
                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1
]

atomparameters.Gamma_decay = [
                 0              0.65              0.65           5300000           5505000
              0.65               1.3               1.3         5300000.7         5505000.7
              0.65               1.3               1.3         5300000.7         5505000.7
           5300000         5300000.7         5300000.7          10600000          10805000
           5505000         5505000.7         5505000.7          10805000          11010000
]

atomparameters.gamma_feed = [
                 0               1.3               1.3                 0                 0
                 0                 0                 0          10600000           1110000
                 0                 0                 0                 0           9900000
                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0
]

atomparameters.mu = [
                 0         40.379947         40.112137                 0                 0
                 0                 0                 0         148310.47         46635.802
                 0                 0                 0                 0         140360.52
                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0
]

laserparameters.alpha_comb = [                 0   ]

laserparameters.beta_pol_comb = [         1.5707963   ]

laserparameters.Bfield = [                 0   ]

laserparameters.v_group = [                 1   ]

laserparameters.v_phase = [                 1   ]

laserparameters.tp = [            5e-014   ]

laserparameters.e0 = [       1.5108e+008   ]

laserparameters.omega_L = [    2.3545645e+015   ]

laserparameters.tau = [    1.2135922e-009   ]

laserparameters.right_integration_limit = [            1e-012   ]

laserparameters.shift_pulse = [          2.5e-013   ]

laserparameters.RelTol = [            3e-014   ]

laserparameters.AbsTol = [            3e-014   ]

propagation_operators.U_I_phi_coeff = [
                 0                 1                 1                 2                 2
```

```
                0                 0                 0                 1                 1
                0                 0                 0                 1                 1
                0                 0                 0                 0                 0
                0                 0                 0                 0                 0
]

laserscanparameters.Niterations = [            50000   ]

laserscanparameters.timeevolution_save_cut = [             1000   ]

laserscanparameters.save_time_evolution = [                 1   ]
```

5.4 Ca 780nm Comb with 3-lvl Trap

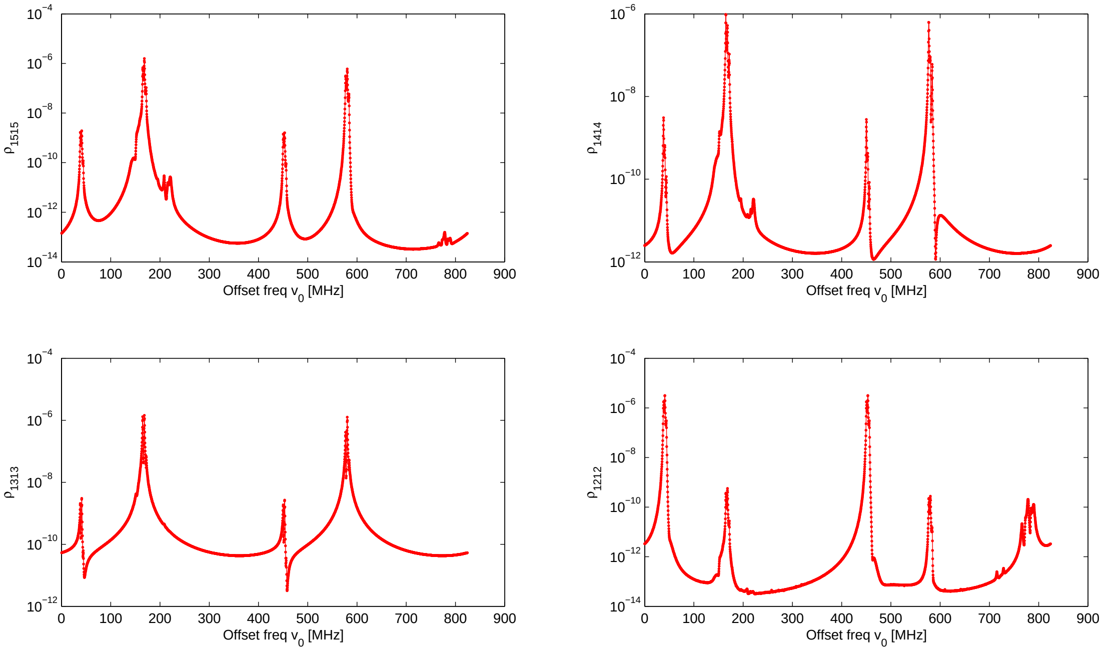

Figure 15: Ca system with three trap levels

```
atomparameters.N = [                 5   ]

atomparameters.no_of_trap_levels = [                 3   ]

atomparameters.atomic_transition_Gamma = [
                0               1.3               1.3                 0                 0
                0                 0                 0          10600000           1110000
                0                 0                 0                 0           9900000
                0                 0                 0                 0                 0
                0                 0                 0                 0                 0
]

atomparameters.atomic_clebsch_gordan = [
                1                 1                 1                 1                 1
                1                 1                 1                 1                 1
                1                 1                 1                 1                 1
                1                 1                 1                 1                 1
                1                 1                 1                 1                 1
]

atomparameters.atomic_allowed_transitions = [
                x                pi                pi                 x                 x
                x                 x                 x                pi                pi
                x                 x                 x                 x                pi
                x                 x                 x                 x                 x
                x                 x                 x                 x                 x
]
```

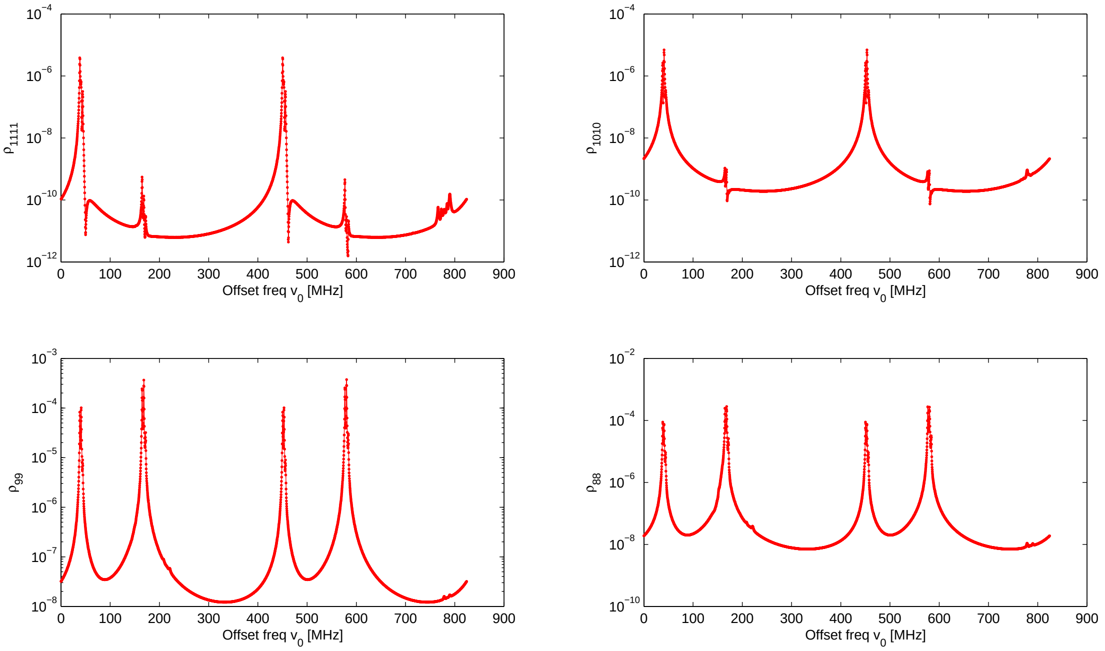

Figure 16: Ca system with three trap levels

```
atomparameters.atomic_rho0 = [                 1                 0                 0                 0                 0   ]

atomparameters.atomic_energies = [                 0    2.7115355e-019    2.7235912e-019    5.0041554e-019    5.0484313e-019   ]

atomparameters.m_factors = [                 0                 0                 0                 0                 0   ]

atomparameters.trap_density = [                 1                 0                 0                 0                 0   ]

atomparameters.omega_trap = [         6283185.3   ]

atomparameters.mass = [    6.6421551e-026   ]

atomparameters.energy_shift_factors = [                 0   ]

atomparameters.do_montecarlo = [                 0   ]

atomparameters.montecarlo_timestep = [    6.0679612e-010   ]

atomparameters.rho0 = [
                 1                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
]

atomparameters.energies = [     3.313034e-028     9.939102e-028     1.656517e-027    2.7115355e-019    2.7115355e-019    2.7115355e-019    2.7235912e-019    2.7235912e-019    2.72

atomparameters.omega = [
                 0         6283185.3          12566371    2.5712202e+015    2.5712202e+015    2.5712202e+015    2.5826521e+015    2.5826521e+015    2.5826521e+015    4.7452027e+01
                 0                 0         6283185.3    2.5712202e+015    2.5712202e+015    2.5712202e+015    2.5826521e+015    2.5826521e+015    2.5826521e+015    4.7452027e+01
                 0                 0                 0    2.5712202e+015    2.5712202e+015    2.5712202e+015     2.582652e+015    2.5826521e+015    2.5826521e+015    4.7452027e+01
                 0                 0                 0                 0         6283185.4          12566371    1.1431881e+013    1.1431888e+013    1.1431894e+013    2.1739826e+01
                 0                 0                 0                 0                 0         6283185.4    1.1431875e+013    1.1431881e+013    1.1431888e+013    2.1739825e+01
                 0                 0                 0                 0                 0                 0    1.1431869e+013    1.1431875e+013    1.1431881e+013    2.1739825e+01
```

