Spring 5-6-2012

Numerical Simulations of Chirped Excitation

Benjamin Iannitelli
University of Connecticut - Storrs, biannitelli@gmail.com

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Benjamin R. Iannitelli

Advisor: Phillip Gould
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Abstract

In this project I developed a general method of finding the optimal laser excitation for an ensemble of two-level atoms with the primary goal of exciting as many atoms as possible, as quickly as possible, for as long as possible, in order of decreasing priority. Specifically, I simulated the laser excitation of a collection of $^{87}$Rb atoms from $^2S_{1/2}$ to $^2P_{3/2}$, by finding numerical solutions to the optical Bloch equations. I optimized the parameters of a linear chirp paired with a Gaussian intensity pulse first neglecting and then including spontaneous emission, and then for a hyperbolic-tangent chirp paired with a squared-hyperbolic-secant intensity pulse including spontaneous emission. Comparing the optimal parameters for the linear chirp both with and without spontaneous emission demonstrated that neglecting spontaneous emission will lead to significant errors, at least when considering $^{87}$Rb. Comparing the linear chirp to the hyperbolic-tangent chirp (both with spontaneous emission) showed that both chirp shapes lead to excitation of greater than 96% of the population, and that based on my simulations, the linear chirp was slightly better at meeting all three goals of ceiling, speed and endurance. The best of all the excitations that I found using a linear chirp is to use a chirp rate between 0.2 and 0.65 GHz/ns and to use a pulse with a FWHM of 100 ns and a peak intensity of $10^6 \text{ W/cm}^2$. 

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Acknowledgements

For every stage of this project that went according to plan, there were two stages that did not. At every stage, rocky or smooth, Charles E. “Chad” Rogers III gave me crucial help, which either prevented me from barking up the wrong tree or turned my mountains into molehills. Thank you, Chad!

Of course, I would like to thank Professor Gould: for agreeing to be my academic advisor when I changed my major to Physics, for additionally agreeing to be my thesis advisor, and for posing the question that drove this project.

I am also grateful to Jennifer Carini, who was available whenever Chad was busy (the nerve of him, having a baby!) and lent me the lab computer when I was experiencing technical difficulties. I am also grateful for the moral support. No, my Nobel Prize hasn’t arrived yet, but I’m sure it’s on its way…

I would also like to thank Tom Collins and Vladislav Zakharov from Stevens Institute of Technology for taking time out of their visit to UConn to share some pointers, both for simulating multi-level atoms and for making Mathematica behave.

I would like to thank my friends for having to write their theses an entire year sooner than me (Crista), with better grammar (Carolyn), and only after learning Old Norse (Claire). Comparing my thesis to each of yours made mine a lot less frightening.

I would like to thank my family for all of their help and love over my whole life. Thank you for your support in all of its forms: moral, practical, and even impractical!
Introduction

In this paper, I will discuss several methods of manipulating the state of a collection of atoms. While an atom has infinitely many bound states before being ionized, in many atoms, states of higher order than the first excited state are only accessible with the contribution of amounts of energy that are significantly larger than that required to access the first excited state. For this reason, I am treating the atom as a two-level quantum mechanical system [1, 2]. Other examples of two-level systems include nuclear magnetic resonance and the states of an optical lattice [5, 6].

Often one desires to put an atom into its first excited state. This may be necessary for quantum information processing, which includes secure signal transmission and efforts to develop quantum computing [7, 1]. A researcher may want the atom in its first excited state merely to examine the properties of the state, or in order to conduct experiments that tangentially involve the first excited state. In all of these situations, one wants as large a population of the atoms as possible in the first excited state (referred to from now on as just “the excited state”, since the two-level treatment means ignoring any others). Often, one also wants the excited population to be produced in the shortest time possible and to remain in the excited state for as long as possible.

One popular means of exciting a collection of atoms is through laser excitation, the result of which depends on the intensity and frequency of the light. Often in the laboratory, a short pulse is used, rather than illuminating the atom continuously. A Gaussian pulse is a realistic option for an intensity pulse in theoretical discussions, since it is a convenient and common option for an intensity pulse in the laboratory. For this reason, in all of the following simulations a Gaussian intensity pulse will be used unless otherwise specified. The frequency of a laser can
also be varied, and when the frequency of a laser is a function of time that variation is referred to as a chirp.

Excitation of a collection of atoms to meet the three stated goals of size, duration, and speed faces two challenges, namely spontaneous emission and stimulated emission.

My aim in these simulations was to compare several different chirp shapes, and for each of these shapes find the parameters for achieving optimal excitation.

Theory and Simulations

All of the simulations featured in this paper\(^1\) were produced first by numerically solving the necessary differential equations. Based on these numerical solutions, I then plotted the relevant populations as fractions of the total population versus time. Both of these tasks were accomplished using the student edition of Mathematica 7. In order to solve differential equations numerically, I used explicit values that represented actual physical quantities in SI units. All of the quantities unique to a species of atom are based on the available data for the transition of \(^{87}\text{Rb}\) from \(^{2}\text{S}_{1/2}\) to \(^{2}\text{P}_{3/2}\).

For my first simulations, I used the Rabi two-level model, which does not account for spontaneous emission. The Rabi treatment is essentially the application of time-dependent perturbation theory, where the radiation of the laser is viewed as a classical field, and the atom is treated as a quantum object \([1]\). The excited state and the ground state will be denoted as \(|2\rangle\) and \(|1\rangle\), respectively. In the two-level Rabi problem, the state \(\Psi\) of an atom is a linear combination of the two states \([1]\):

\[
\Psi = c_1(t)|1\rangle e^{-i\frac{E_1}{\hbar}t} + c_2(t)|2\rangle e^{-i\frac{E_2}{\hbar}t}.
\]  

\(^1\) unless otherwise noted
If a laser is shone on the atoms at a frequency $\omega_l$, then the electric field from the laser is

$$\vec{E}_l = \vec{E}_0 \sin(\omega_l t).$$  \hspace{1cm} (2)

Since the atoms are small compared to the wavelength of the laser shone on them, the electric dipole approximation can be applied in order to describe the interaction between an atom and the electric field from the laser [1, 2]. Almost immediately it proves convenient to introduce two new quantities. The first of these is the detuning $\delta$ defined as

$$\delta \equiv \omega_l - \omega_a,$$  \hspace{1cm} (3)

where $\omega_a = \frac{E}{\hbar}$ is the atomic resonance frequency, proportional to the transition energy $E$ between the two states [1, 2]. From Eq. 3 it is clear that if $\omega_l$ is made a function of time, $\delta$ will have the same shape.

The second convenient quantity is the Rabi frequency, $\Omega$, which in this derivation is defined [2]

$$\Omega \equiv \frac{-eE_0}{\hbar} \langle 2|r|1 \rangle.$$  \hspace{1cm} (4)

Here $r$ denotes an electron’s distance from the nucleus [2]. The Rabi frequency, as will be apparent later, is the frequency at which both the excited and the ground populations are expected to oscillate if the detuning is zero (i.e., when the laser’s frequency is the resonance frequency).

It turns out that from the Schrodinger equation, a valence electron’s state follows the pattern [2]

$$i \dot{c}_1 = \Omega \cos(\omega_l) e^{-i\omega_a t}$$ \hspace{1cm} (5a)

$$i \dot{c}_2 = \Omega^* \cos(\omega_l) e^{-i\omega_a t}.$$ \hspace{1cm} (5b)

Applying the rotating wave approximation, and assuming the atom starts out in the ground state, one finds that [1]
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\[ i \dot{c}_1 = c_2 e^{i \delta t \frac{\Omega}{2}} \]  
\[ i \dot{c}_2 = c_1 e^{-i \delta t \frac{\Omega'}{2}} \]  
\[ c_1(0) = 1 \]  
\[ c_2(0) = 0, \]

or equivalently [1],

\[ i \dot{\tilde{c}}_1 = \frac{1}{2} (\delta \tilde{c}_1 + \Omega \tilde{c}_2) \]  
\[ i \dot{\tilde{c}}_2 = \frac{1}{2} (\Omega \tilde{c}_1 - \delta \tilde{c}_2) \]  
\[ \tilde{c}_1(0) = 1 \]  
\[ \tilde{c}_2(0) = 0, \]

where

\[ \tilde{c}_1 \equiv c_1 e^{-i \frac{\delta t}{2}} \]  
\[ \tilde{c}_2 \equiv c_2 e^{i \frac{\delta t}{2}}. \]

If \( \delta \) and \( \Omega \) are both constant, the solution to the original system is [2]:

\[ c_1 = e^{i \frac{\delta t}{2}} \left[ \cos \left( \frac{\Omega t}{2} \right) - i \frac{\delta}{\Omega} \sin \left( \frac{\Omega t}{2} \right) \right] \]  
\[ c_2 = -i \frac{\Omega}{\Omega'} \sin \left( \frac{\Omega t}{2} \right) e^{-i \frac{\delta t}{2}}. \]

In Eqs. 8a and 8b, \( \Omega' \) is the generalized Rabi frequency,

\[ \Omega' \equiv \sqrt{\Omega'^2 + \delta^2}. \]

The physical relevance of the generalized Rabi frequency is that it is the frequency of oscillation of the fractional populations \( |c_1|^2 \) and \( |c_2|^2 \).