```
               0               0               0               0               0               0               0       6283185.4        12566371  2.1625507e+01
               0               0               0               0               0               0               0               0       6283185.4  2.1625507e+01
               0               0               0               0               0               0               0               0               0  2.1625507e+01
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
]

atomparameters.wavelengths = [
               0       299.79246       149.89623  7.3259054e-007  7.3259053e-007  7.3259053e-007  7.2934779e-007  7.2934779e-007  7.2934778e-007  3.9695913e-00
               0               0       299.79246  7.3259054e-007  7.3259054e-007  7.3259053e-007  7.2934779e-007  7.2934779e-007  7.2934779e-007  3.9695913e-00
               0               0               0  7.3259054e-007  7.3259054e-007  7.3259054e-007  7.2934779e-007  7.2934779e-007  7.2934779e-007  3.9695914e-00
               0               0               0               0       299.79245       149.89623   0.00016477179    0.0001647717   0.00016477161  8.6645202e-00
               0               0               0               0               0       299.79245   0.00016477188   0.00016477179    0.0001647717  8.6645202e-00
               0               0               0               0               0               0   0.00016477197   0.00016477188   0.00016477179  8.6645202e-00
               0               0               0               0               0               0               0       299.79245       149.89623  8.7103234e-00
               0               0               0               0               0               0               0               0       299.79245  8.7103234e-00
               0               0               0               0               0               0               0               0               0  8.7103234e-00
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
]

atomparameters.lamb_dicke = [
               0     0.096404462     0.096833085               0               0
               0               0               0     0.081510568     0.083084729
               0               0               0               0     0.082656106
               0               0               0               0               0
               0               0               0               0               0
]

atomparameters.transition_Gamma = [
               0               0               0             1.3     0.012081966               0             1.3      0.01218964               0
               0               0               0     0.012081966       1.2759484     0.024163933      0.01218964        1.275735     0.024379281
               0               0               0               0     0.024163933       1.2521213               0     0.024379281       1.2516986
               0               0               0               0               0               0               0               0               0         1060000
               0               0               0               0               0               0               0               0               0        70426.11
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
]

atomparameters.allowed_Gamma = [
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
               0               0               0               0               0               0               0               0               0
]

atomparameters.allowed_transitions = [
               x               x               x              pi              pi               x              pi              pi               x
               x               x               x              pi              pi              pi              pi              pi              pi
               x               x               x               x              pi              pi               x              pi              pi
               x               x               x               x               x               x               x               x               x              p
               x               x               x               x               x               x               x               x               x              p
               x               x               x               x               x               x               x               x               x
               x               x               x               x               x               x               x               x               x
               x               x               x               x               x               x               x               x               x
               x               x               x               x               x               x               x               x               x
               x               x               x               x               x               x               x               x               x
               x               x               x               x               x               x               x               x               x
               x               x               x               x               x               x               x               x               x
               x               x               x               x               x               x               x               x               x
               x               x               x               x               x               x               x               x               x
               x               x               x               x               x               x               x               x               x
]

atomparameters.clebsch_gordan = [
                 1                 1                 1                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1                 1                 1                 1
]

atomparameters.Gamma_decay = [
                 0                 0                 0        0.65604098        0.65609713        0.63814261        0.65609482        0.65615197        0.63803896          5335213.
                 0                 0                 0        0.65604098        0.65609713        0.63814261        0.65609482        0.65615197        0.63803896          5335213.
                 0                 0                 0        0.65604098        0.65609713        0.63814261        0.65609482        0.65615197        0.63803896          5335213.
        0.65604098        0.65604098        0.65604098          1.312082         1.3121381         1.2941836         1.3121358          1.312193         1.2940799          5335213.
        0.65609713        0.65609713        0.65609713         1.3121381         1.3121943         1.2942397         1.3121919         1.3122491         1.2941361          5335213.
        0.63814261        0.63814261        0.63814261         1.2941836         1.2942397         1.2762852         1.2942374         1.2942946         1.2761816          5335213.
        0.65609482        0.65609482        0.65609482         1.3121358         1.3121919         1.2942374         1.3121896         1.3122468         1.2941338          5335213.
        0.65615197        0.65615197        0.65615197          1.312193         1.3122491         1.2942946         1.3122468         1.3123039         1.2941909          5335213.
        0.63803896        0.63803896        0.63803896         1.2940799         1.2941361         1.2761816         1.2941338         1.2941909         1.2760779          5335213.
         5335213.1         5335213.1         5335213.1         5335213.7         5335213.7         5335213.7         5335213.7         5335213.7         5335213.7           1067042
           5335447           5335447           5335447         5335447.7         5335447.7         5335447.6         5335447.7         5335447.7         5335447.6           1067066
         5230509.7         5230509.7         5230509.7         5230510.4         5230510.4         5230510.3         5230510.4         5230510.4         5230510.3           1056572
         5542649.8         5542649.8         5542649.8         5542650.4         5542650.4         5542650.4         5542650.4         5542650.4         5542650.4           1087786
         5542907.3         5542907.3         5542907.3         5542907.9         5542907.9         5542907.9         5542907.9         5542907.9         5542907.9           1087812
         5430730.5         5430730.5         5430730.5         5430731.1         5430731.1         5430731.1         5430731.1         5430731.1         5430731.1           1076594
]

atomparameters.gamma_feed = [
                 0                 0                 0               1.3       0.012081966                 0               1.3        0.01218964                 0
                 0                 0                 0       0.012081966         1.2759484       0.024163933        0.01218964          1.275735       0.024379281
                 0                 0                 0                 0       0.024163933         1.2521213                 0       0.024379281         1.2516986
                 0                 0                 0                 0                 0                 0                 0                 0                 0           1060000
                 0                 0                 0                 0                 0                 0                 0                 0                 0          70426.11
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
]

atomparameters.mu = [
                 0                 0                 0         40.379947         3.8928071                 0         40.112137         3.8841819                 0
                 0                 0                 0         3.8928071         40.004663         5.5052606          3.884182         39.736019         5.4930628
                 0                 0                 0                 0         5.5052606         39.629379                 0         5.4930628         39.359902
                 0                 0                 0                 0                 0                 0                 0                 0                 0          148310.4
                 0                 0                 0                 0                 0                 0                 0                 0                 0          12088.87
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
]

laserparameters.alpha_comb = [                0   ]

laserparameters.beta_pol_comb = [        1.5707963   ]

laserparameters.Bfield = [                0   ]

laserparameters.v_group = [                1   ]

laserparameters.v_phase = [                1   ]

laserparameters.tp = [           5e-014   ]

laserparameters.e0 = [      1.5108e+008   ]

laserparameters.omega_L = [   2.3545645e+015   ]

laserparameters.tau = [   1.2135922e-009   ]

laserparameters.right_integration_limit = [           1e-012   ]

laserparameters.shift_pulse = [         2.5e-013   ]
laserparameters.RelTol = [            3e-014   ]

laserparameters.AbsTol = [            3e-014   ]

propagation_operators.U_I_phi_coeff = [
                 0                 0                 0                 1                 1                 1                 1                 1                 1
                 0                 0                 0                 1                 1                 1                 1                 1                 1
                 0                 0                 1                 1                 1                 1                 1                 1                 1
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
]

laserscanparameters.Niterations = [             50000   ]

laserscanparameters.timeevolution_save_cut = [              5000   ]