Rather than rely directly on Eq. 4 to run realistic simulations, I derived the relation between \( \Omega \) and the intensity \( I \). For a laser described by Eq. 2,

\[ I = \frac{E_0^2}{2 \epsilon_0 n_0}. \]
I then solved Eq. 10 for $E_0$, and substituted it into Eq. 4. I combined that result with a relation between the mean lifetime $\tau$ of the excited state and the matrix element $\langle 1|\tau|2 \rangle$ [1, 2, 4]:

$$\frac{1}{\tau} = \frac{g_1}{g_2} \frac{4\alpha}{3c^2} \omega_\alpha \left| \langle 1|\tau|2 \rangle \right|^2,$$

(11)

where $g_n$ denotes the degeneracy of state $n$ and $\alpha$ is the fine-structure constant. This enabled me to make a formula for $\Omega$ in terms of $I$ and properties of the atom:

$$\Omega = \sqrt{\frac{6\pi g_2}{g_1 \hbar \omega_\alpha^3 \tau}} I.$$

(12)

For the transition of $^{87}\text{Rb}$ from $5^2S_{1/2}$ to $5^2P_{3/2}$ ($\text{D}_2$ line), $\tau = 26.2$ ns and $\omega_\alpha = 2.414 \times 10^{15}$ rad/s, and for a two-level atom $g_1 = g_2 = 1$ [3, 1]. Therefore, in my simulations

$$\Omega = \sqrt{\frac{6\pi \frac{c^2}{\hbar \omega_\alpha^3 \tau}} I}. $$

(13)

Before running any simulations for a varying frequency or a Gaussian intensity pulse, I first solved the fixed-frequency, fixed-intensity situation numerically. As shown in Fig. 1, I used $2\pi \times 80$ MHz for a realistic value of $\delta$, and $500 \text{W/cm}^2$ for $I$, since reasonable ranges for $\delta$ and $I$ were from 0 to $2\pi \times 1$ GHz, and from 0 to 1000 $\text{W/cm}^2$ respectively. Inserting all of the preceding values into Eq. 13 led to the values $\Omega = 14.8 \times 10^9$ rad/s, and $\Omega' \approx 14.8 \times 10^9$ rad/s, which then allowed me to solve Eqs. 6a-d numerically with a realistic set of numbers.

The graphs of the numerical solution and the analytical solution to Eqs. 6a-d are given in Figs. 2 and 3, using the values $\delta = 0.5 \text{Grad/s}$, $\Omega = 14.8 \text{Grad/s}$, and $\Omega' \approx 14.8 \text{Grad/s}$. These are graphs of the probabilities $|c_1|^2$ and $|c_2|^2$, and they show that my simulation based on the numerical solution to Eq. 8 matches that based on the analytical solution.
Figure 1: Graph of the detuning (blue) and Rabi frequency (purple) used in the simulations of constant detuning and constant Rabi frequency (shown in Figs. 2 and 3). The horizontal axis is time in nanoseconds, and the vertical axis is angular frequency in $\text{Grad}/\text{s}$. 
Figure 2: Graph of the numerical solution from Mathematica. The blue line represents $|c_1|^2$ and the red line represents $|c_2|^2$. The horizontal axis represents time in nanoseconds; the vertical axis is dimensionless, since $|c_1|^2$ and $|c_2|^2$ are probabilities. The parameters are given in Fig. 1.
Next I simulated a constant detuning and a Gaussian intensity pulse. To accomplish this, I used Eq. 13 and an intensity of the form:

\[ I(t) = I_m e^{-\frac{(t-m)^2}{2\sigma^2}}, \]  

with these parameters:

| \( I_m \) | 100 W/cm² |
| \( m \) | 50 ns |
| \( \sigma \) | 17.0 ns |

This pulse has a full width at half-max (FWHM) of 40 ns. Once again I set \( \delta \) at 0.5 Grad/s. The resulting simulation is shown in Figure 4.
Fig. 4.1: Graph of the numerical solution for a Gaussian intensity and constant detuning. The blue line represents $|c_1|^2$ and the red line represents $|c_2|^2$. The horizontal axis represents time in seconds; the vertical axis is dimensionless, since $|c_1|^2$ and $|c_2|^2$ are probabilities. The sudden jerk in the probabilities in the neighborhood of 50 ns is due to a technical limitation in the resolution of Mathematica’s “Plot” command, as evidenced by Fig. 4.2, which shows exactly the same probabilities but in a narrower time window.
Figure 4.2: Graph of $|c_1|^2$ and $|c_2|^2$, strictly from 40 ns to 60 ns. This plot does not show the sudden lack of oscillations near 50 ns that appears in Fig. 4.1. Evidently the reason for the strange behavior in Fig. 4.1 is that Mathematica is unable to produce a perfectly loyal plot of the entire numerical solution, no matter how high one sets MaxRecursions.

The simulation with a Gaussian intensity resembles an evolution of the solutions with constant intensities, as shown in Figs. 5-9.
Fig. 5: Solution with $I = 1.3 \frac{W}{cm^2}$.
Fig. 6: Solution with $I = 6.3 \, \text{W/cm}^2$.

Fig. 7: Solution with $I = 21 \, \text{W/cm}^2$. 
Fig. 8: Solution with $I = 50 \, W/cm^2$.

Fig. 9: Solution with $I = 84 \, W/cm^2$. 
Once I had simulated excitation of a collection of atoms with a Gaussian pulse and constant detuning, I was ready to simulate excitation with a Gaussian pulse and a linear chirp, i.e.

with a frequency of the form

\[ \omega(t) = \alpha t + \nu, \]  

which is mathematically equivalent to using a detuning of the form

\[ \delta(t) = \alpha t + \nu - \omega_a. \]  

In these simulations I set the parameters \(\alpha\) and \(\nu\) such that

\[ \delta(t) = 2\pi \times 1.6 \times 10^{15} \text{Hz/s} \times t - 2\pi \times 80 \text{MHz}, \]  

and \(I\) was set to \(50 \text{W/cm}^2\). A 40 ns FWHM Gaussian pulse was assumed. This led to the result shown in Fig. 10.

Fig. 10: Simulation of excitation with a linear chirp and with a Gaussian pulse. The blue line represents \(|c_1|^2\) and the red line represents \(|c_2|^2\). The horizontal axis represents time in seconds; the vertical axis is dimensionless, since \(|c_1|^2\) and \(|c_2|^2\) are probabilities.
Along the time interval from 0 to 50 ns I measured the period $T$ along several subintervals.

Measuring $T$ gave me a measurement $\Omega_{\text{meas}}$ of the generalized Rabi frequency. For each subinterval, I found the midpoint $t$ and calculated the value $\Omega'_{\text{calc}}$ for the generalized Rabi frequency. The results are shown in Table 1.

Table 1: Measurements from the graph based on linear chirp and Gaussian intensity compared to calculations based on the same detuning and intensity.

<table>
<thead>
<tr>
<th>$t$ (ns)</th>
<th>$T$ (ns)</th>
<th>$\Omega'_{\text{meas}}$ (rad/s)</th>
<th>$\Omega'_{\text{calc}}$ (rad/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.83</td>
<td>4.17</td>
<td>1.51E+09</td>
<td>1.48E+09</td>
</tr>
<tr>
<td>16</td>
<td>2.58</td>
<td>2.44E+09</td>
<td>2.45E+09</td>
</tr>
<tr>
<td>27.36</td>
<td>1.45</td>
<td>4.33E+09</td>
<td>4.24E+09</td>
</tr>
<tr>
<td>37.36</td>
<td>1.09</td>
<td>5.76E+09</td>
<td>5.75E+09</td>
</tr>
<tr>
<td>45.5</td>
<td>1</td>
<td>6.28E+09</td>
<td>6.49E+09</td>
</tr>
</tbody>
</table>

These results show that the oscillations in Fig. 10 are indeed Rabi oscillations. This indicates that within the constraints of only two levels and neglecting spontaneous emission, my simulations are accurate for chirped excitation with intensities that vary with time.

As another consistency check, for all of these simulations I graphed the sum of the two probabilities, which in a two-level treatment should be 1. Within machine error, it was, indicating that all of the preceding simulations were consistent with conservation of probability. The plots from several of these tests are shown in Figs. 11-13.
Figure 11: Mathematica graph of $|c_1|^2 + |c_2|^2$ from the numerical solution for $\delta = 0.5 \text{ Grad/s}$ and $\Omega = 14.8 \text{ Grad/s}$. The deviation from unity is so small that it is most likely from rounding of numbers by the computer. This means that within the limitations of the computer used, the numerical solution obeys the normalization condition. These axes have the same dimensions as those of Fig.1.

Figure 12: Mathematica graph of $|c_1|^2 + |c_2|^2$ from the simulation for $\delta = 0.5 \text{ Grad/s}$ and a Gaussian intensity pulse. The deviation from unity is again so small that within the limitations...
of the computer used, the numerical solution obeys the normalization condition. These axes have the same dimensions as those of Fig.10.

![Graph](image)

Fig. 13: graph of $|c_1|^2 + |c_2|^2$ from the simulation for a linear chirp and a Gaussian intensity pulse. The deviation from unity is again so small that within the limitations of the computer used, the numerical solution obeys the normalization condition. These axes have the same dimensions as those of Fig.12.

To account for spontaneous emission, it proved necessary to view the problem in a different theoretical framework. Therefore as an intermediate step, I next simulated exactly the same system with the Bloch equations [1]²:

\begin{align}
\dot{u} &= \delta v \\
\dot{v} &= -\delta u + \Omega w \\
\dot{w} &= -\Omega v, \\
u &\equiv \bar{\rho}_{12} + \bar{\rho}_{21} \\
v &\equiv -i(\bar{\rho}_{12} - \bar{\rho}_{21})
\end{align}

² The Bloch equations as they appear in Eqs. 18 and 19 still neglect spontaneous emission, but it will be evident later that Eqs. 18 can be corrected to account for spontaneous emission, which would be inconvenient to attempt with Eqs. 6 or 7 [5, 1]. In this paper, I will refer to Eqs. 18 as “the Bloch equations” and I will refer to the model corrected for spontaneous emission (Eqs. 23 and 24) as “the optical Bloch equations,” as did Allen and Eberly.
The quantities $u$, $v$, and $w$ are the components of a quantity called the Bloch vector, which represents the state of the system in a three-dimensional state space, analogous to the position of a particle in traditional 3-D space [1]. As a consequence of this framework, the generalized Rabi frequency becomes analogous to the angular velocity of the system, with the Rabi frequency and the detuning acting as its components in state space [1]. In this state space, one can define the Bloch sphere, which is a sphere of radius 1, and represents all of the possible states in which the system could be [1]. In the state space corresponding to Eqs. 18 and 19, the “North pole” of the Bloch sphere represents the entire population being in the ground state, and the “South pole” represents the entire population being in the excited state [1]. Therefore the goal stated in this paper can be viewed as moving the Bloch vector from the North pole to the South pole, by an appropriate manipulation of angular velocity. The components of the Bloch vector are defined based on the transformed coherences of the system, and it happens that $\rho_{kk}$ is the fractional population in state $k$, so $w$ is the difference in fractional population between the two states. Since $\rho_{kk}$ are fractional populations, it still holds that

$$\rho_{11} + \rho_{22} = 1. \tag{20}$$

Combining Eqs. 19c and 20 leads to the result that

$$\rho_{22} = |c_2|^2 = \frac{1}{2} - \frac{w}{2} \tag{21}$$

I solved Eqs. 18 numerically with the same linear chirp and Gaussian intensity pulse (Eqs. 14 and 15) as I had used for the Rabi two-level problem, and found that the two treatments agree. Fig.14 shows the time-dependent Rabi frequency and detuning used in this comparison. Figs. 15 and 16 show the resulting graphs for the fractional population in the excited state.
Figure 14: The time-dependent Rabi frequency (purple) and detuning (blue) used in comparing the Rabi-based simulations to the Bloch-based simulations. The horizontal axis is time in seconds; the vertical axis is angular frequency in rad/s.

Figure 15: Graph of the excited fractional population based on the Rabi treatment for linear chirp and Gaussian intensity.
Conservation of probability takes a new form in the Bloch framework:

\[ u^2 + v^2 + w^2 = 1 \]  

This means that to do a normalization test (Fig. 17), I had to graph the quantity on the left-hand side of Eq. 22, which is equivalent to \(|c_1|^2 + |c_2|^2\). The results show that the Bloch simulation for a linear chirp and Gaussian intensity pulse also agrees with the normalization condition.
The agreement of these two treatments allowed me to get even more realistic, by solving the optical Bloch equations [1] (OBE), which account for spontaneous emission:\(^3\):

\[
\begin{align*}
\dot{u} &= \delta v - \frac{\Gamma}{2} u \\
\dot{v} &= -\delta u + \Omega w - \frac{\Gamma}{2} v \\
\dot{w} &= -\Omega v - \Gamma (w - 1),
\end{align*}
\]

\[\Gamma = \frac{1}{\tau}\]  