laserscanparameters.save_time_evolution = [                 1   ]
```

5.5 Ca 780nm Comb Including 397nm Decay with 3-lvl Trap

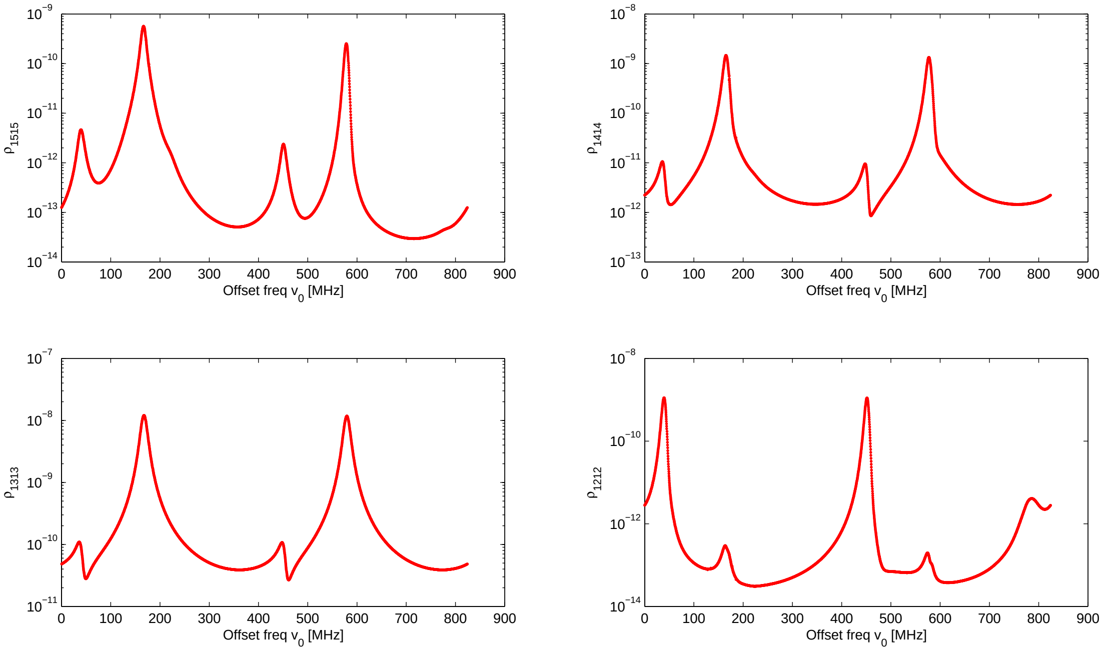

Figure 17: Ca system including 397nm decay channels and three trap levels

```
atomparameters.N = [                 5   ]

atomparameters.no_of_trap_levels = [                 3   ]

atomparameters.atomic_transition_Gamma = [
                 0               1.3               1.3           1.4e+008          1.47e+008
                 0                 0                 0           10600000            1110000
                 0                 0                 0                  0            9900000
                 0                 0                 0                  0                  0
                 0                 0                 0                  0                  0
```

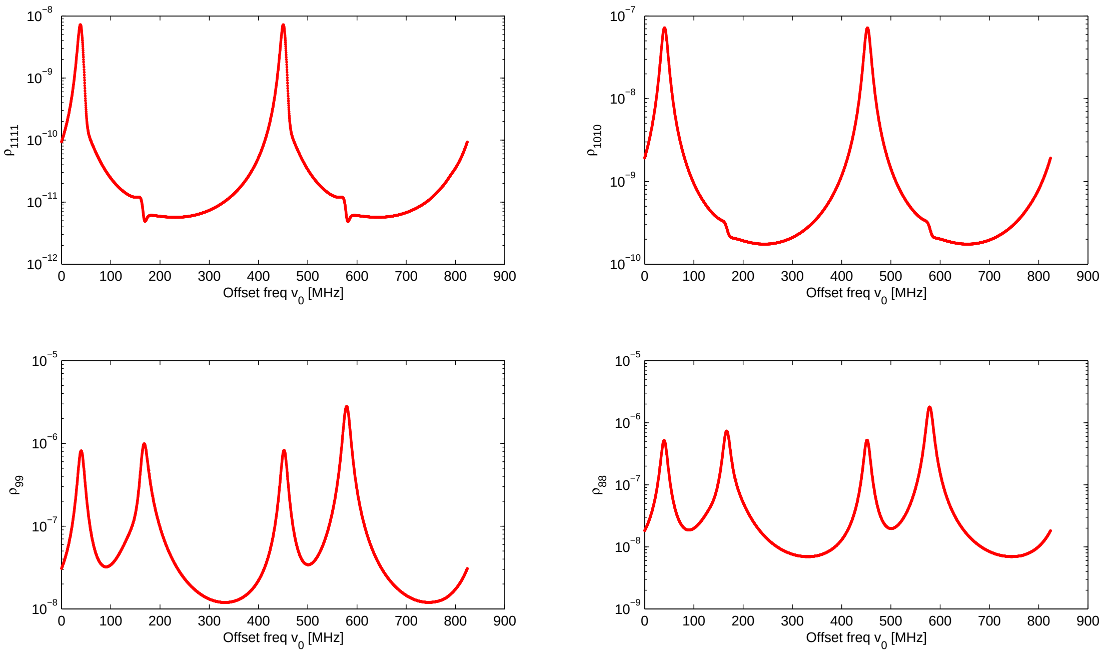

Figure 18: Ca system including 397nm decay channels and three trap levels

```
]

atomparameters.atomic_clebsch_gordan = [
                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1
]

atomparameters.atomic_allowed_transitions = [
                 x                pi                pi                 x                 x
                 x                 x                 x                pi                pi
                 x                 x                 x                 x                pi
                 x                 x                 x                 x                 x
                 x                 x                 x                 x                 x
]

atomparameters.atomic_rho0 = [                 1                 0                 0                 0                 0   ]

atomparameters.atomic_energies = [                 0     2.7115355e-019    2.7235912e-019    5.0041554e-019    5.0484313e-019   ]

atomparameters.m_factors = [                 0                 0                 0                 0                 0   ]

atomparameters.trap_density = [                 1                 0                 0                 0                 0   ]

atomparameters.omega_trap = [          6283185.3   ]

atomparameters.mass = [    6.6421551e-026   ]

atomparameters.energy_shift_factors = [                 0   ]

atomparameters.do_montecarlo = [                 0   ]

atomparameters.montecarlo_timestep = [    6.0679612e-010   ]

atomparameters.rho0 = [
                 1                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
]

atomparameters.energies = [     3.313034e-028     9.939102e-028     1.656517e-027    2.7115355e-019    2.7115355e-019    2.7115355e-019    2.7235912e-019    2.7235912e-019    2.72

atomparameters.omega = [
                 0         6283185.3          12566371    2.5712202e+015    2.5712202e+015    2.5712202e+015    2.5826521e+015    2.5826521e+015    2.5826521e+015   4.7452027e+01
                 0                 0         6283185.3    2.5712202e+015    2.5712202e+015    2.5712202e+015    2.5826521e+015    2.5826521e+015    2.5826521e+015   4.7452027e+01
                 0                 0                 0    2.5712202e+015    2.5712202e+015    2.5712202e+015     2.582652e+015    2.5826521e+015    2.5826521e+015   4.7452027e+01
                 0                 0                 0                 0         6283185.4          12566371    1.1431881e+013    1.1431888e+013    1.1431894e+013   2.1739826e+01
                 0                 0                 0                 0                 0         6283185.4    1.1431875e+013    1.1431881e+013    1.1431888e+013   2.1739825e+01
                 0                 0                 0                 0                 0                 0    1.1431869e+013    1.1431875e+013    1.1431881e+013   2.1739825e+01
                 0                 0                 0                 0                 0                 0                 0         6283185.4          12566371   2.1625507e+01
                 0                 0                 0                 0                 0                 0                 0                 0         6283185.4   2.1625507e+01
                 0                 0                 0                 0                 0                 0                 0                 0                 0   2.1625507e+01
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
]

atomparameters.wavelengths = [
                 0         299.79246         149.89623    7.3259054e-007    7.3259053e-007    7.3259053e-007    7.2934779e-007    7.2934779e-007    7.2934778e-007   3.9695913e-00
                 0                 0         299.79246    7.3259054e-007    7.3259054e-007    7.3259053e-007    7.2934779e-007    7.2934779e-007    7.2934779e-007   3.9695913e-00
                 0                 0                 0    7.3259054e-007    7.3259054e-007    7.3259054e-007    7.2934779e-007    7.2934779e-007    7.2934779e-007   3.9695914e-00
                 0                 0                 0                 0         299.79245         149.89623     0.00016477179      0.0001647717     0.00016477161   8.6645202e-00
                 0                 0                 0                 0                 0         299.79245     0.00016477188     0.00016477179      0.0001647717   8.6645202e-00
                 0                 0                 0                 0                 0                 0     0.00016477197     0.00016477188     0.00016477179   8.6645202e-00
                 0                 0                 0                 0                 0                 0                 0         299.79245         149.89623   8.7103234e-00
                 0                 0                 0                 0                 0                 0                 0                 0         299.79245   8.7103234e-00
                 0                 0                 0                 0                 0                 0                 0                 0                 0   8.7103234e-00
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
]

atomparameters.lamb_dicke = [
                 0       0.096404462       0.096833085        0.17791503        0.17948919
                 0                 0                 0       0.081510568       0.083084729
                 0                 0                 0                 0       0.082656106
                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0
]

atomparameters.transition_Gamma = [
                 0                 0                 0               1.3       0.012081966                 0               1.3        0.01218964                 0         1.4e+00
                 0                 0                 0       0.012081966         1.2759484       0.024163933        0.01218964          1.275735       0.024379281        4431526.
                 0                 0                 0                 0       0.024163933         1.2521213                 0       0.024379281         1.2516986
                 0                 0                 0                 0                 0                 0                 0                 0                 0         1060000
                 0                 0                 0                 0                 0                 0                 0                 0                 0        70426.11
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
]

atomparameters.allowed_Gamma = [
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
]