\(^\Gamma\) represents the decay constant of the excited state, so I tested that it fulfilled this role in the OBE by numerically solving the OBE for a pi-pulse [1] (Fig. 18). To achieve a pi-pulse, I set the detuning and intensity so that

\[
\delta(t) = 0,
\]

\(^3\) This was the ultimate reason for the transition from the Rabi treatment to the Bloch equations (Eqs. 18 and 19).
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\[ I(t) = \begin{cases} \frac{1}{2} I_m, & t < \sqrt{\frac{\pi \hbar \omega_0^3 \gamma}{3 c^2 I_m}} = \frac{\pi}{\alpha(T_m)}, \\ 0, & \text{otherwise} \end{cases} \quad (25b) \]

Under the influence of a pi-pulse, the excited fractional population should reach nearly 1, and should then decay at a rate \( \Gamma \).

Figure 18: The graphical result of illuminating the system with a pi-pulse, according to the OBE.

I found from measuring several points in Fig. 18 that the population did indeed decay exponentially. Knowing that the Bloch equations could handle two levels without spontaneous emission, and additionally knowing that the OBE properly accounted for spontaneous emission, I proceeded to numerically solve the OBE with a beam described by Eqs. 14 and 16, with these parameters:

<table>
<thead>
<tr>
<th>( I_m )</th>
<th>100 W/cm²</th>
</tr>
</thead>
<tbody>
<tr>
<td>( m )</td>
<td>50 ns</td>
</tr>
</tbody>
</table>
The results are shown in Fig. 19.

![Numerical solution of the OBE. This was calculated for a time span of 300 ns, instead of the 100 ns used in previous numerical solutions.](image)

Having been introduced to the concept of a pi-pulse, one may question the need to bother employing a chirp, since in theory a pi-pulse should provide 100% excitation\(^4\) [5]. While the square pulse in Eq. 25b is physically impossible, it is possible to produce Gaussian intensity pulses which result in a pulse area (integral of $\Omega$ with respect to time) equal to $\pi$. This would suggest that one should use a pi-pulse and set $\omega_l$ to $\omega_a$ in order to achieve optimal excitation, with no chirp required. It turns out that chirped excitation is more robust than pi-pulse excitation -or phrased differently, chirped excitation is more forgiving to variations in intensity.

\(^4\) ignoring spontaneous emission in both cases
I compared the effect on the two excitation schemes of varying the peak intensity, still ignoring spontaneous emission. To accomplish this I ran simulations for a pi-pulse\(^5\) at zero detuning and for a linear chirp with a Gaussian pulse\(^6\) of the same peak intensity\(^7\). For each of the two schemes I ran an additional simulation with 0.81 of the peak intensity of the pi-pulse, and a third with 1.21 of the “pi” peak. Therefore for each scheme the peak Rabi frequency was that for a pi-pulse, or 10% less, or 10% more. Varying the peak intensity in this way simulates the variation of laser power in an experiment. This resulted in Figs. 20-22 for a pi-pulse or “near-pi-pulse” and Figs. 23-25 for a linear chirp.

Figure 20: The excited fraction (left) for a near-pi pulse at resonance (right) with a peak Rabi frequency of 10% less than that of a pi pulse and a FWHM of 1 ns. In both plots the horizontal axis is time from -1.25 ns to 1.25 ns. The left-hand vertical axis is dimensionless; the right-hand vertical axis is angular frequency in \(\text{Grad/s}\).

\(^5\) \((\text{FWHM, } I_m) = (1 \text{ ns, } 10 \text{ W/cm}^2)\)
\(^6\) \(\alpha = 2\pi \times 0.09 \text{ GHz/ns, } (\text{FWHM, } I_m) = (10 \text{ ns, } 10 \text{ W/cm}^2)\), which I will show later would be a set of optimal parameters for a linear chirp if not for spontaneous emission.
\(^7\) In principle, using a pulse of a different width with the chirp should be fine. A pi pulse was only used at resonance because my references indicated that it was specifically needed. My references had nothing to say about linear chirps, so I am obligated to test for an arbitrary pulse-except that the two pulses must have some common trait if I am to make a comparison. I chose the peak intensity to be that common trait because of its relation to the peak Rabi frequency.
Figure 21: The excited fraction (left) for a pi pulse at resonance (right) with a FWHM of 1 ns. This figure has the same time interval and units as Fig. 20, and one will notice that the final excited fractions in Figs. 20 and 22 are visibly less than that of this figure.

Figure 22: The excited fraction (left) for a near-pi pulse at resonance (right) with a peak Rabi frequency of 10\% more than that of a pi pulse. This figure has the same time interval and units as Figs. 20 and 21.
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Figure 23: The excited fraction (left) for a Gaussian pulse and a linear chirp (right) with a peak Rabi frequency of 10% less than that of a pi pulse and a FWHM of 10 ns. In both plots the horizontal axis is time from -12.5 ns to 12.5 ns. The left-hand vertical axis is dimensionless; the right-hand vertical axis is angular frequency in Grad/s.

Figure 24: The excited fraction (left) for a Gaussian pulse and a linear chirp (right) with the same peak Rabi frequency as the pi pulse from Fig. 21. This figure has the same time interval and units as Fig. 23. There is no visible difference between the left-hand plots of Figs. 23-25.

Figure 25: The excited fraction (left) for a Gaussian pulse and a linear chirp (right) with a peak Rabi frequency of 10% more than the pi pulse from Fig. 21. This figure has the same time interval and units as Figs. 23-24.

In Figs. 20-25, one can see that varying the peak intensity has a visible effect on the final excited fraction when using a “pi” pulse at resonance, but not when using a pulse of the same peak intensity and the appropriate linear chirp. This demonstrates that the (linear) chirp is more robust
than use of a pi pulse at resonance; one can afford a greater uncertainty in the power of the laser when employing a chirp.

Once I knew that my simulations could properly account for spontaneous emission, I divided my optimization for each chirp shape into one optimization ignoring spontaneous emission (by setting $\Gamma$ to zero) and another that accounted for spontaneous emission (setting $\Gamma$ to its real value, $\frac{1}{\tau}$). Comparing simulations that ignore spontaneous emission to simulations that do not shows (at least qualitatively) the influence of spontaneous emission on the behavior of a two-level atom.

Before running simulations for the various chirp shapes and for each of the two values of $\Gamma$, I employed a routine in order to reduce the numerical error in my simulations. I set the laser parameters for the most rapidly changing chirp and for the most intense, longest lasting pulse that I was willing to consider, and varied the maximum number of steps that Mathematica could use to produce each datum of its solution. This limit is referred to as “MaxSteps” in Mathematica and its default value for the NDSolve command is $10^4$. I first established the minimum number of steps necessary to ensure that the simulations were consistent with the axioms of probability\(^8\) by plotting simulations based on MaxSteps with successive powers of ten (starting from the default setting). I found the lowest value of MaxSteps which did not result in an impossible plot by comparing plots like those in Fig. 26.

\(^8\) i.e., that the excited fraction must always be non-negative and never greater than 1
Figure 26: Graphs of excitation with a linear chirp and no spontaneous emission for a chirp rate of \(1 \text{ GHz/ns}\), a FWHM of 100 ns, peak intensity of \(100 \text{ W/cm}^2\), and MaxSteps from \(10^4\) to \(10^7\). These plots show the entire time range over which the numerical solution was calculated, which in this case is from -625 ns to 625 ns. It is clear that \(10^7\) is the minimum MaxSteps setting to produce reasonable probabilities for a linear chirp with no spontaneous emission.

After ensuring convergence with this qualitative check, I needed to find the minimum setting of MaxSteps for which the simulations did not differ from each other. I accomplished this by varying MaxSteps as previously only starting at the new value, in case there was a visible difference in the plots. Often, there was not a visible difference, which made it necessary for me to calculate the excited population at the final point in time of the simulation, and compare how the calculated value varied with MaxSteps. This would result in a set of data like that shown in Table 2.
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Table 2: Final excited population with spontaneous emission for a chirp rate of 1 GHz/ns, a FWHM of 100 ns, peak intensity of 100 W/cm², for several settings of MaxSteps. In this case the final time is 625 ns. Evidently the minimum setting of max steps for a linear chirp and spontaneous emission is 10⁷. In this case it happens that my minimum MaxSteps setting is also the minimum setting determined from Fig. 26.

<table>
<thead>
<tr>
<th>MaxSteps</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
</tr>
</thead>
<tbody>
<tr>
<td>Final population</td>
<td>−6157.73</td>
<td>4.51816 × 10⁻¹¹</td>
<td>4.51816 × 10⁻¹¹</td>
<td>4.51816 × 10⁻¹¹</td>
</tr>
</tbody>
</table>

In this way I determined the minimum setting of MaxSteps for use in my simulations for each chirp shape and for each of the two values of Γ considered.