atomparameters.allowed_transitions = [
                 x                 x                 x                pi                pi                 x                pi                pi                 x
                 x                 x                 x                pi                pi                pi                pi                pi                pi
                 x                 x                 x                 x                pi                pi                 x                pi                pi
                 x                 x                 x                 x                 x                 x                 x                 x                 x                 p
                 x                 x                 x                 x                 x                 x                 x                 x                 x                 p
                 x                 x                 x                 x                 x                 x                 x                 x                 x
                 x                 x                 x                 x                 x                 x                 x                 x                 x
                 x                 x                 x                 x                 x                 x                 x                 x                 x
                 x                 x                 x                 x                 x                 x                 x                 x                 x
                 x                 x                 x                 x                 x                 x                 x                 x                 x
                 x                 x                 x                 x                 x                 x                 x                 x                 x
                 x                 x                 x                 x                 x                 x                 x                 x                 x
                 x                 x                 x                 x                 x                 x                 x                 x                 x
                 x                 x                 x                 x                 x                 x                 x                 x                 x
                 x                 x                 x                 x                 x                 x                 x                 x                 x
]

atomparameters.clebsch_gordan = [
                 1                 1                 1                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1                 1                 1                 1
                 1                 1                 1                 1                 1                 1                 1                 1                 1
]

atomparameters.Gamma_decay = [
                 0                 0                 0        0.65604098        0.65609713        0.63814261        0.65609482        0.65615197        0.63803896           7755097
                 0                 0                 0        0.65604098        0.65609713        0.63814261        0.65609482        0.65615197        0.63803896           7755097
                 0                 0                 0        0.65604098        0.65609713        0.63814261        0.65609482        0.65615197        0.63803896           7755097
        0.65604098        0.65604098        0.65604098          1.312082         1.3121381         1.2941836         1.3121358          1.312193         1.2940799           7755097
        0.65609713        0.65609713        0.65609713         1.3121381         1.3121943         1.2942397         1.3121919         1.3122491         1.2941361           7755097
        0.63814261        0.63814261        0.63814261         1.2941836         1.2942397         1.2762852         1.2942374         1.2942946         1.2761816           7755097
        0.65609482        0.65609482        0.65609482         1.3121358         1.3121919         1.2942374         1.3121896         1.3122468         1.2941338           7755097
        0.65615197        0.65615197        0.65615197          1.312193         1.3122491         1.2942946         1.3122468         1.3123039         1.2941909           7755097
        0.63803896        0.63803896        0.63803896         1.2940799         1.2941361         1.2761816         1.2941338         1.2941909         1.2760779           7755097
          77550976          77550976          77550976          77550977          77550977          77550977          77550977          77550977          77550977     1.5510195e+00
          77621347          77621347          77621347          77621348          77621348          77621348          77621348          77621348          77621348     1.5517232e+00
          71079532          71079532          71079532          71079533          71079533          71079533          71079533          71079533          71079533     1.4863051e+00
          81410553          81410553          81410553          81410554          81410554          81410554          81410554          81410554          81410554     1.5896153e+00
          81487096          81487096          81487096          81487096          81487096          81487096          81487096          81487096          81487096     1.5903807e+00
          74500065          74500065          74500065          74500066          74500066          74500066          74500066          74500066          74500066     1.5205104e+00
]

atomparameters.gamma_feed = [
                 0                 0                 0               1.3       0.012081966                 0               1.3        0.01218964                 0           1.4e+00
                 0                 0                 0       0.012081966         1.2759484       0.024163933        0.01218964          1.275735       0.024379281          4431526.
                 0                 0                 0                 0       0.024163933         1.2521213                 0       0.024379281         1.2516986
                 0                 0                 0                 0                 0                 0                 0                 0                 0           1060000
                 0                 0                 0                 0                 0                 0                 0                 0                 0          70426.11
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
]

atomparameters.mu = [
                 0                 0                 0         40.379947         3.8928071                 0         40.112137         3.8841819                 0
                 0                 0                 0         3.8928071         40.004663         5.5052606          3.884182         39.736019         5.4930628
                 0                 0                 0                 0         5.5052606         39.629379                 0         5.4930628         39.359902
                 0                 0                 0                 0                 0                 0                 0                 0                 0          148310.4
                 0                 0                 0                 0                 0                 0                 0                 0                 0          12088.87
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
]

laserparameters.alpha_comb = [                 0   ]

laserparameters.beta_pol_comb = [         1.5707963   ]
laserparameters.Bfield = [                 0   ]

laserparameters.v_group = [                 1   ]

laserparameters.v_phase = [                 1   ]

laserparameters.tp = [           5e-014   ]

laserparameters.e0 = [      1.5108e+008   ]

laserparameters.omega_L = [    2.3545645e+015   ]

laserparameters.tau = [    1.2135922e-009   ]

laserparameters.right_integration_limit = [           1e-012   ]

laserparameters.shift_pulse = [         2.5e-013   ]

laserparameters.RelTol = [           3e-014   ]

laserparameters.AbsTol = [           3e-014   ]

propagation_operators.U_I_phi_coeff = [
                 0                 0                 0                 1                 1                 1                 1                 1                 1
                 0                 0                 0                 1                 1                 1                 1                 1                 1
                 0                 0                 0                 1                 1                 1                 1                 1                 1
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
                 0                 0                 0                 0                 0                 0                 0                 0                 0
]

laserscanparameters.Niterations = [            50000   ]

laserscanparameters.timeevolution_save_cut = [             5000   ]

laserscanparameters.save_time_evolution = [                1   ]
```

A Calculations

A.1 Comb Structure

We discuss the function that results in the comb structure. The sum itself equals the geometric sum so that we can directly write down the solution

$$S_p = \sum_{k=0}^{p} e^{i\alpha k} = \frac{1-e^{i\alpha(p+1)}}{1-e^{i\alpha}} \tag{112}$$

Splitting the sum in real and imaginary part yields

$$\Re(S_p) = \cos\left(\frac{1}{2}\alpha p\right)\csc\left(\frac{\alpha}{2}\right)\sin\left(\frac{1}{2}\alpha(p+1)\right) \tag{113}$$

$$\Im(S_p) = \sin\left(\frac{1}{2}\alpha p\right)\csc\left(\frac{\alpha}{2}\right)\sin\left(\frac{1}{2}\alpha(p+1)\right) \tag{114}$$

Thus the complete sum results in

$$S_p = \sin\left(\frac{1}{2}\alpha p\right)\csc\left(\frac{\alpha}{2}\right)e^{i\frac{\alpha p}{2}} \tag{115}$$

Taking the square yields

$$|S_p|^2 = \frac{\cos(\alpha(p+1))-1}{\cos\alpha - 1} \tag{116}$$

A.2 Interaction Picture

A state is transformed into the interaction picture via

$$\left|\psi^I\right\rangle = U_0^\dagger(t)\left|\psi^S\right\rangle \quad \text{with} \quad U_0(t) = e^{-iH_0t/\hbar} \tag{117}$$

The transformation of an operator and the density matrix is given by

$$O^I = U_0^\dagger(t)\cdot O\cdot U_0(t) \quad ; \quad \rho^I = U_0^\dagger(t)\cdot\rho\cdot U_0(t) \tag{118}$$

The time evolution of a state $\psi^I(t)$ and the density matrix $\rho^I(t)$ in the interaction picture is given by

$$\left|\psi^I(t)\right\rangle = U_I(t)\left|\psi^I(0)\right\rangle \quad ; \quad \rho^I(t) = U_I(t)\cdot\rho^I(0)\cdot U_I^\dagger(t) \tag{119}$$

where $U_I(t)$ denotes the time propagation operator. It is determined by the Schrödinger equation

$$i\hbar\left|\dot{\psi}^I(t)\right\rangle = H_{int}^I(t)\left|\psi^I(t)\right\rangle \longrightarrow i\hbar\dot{U}_I(t)\left|\psi^I(0)\right\rangle = H_{int}^I(t)U_I(t)\left|\psi^I(0)\right\rangle \tag{120}$$

A.3 Formulas

$$\begin{aligned} FFT(f(t)) &= F(\omega) = \frac{1}{\sqrt{2\pi}}\int e^{-i\omega t}f(t)dx && (121)\\ FFT(f(at+b)) &= \frac{1}{a}e^{i\omega\frac{b}{a}}\cdot F\left(\frac{\omega}{a}\right) && (122)\\ FFT(f^*(t)) &= F(-\omega) && (123)\end{aligned}$$

A.4 Unitary Transformation for the Phase Dependence

In the following three examples of the unitary transformation to cancel out the phase dependence of the time propagation operator is shown. The Hamiltonian and the time propagation are transformed in the following way

$$\begin{aligned} U_I(t,\phi) &= K(\phi)\cdot U_I(t)\cdot K^\dagger(\phi) && (124)\\ H_{\text{int}}^I(t,\phi) &= K(\phi)\cdot H_{\text{int}}^I(t)\cdot K^\dagger(\phi) && (125)\\ K(\phi)\cdot K^\dagger(\phi) &= \mathbb{1} && (126)\end{aligned}$$

2-Level System This is an example for a generic two-level system. For convenience we leave out the time arguments.

$$\begin{aligned} K &= \begin{pmatrix} e^{i\phi} & 0 \\ 0 & 1 \end{pmatrix} && (127)\\ H_{\text{int}}^I &= \begin{pmatrix} 0 & h_{12} \\ h_{21} & 0 \end{pmatrix} && (128)\\ H_{\text{int}}^I(\phi) &= KH_{\text{int}}^IK^\dagger && (129)\end{aligned}$$

$$= \begin{pmatrix} 0 & h_{12}e^{i\phi} \\ h_{21}e^{-i\phi} & 0 \end{pmatrix} \tag{130}$$

$$U_I = \begin{pmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{pmatrix} \tag{131}$$

$$U_I(\phi) = KU^I K^\dagger \tag{132}$$

$$= \begin{pmatrix} u_{11} & u_{12}e^{i\phi} \\ u_{21}e^{-i\phi} & u_{22} \end{pmatrix} \tag{133}$$

$$\tag{134}$$

3-Level System Regarding the three-level system we have two possibilities.

$$K = \begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{i\phi} & 0 \\ 0 & 0 & e^{2i\phi} \end{pmatrix} \tag{135}$$

$$H^I_{\text{int}} = \begin{pmatrix} 0 & h_{12} & 0 \\ h_{21} & 0 & h_{23} \\ 0 & h_{32} & 0 \end{pmatrix} \tag{136}$$

$$H^I_{\text{int}}(\phi) = \begin{pmatrix} 0 & h_{12}e^{i\phi} & 0 \\ h_{21}e^{-i\phi} & 0 & h_{23}e^{i\phi} \\ 0 & h_{32}e^{-i\phi} & 0 \end{pmatrix} \tag{137}$$

$$U^I(\phi) = \begin{pmatrix} u_{11} & u_{12}e^{i\phi} & u_{13}e^{2i\phi} \\ u_{21}e^{-i\phi} & u_{22} & u_{23}e^{i\phi} \\ u_{31}e^{-2i\phi} & u_{32}e^{-i\phi} & u_{33} \end{pmatrix} \tag{138}$$

$$\tag{139}$$

$$K = \begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{-i\phi} & 0 \\ 0 & 0 & e^{-i\phi} \end{pmatrix} \tag{140}$$

$$H^I_{\text{int}} = \begin{pmatrix} 0 & h_{12} & h_{13} \\ h_{21} & 0 & 0 \\ h_{31} & 0 & 0 \end{pmatrix} \tag{141}$$

$$H^I_{\text{int}}(\phi) = \begin{pmatrix} 0 & h_{12}e^{i\phi} & h_{13}e^{i\phi} \\ h_{21}e^{-i\phi} & 0 & 0 \\ h_{31}e^{-i\phi} & 0 & 0 \end{pmatrix} \tag{142}$$

$$U^I(\phi) = \begin{pmatrix} u_{11} & u_{12}e^{i\phi} & u_{13}e^{i\phi} \\ u_{21}e^{-i\phi} & u_{22} & u_{23} \\ u_{31}e^{-i\phi} & u_{32} & u_{33} \end{pmatrix} \tag{143}$$

$$\tag{144}$$

B Scripts to Operate the GRID

Here you find the source code of several scripts used to communicate with the different clusters.

B.1 Useful Stuff for Operating the GRID Machines

- Copy files including directories
  `globus-url-copy -cd -r file:<source> gsiftp://altix1/<destiny>`
-

globus commands qsub commands qdel qstat nohup

Deleting multiple jobs

```
#!/bin/bash

echo 'Deleting job ...'
for ((i=$2;i<=$3;i+=1)); do
qdel $1$i
echo $1$i
done
echo 'done.'
```

B.2 Agrid1 Cluster

do_compile.pl

```
#!/usr/bin/perl

#use strict;
use warnings;

#my $direc                 = $ARGV[0];  # only if you want to use it as a parameter

my $direc = "simulations/fs_comb/141007/";
my $server = "agrid1.uibk.ac.at";
my $main_cp_cmd = "globus-url-copy file:/home/c704/c704290/".${direc};

# copy the necessary files to the grid and compiles calc_u_i and scan_job

my $str = "";

$str = "${main_cp_cmd}compile_job gsiftp://".$server."/~/".$direc."\n";
print $str;
system ($str);

$str = "${main_cp_cmd}scan_comb.m gsiftp://".$server."/~/".$direc."\n";
print $str;
system ($str);

$str = "${main_cp_cmd}calc_U_I.m gsiftp://".$server."/~/".$direc."\n";
print $str;
system ($str);

$str = "${main_cp_cmd}direct_int_timeprop_3lvl.m gsiftp://".$server."/~/".$direc."\n";
print $str;
system ($str);

$str = "${main_cp_cmd}do_time_evolution.m gsiftp://".$server."/~/".$direc."\n";
print $str;
system ($str);

$str = "${main_cp_cmd}feed_diagonal_terms.m gsiftp://".$server."/~/".$direc."\n";
print $str;
system ($str);
```

compile_job

```
#!/bin/bash
# PBS -l nodes=1
. /usr/site/matlab/matlab-R2007a.login
cd $arg1
##mcc -m -R -nojvm -R -nodisplay $arg1 -N
mcc -m -R -nojvm -R -nodisplay $arg2
```

do_calc_u.pl

calc_u_job

do_grid_scan.pl

B.3 HC Cluster

do_compile_hc

```
#!/bin/bash

qsub -v arg1=calc_U_I.m  compile_job
qsub -v arg1=scan_comb.m  compile_job
```

compile_job

```
#!/bin/bash
# The job should be placed into the queue 'all.q'.
#$ -q all.q
#$ -cwd

mcc -m -R -nojvm -R -nodisplay $arg1
```

do_calc_u_hc.pl

```
#!/usr/bin/perl

#use strict;
use warnings;

my $atomfingerprint = $ARGV[0];
my $ufingerprint    = $ARGV[1];

# run the time propagation calculation

$str = "qsub -v arg1=$atomfingerprint,arg2=$ufingerprint calc_u_job\n\n";
print $str;
system ($str);
```

calc_u_job

```
#!/bin/bash

# The job should be placed into the queue 'all.q'.
#$ -q all.q
#$ -cwd

./run_calc_U_I.sh $MATLAB $arg1 $arg2
```

scan_job

```
#!/bin/bash

# The job should be placed into the queue 'all.q'.
#$ -q all.q
#$ -cwd

./run_scan_comb.sh $MATLAB $arg2 $arg3 $arg4 $arg5 $arg6 $arg7 $arg8
```

C Information On the Elements

Isotope shifts? Source??? fermis golden rule

$$\Gamma_{ab} = \frac{8\pi^2}{3\epsilon_0\hbar\lambda_{ab}^3}\cdot|\mu_{ab}|^2 \tag{145}$$

$$\tag{146}$$

saturation intensity

$$I_S = \frac{\pi hc}{3\tau\lambda^3} \tag{147}$$

Einstein coefficients

$$A = \frac{hbar\omega_0^3 g_1}{\pi^2 c^3 g_2}B \tag{148}$$

$$B = \frac{\pi e^2}{3\epsilon_0\hbar^2}|\mu|^2 \tag{149}$$

fine structure

$$g_J = 1 + \frac{J(J+1)+S(S+1)-L(L+1)}{2J(J+1)} \tag{150}$$

$$\Delta E^Z_{m_J} = m_J g_J \mu_B B_0 \tag{151}$$

hyperfine structure

$$\Delta E_{hfs} = \frac{K_1}{2}A + K_2 B \tag{152}$$

$$K_1 = F(F+1) - J(J+1) - I(I+1) \tag{153}$$

$$K_2 = \frac{\frac{3}{2}K_1(K_1+1) - 2I(I+1)J(J+1)}{2I(2I-1)2J(2J-1)} \tag{154}$$

$$A = \frac{g_I\mu_K B_J}{\sqrt{J(J+1)}} \quad \text{dipole part} \tag{155}$$

$$B = \quad \text{quadrupole part} \tag{156}$$

hyperfine zeeman

$$\Delta E^Z_{m_F} = g_F\mu_B m_F B_0 \tag{157}$$

$$g_F = g_J\frac{F(F+1)+J(J+1)-I(I+1)}{2F(F+1)} - g_I \underbrace{\frac{\mu_K}{\mu_B}}_{=1/1836\approx 0} \cdots \tag{158}$$

C.1 Magnesium

Ionisation energy 7.646235 eV

Element	Mass	Abundance	Spin	Mag. Moment
24Mg	23.985042	78.99%	0	
25Mg	24.985837	10.00%	5/2	-0.85545
26Mg	25.982593	11.01%	0	

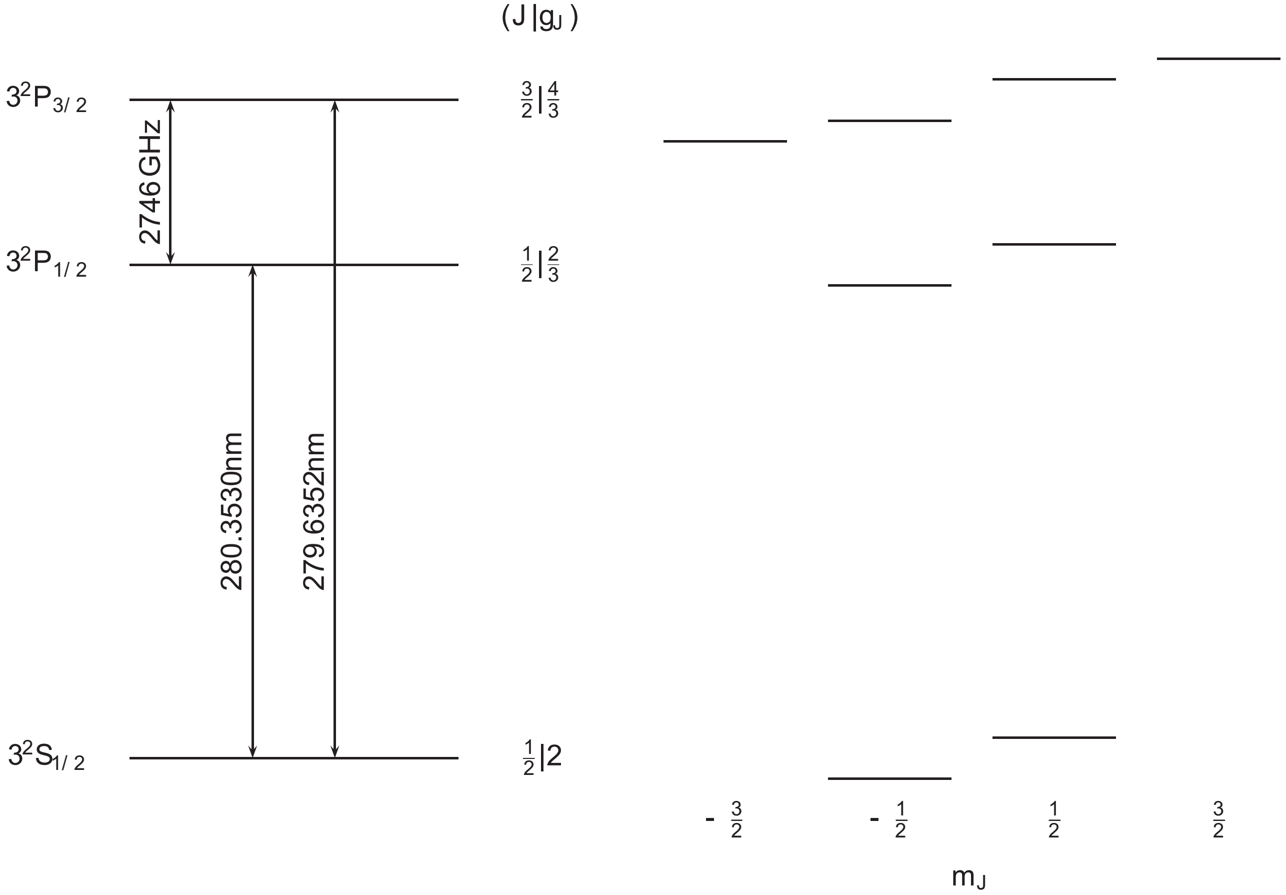

Figure 19: Magnesium-24 term scheme

C.1.1 Magnesium-24

Configuration	Term	J	Landé-g	Level [cm^{-1}]
2p^{6}3s	^{2}S	1/2	2	0
2p^{6}3p	^{2}P^0	1/2 3/2	2/3 4/3	35669.31 35760.88

λ [nm]	Ritz-λ [nm]	Terms	J$_i$ - J$_k$	A$_{ki}$ [s^{-1}]	f$_{ik}$	Type
279.6352	279.6352	^{2}S - ^{2}P^0	1/2 - 3/2	2.60e8	6.08e-1	
					3.8e-3	M2
280.3530	280.3531	^{2}S - ^{2}P^0	1/2 - 1/2	2.57e8	3.03e-1	

C.1.2 Magnesium-25

Configuration	Term	J	Landé-g	Level [cm^{-1}]
2p^{6}3s	^{2}S	1/2	2	0
2p^{6}3p	^{2}P^0	1/2 3/2	2/3 4/3	35669.31 35760.88

λ [nm]	Ritz-λ [nm]	Terms	J$_i$ - J$_k$	A$_{ki}$ [s^{-1}]	f$_{ik}$	Type
279.6352	279.6352	^{2}S - ^{2}P^0	1/2 - 3/2	2.60e8	6.08e-1	
					3.8e-3	M2
280.3530	280.3531	^{2}S - ^{2}P^0	1/2 - 1/2	2.57e8	3.03e-1	

C.2 Calcium-40

source: NIST database

Ionisation energy 6.11316 eV

Element	Mass	Abundance	Spin	Mag. Moment
40Ca	39.962591	96.941%	0	
42Ca	41.958618	0.647%	0	
43Ca	42.958766	0.135%	7/2	+1.3173
44Ca	43.955480	2.086%	0	
46Ca	45.953689	0.004%	0	
48Ca	47.952553	0.187%	0	

No	Level	Wavenumber [cm^{-1}]
5	4P3/2	25414.40
4	4P1/2	25191.51
3	3D5/2	13710.88
2	3D3/2	13650.19
1	4S1/2	0

Transition	Wavelength [nm]
S1/2 - P1/2	397
S1/2 - D5/2	729
D3/2 - P1/2	866
D5/2 - P3/2	854

Einstein coefficients and feeding terms

$$A = \begin{pmatrix} 0 & 0 & 1.3 & 1.4e8 & 0 \\ 0 & 0 & 0 & 1.06e7 & 0 \\ 0 & 0 & 0 & 0 & 9.9e6 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \frac{1}{s} \tag{159}$$

$$\gamma = \begin{pmatrix} 0 & 0 & 1 & 14/15 & 0 \\ 0 & 0 & 0 & 1/15 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \tag{160}$$

C.3 Titanium

Ionisation energy 6.82812 eV

Element	Mass	Abundance	Spin	Mag. Moment
46Ti	45.952629	8.0%	0	
47Ti	46.951764	7.43%	5/2	-0.7885
48Ti	47.947947	73.8%	0	
49Ti	48.947871	5.5%	7/2	-1.0417
50Ti	49.944792	5.4%	0	

C.4 Iron

Ionisation energy 7.9024 eV

Element	Mass	Abundance	Spin	Mag. Moment
54Fe	53.939612	5.82%	0	
56Fe	55.934939	91.18%	0	
57Fe	56.935396	2.1 %	1/2	+0.09044
58Fe	57.933277	0.28%	0	

Conifguration	Term	J	Level [cm^{-}1]	Lange-g
3d^6(^{5}D)4s	a^{6}D	9/2	0	1.58
		7/2	384.790	1.58
		5/2	667.683	1.655
		3/2	862.613	1.862
		1/2	977.053	3.31
3d^6(^{5}D)4p	z^{6}D^0	9/2	38458.981	1.542
		7/2	38660.043	1.584
		5/2	38858.958	1.653
		3/2	39013.206	1.86
		1/2	39109.307	3.35
3d^6(^{5}D)4p	z^{6}F^0	11/2	41968.046	-
		9/2	42114.818	1.43
		7/2	42237.033	1.399
		5/2	42334.822	1.304
		3/2	42401.302	1.04
		1/2	42439.822	-0.647
3d^6(^{5}D)4p	z^{6}P^0	7/2	42658.224	1.702
		5/2	43238.586	1.869
		3/2	43620.957	2.398
3d^6(^{5}D)4p	z^{4}F^0	9/2	44232.512	1.32
		7/2	44753.799	1.29
		5/2	45079.879	1.069
		3/2	45289.801	0.445
3d^6(^{5}D)4p	z^{4}D^0	7/2	44446.878	1.40
		5/2	44784.761	1.35
		3/2	45044.168	1.15
		1/2	45206.450	-0.021

λ [nm]	Ritz-λ [nm]	A$_{ki}$ [s^{-1}]	f$_{ik}$	Terms	J$_i$ - J$_k$	g$_i$ - g$_k$	Type
	224.9180	4.1e+06	2.5e-03	a^{6}D - z^{4}D^0	9/2 - 7/2	10 - 8	
	225.0176	1.5e+06	1.1e-03	a^{6}D - z^{4}F^0	3/2 - 3/2	4 - 4	
	225.0936	3.1e+06	2.4e-03		5/2 - 5/2	6 - 6	
	225.3127	5.1e+06	3.9e-03		7/2 - 7/2	8 - 8	
	226.0081	4.9e+06	3.8e-03		9/2 - 9/2	10 - 10	
	226.0860	2.1e+06	2.4e-03		3/2 - 5/2	4 - 6	
	226.2688	1.8e+06	1.4e-03	a^{6}D - z^{4}D^0	3/2 - 3/2	4 - 4	
	226.7587	3.1e+06	3.2e-03	a^{6}D - z^{4}F^0	5/2 - 7/2	6 - 8	
	226.8564	5.5e+05	8.5e-04	a^{6}D - z^{4}D^0	1/2 - 3/2	2 - 4	
	227.9916	3.9e+06	3.8e-03	a^{6}D - z^{4}F^0	7/2 - 9/2	8 - 10	
232.740	232.7397	5.9e+07	3.2e-02	a^{6}D - z^{6}P^0	5/2 - 3/2	6 - 4	
233.280	233.2800	1.5e+08	9.2e-02		7/2 - 5/2	8 - 6	
233.801	233.8008	1.1e+08	9.0e-02		3/2 - 3/2	4 - 4	
234.349	234.3496	1.7e+08	1.1e-01		9/2 - 7/2	10 - 8	
234.428	234.4283	8.2e+07	1.4e-01		1/2 - 3/2	2 - 4	
234.830	234.8303	1.2e+08	9.9e-02		5/2 - 5/2	6 - 6	
236.483	236.4829	6.1e+07	5.1e-02		7/2 - 7/2	8 - 8	
237.374	237.3736	3.3e+07	2.8e-02	a^{6}D - z^{6}F^0	9/2 - 9/2	10 - 10	
238.076	238.0762	3.1e+07	3.5e-02	a^{6}D - z^{6}P^0	5/2 - 7/2	6 - 8	
238.204	238.2039	3.8e+08	3.9e-01	a^{6}D - z^{6}F^0	9/2 - 11/2	10 - 12	
238.863	238.8630	1.0e+08	8.6e-02		7/2 - 7/2	8 - 8	
239.542	239.5420	3.3e+07	1.9e-02		5/2 - 3/2	6 - 4	
239.562	239.5626	2.5e+08	2.7e-01		7/2 - 9/2	8 - 10	
239.924	239.9242	1.4e+08	1.2e-01		5/2 - 5/2	6 - 6	
240.443	240.4432	7.1e+07	3.1e-02		3/2 - 1/2	4 - 2	
240.488	240.4887	1.7e+08	2.0e-01		5/2 - 7/2	6 - 8	
240.666	240.6662	1.6e+08	1.4e-01		3/2 - 3/2	4 - 4	
241.052	241.0520	1.5e+08	2.0e-01		3/2 - 5/2	4 - 6	
241.107	241.1069	2.4e+08	2.1e-01		1/2 - 1/2	2 - 2	
241.331	241.3311	1.1e+08	1.9e-01		1/2 - 3/2	2 - 4	
258.588	258.5876	8.1e+07	6.5e-02	a^{6}D - z^{6}D^0	9/2 - 7/2	10 - 8	
259.837	259.8370	1.3e+08	9.9e-02		7/2 - 5/2	8 - 6	
259.940	259.9396	2.2e+08	2.2e-01		9/2 - 9/2	10 - 10	
260.709	260.7088	1.7e+08	1.2e-01		5/2 - 3/2	6 - 4	
261.187	261.1874	1.1e+08	1.1e-01		7/2 - 7/2	8 - 8	
261.382	261.3825	2.0e+08	1.0e-01		3/2 - 1/2	4 - 2	
261.762	261.7618	4.4e+07	4.5e-02		5/2 - 5/2	6 - 6	
262.041	262.0409	3.6e+06	3.7e-03		3/2 - 3/2	4 - 4	
262.167	262.1670	4.9e+07	5.1e-02		1/2 - 1/2	2 - 2	
262.567	262.5668	3.4e+07	4.4e-02		7/2 - 9/2	8 - 10	
262.829	262.8294	8.6e+07	1.8e-01		1/2 - 3/2	2 - 4	
263.105	263.1048	7.7e+07	1.2e-01		3/2 - 5/2	4 - 6	
263.132	263.1324	6.0e+07	8.3e-02		5/2 - 7/2	6 - 8	

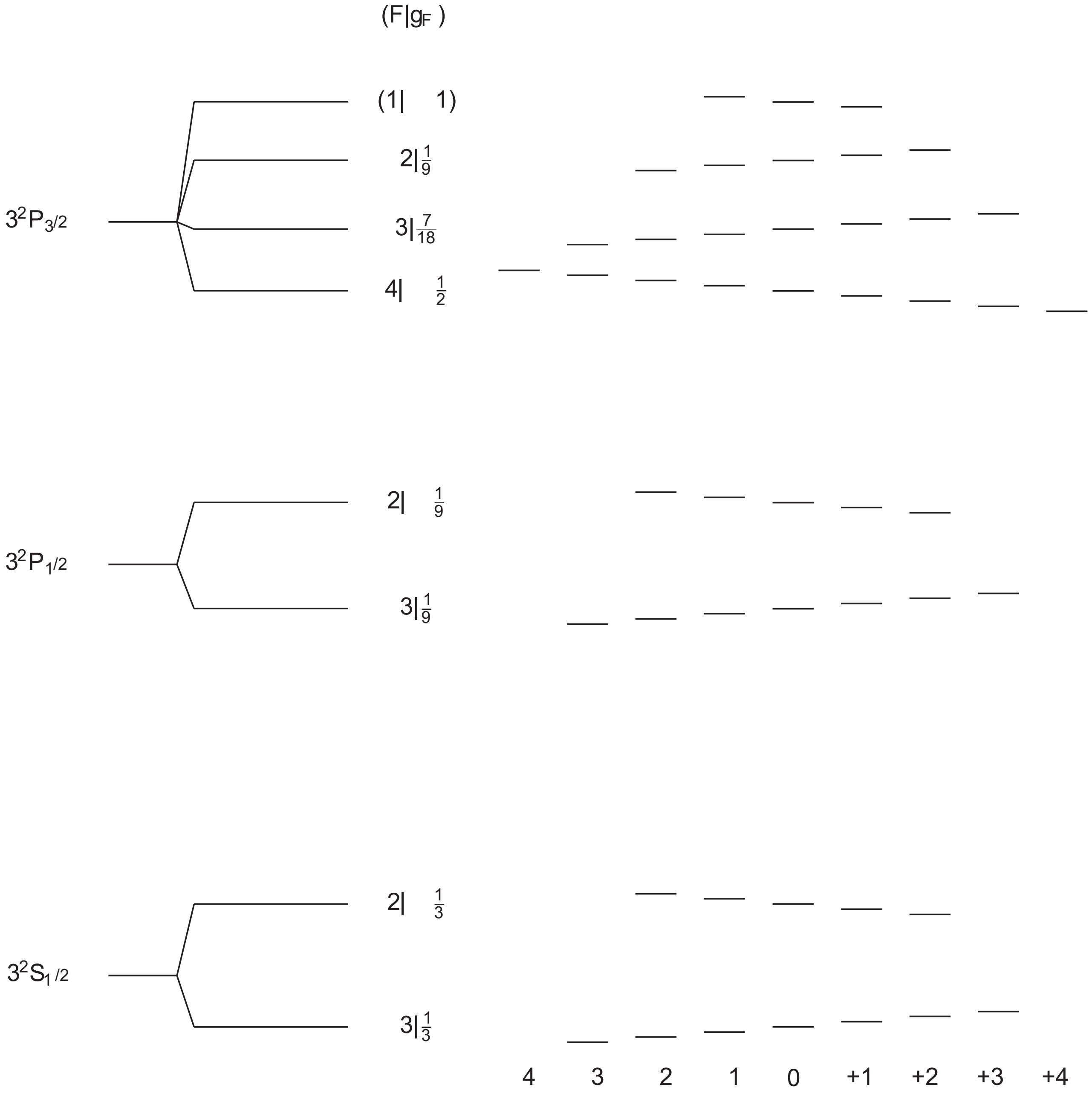

Figure 20: Magnesium-24 term scheme

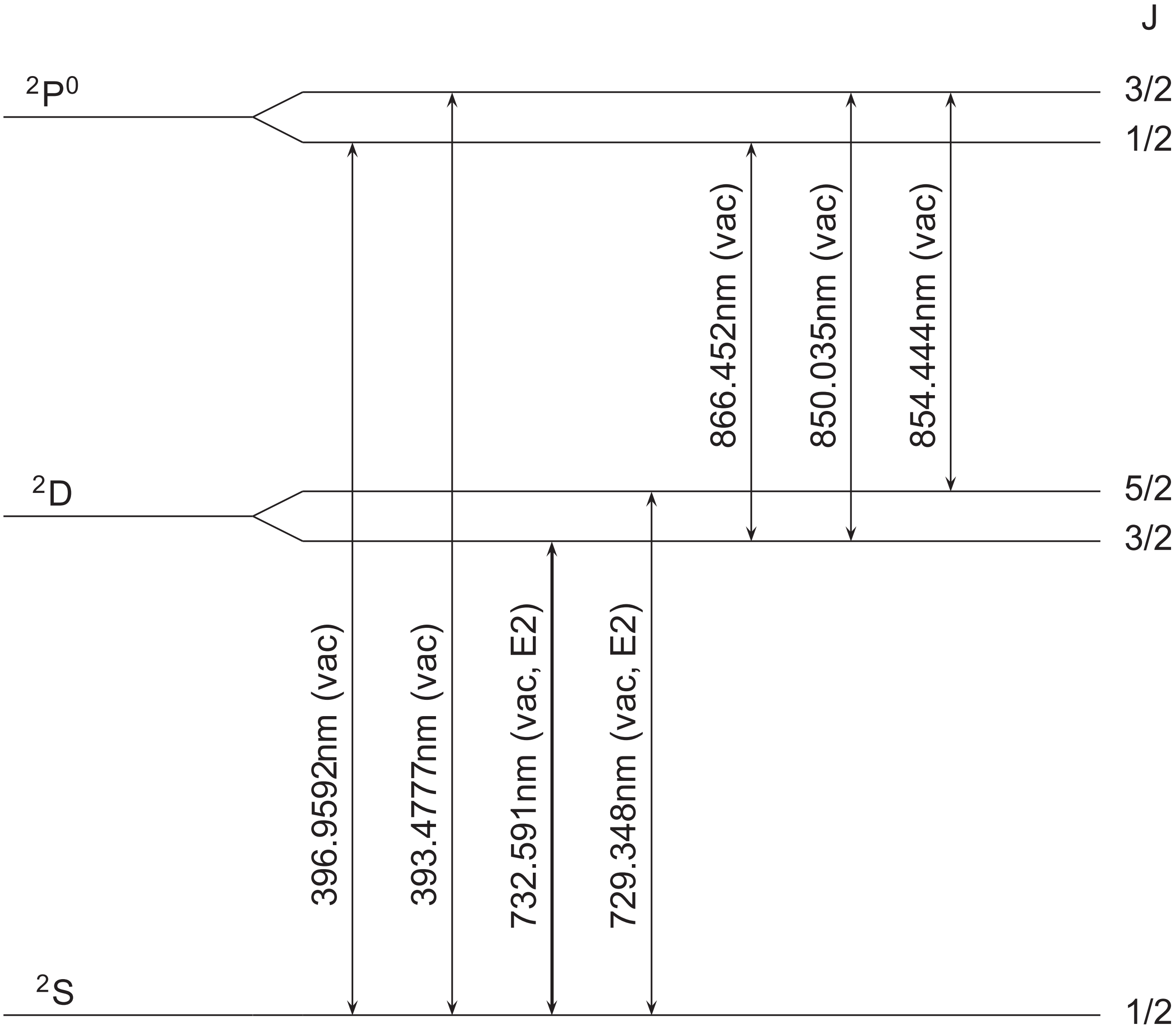

Figure 21: Calcium-40 term scheme

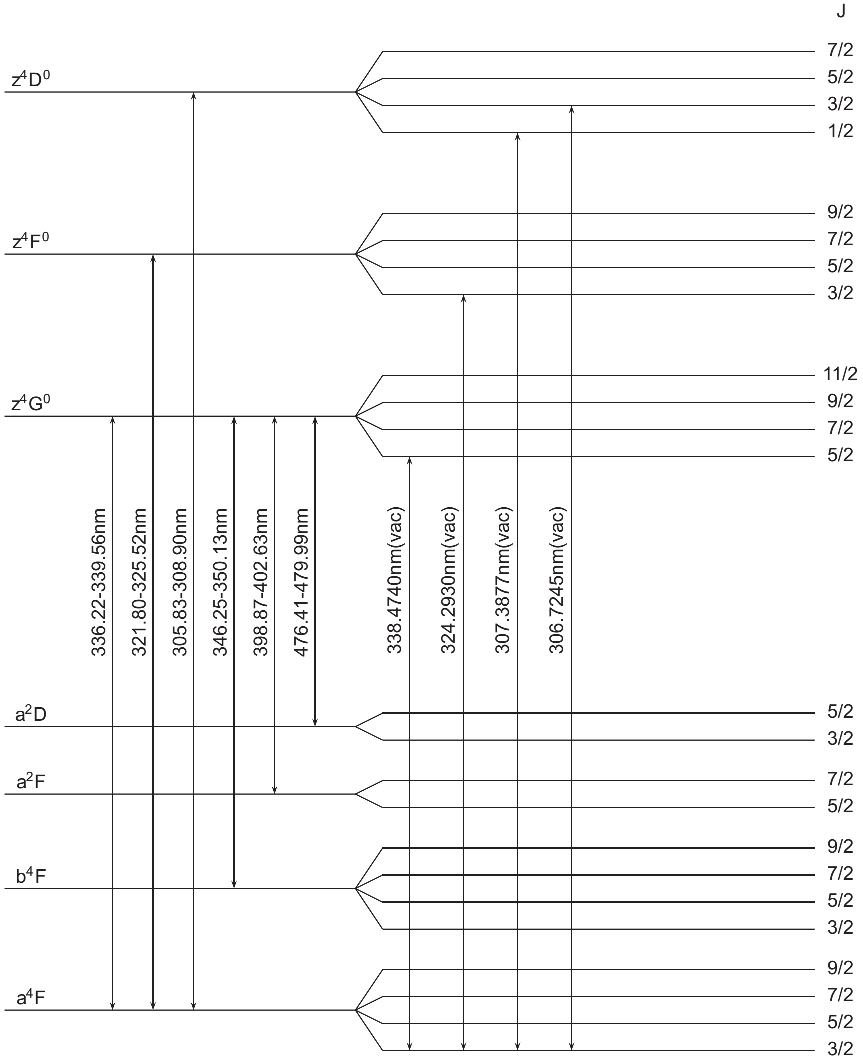

Figure 22: Ti-II level scheme, only the transitions of Flambaum's interest are shown

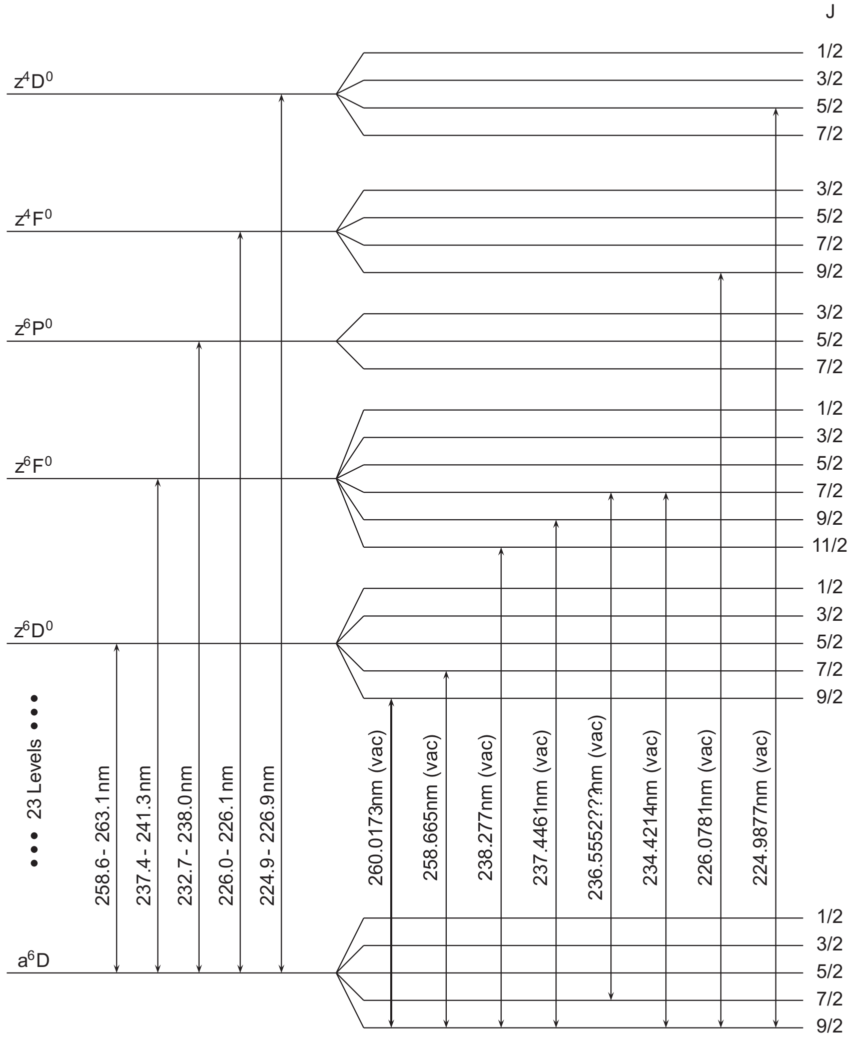

Figure 23: Fe-II level scheme, only the transitions of Flambaum's interest are shown

D So Far Unsolved Questions and Problems to Tackle

- Analytical approximation of the comb lines
- General solution for the feeding terms
- how to tune unknown frequencies of the atom
- $\Sigma(t - t_k)$

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