Next, for the simulations ignoring spontaneous emission I calculated the maximum excited fraction for each set of parameters, which I labeled maxpop. For each pair of intensities and pulse widths shown in Table 3, I optimized the chirp parameters by viewing maxpop as a function of them, and iteratively refined the set of chirp parameters for a given pulse parameter pair until I had found an interval in (chirp) parameter space in which the minimum value of the maximum excited fraction was no less than 90% of the greatest value of the maximum fraction for the peak intensity under consideration.

Table 3: The pulse parameters considered for chirp optimization. The pulse widths considered included τ, two widths on the order of τ, and two widths different from τ by an order of magnitude. The peak intensity Iₚ was varied by factors of 10.

<table>
<thead>
<tr>
<th>FWHM (ns)</th>
<th>1</th>
<th>10</th>
<th>26.2</th>
<th>40</th>
<th>100</th>
</tr>
</thead>
<tbody>
<tr>
<td>Iₚ (W/cm²)</td>
<td>0.01</td>
<td>0.1</td>
<td>1</td>
<td>10</td>
<td>100</td>
</tr>
</tbody>
</table>

These steps enabled me to find the optimal parameters for the largest excited fraction possible.

Because of its importance in applications, the value of the excited population became the primary goal in my optimizations. Therefore other goals such as minimizing the time at which the excited fraction reached its peak were deemed secondary goals.
Whenever possible without harming the primary goal of size, parameters were refined with the goal of minimizing this time of maximum excitation, which I labeled $t_{\text{max}}$. Rather than directly compare values of $t_{\text{max}}$ corresponding to different pulse widths, I defined the relative time of maximum excitation, $t_{\text{maxrel}}$:

$$t_{\text{maxrel}} = \frac{t_{\text{max}}}{FWHM} \quad (26)$$

This was necessary because in my simulations the width of each pulse determined the relevant timescale. Unlike the time of maximum excitation, $t_{\text{maxrel}}$ is intensive\(^9\), which is convenient for directly comparing the results of two different pulse widths, or even the same pulse width with differences in other parameters. When I optimized with regard for $t_{\text{maxrel}}$, I optimized parameters so that $t_{\text{maxrel}}$ was no greater than 6.

In the simulations neglecting spontaneous emission the goal of duration was moot, so no additional steps needed to be taken in order to optimize the laser parameters. According to my resources optimization of a hyperbolic-tangent chirp when ignoring spontaneous emission was unnecessary [5,8], so as an exception to this general process I compared how closely my numerical solution agreed with the analytical solution instead of optimizing parameters for a “tanh($t$)” chirp when $\Gamma = 0$.

In the simulations that accounted for spontaneous emission, my previously stated processes for optimizing size and speed required no modification. However, in these simulations it was additionally necessary to measure duration. Originally, I hoped to pick a threshold excitation level and simply find the time at which the excited fraction permanently ceased to be at or above this threshold. I later decided to integrate the excited fraction over time, in order both to have a measure that was less arbitrary (it doesn’t require picking a threshold) and that

\(^9\) and dimensionless
required no attention on my part to account for oscillations (which I would have needed to examine closely to discern when $\rho_{22}$ fell permanently below a threshold). The relevant region of integration would have started at $t_{\text{max}}$ and ended at the final time used in my simulations\(^{10}\). This would have meant measuring endurance with the quantity

$$\int_{t_{\text{max}}}^{25\text{FWHM}} \rho_{22} dt.$$  \hfill (27)

For technical reasons, this integration proved difficult to accomplish, and instead I defined the duration $d$ with a discrete sum:

\begin{align*}
\sum_{m=0}^{1000} \rho_{22}(t_{\text{max}} + m \ast \Delta t) \ast \Delta t, \hfill (28a) \\
\Delta t \equiv \frac{25\text{FWHM} - t_{\text{max}}}{1000}. \hfill (28b)
\end{align*}

This definition was chosen because the duration as calculated in Eqs. 28 approximates the quantity in Eq. 27. When it was possible to optimize duration at no cost with respect to both $\text{maxpop}$ and $t_{\text{maxrel}}$,\(^{11}\) the goal was simply to have the longest duration possible, and I was satisfied with whatever duration I could achieve within the bounds already established for size and speed.

\(^{10}\) which I had previously selected to always be $\frac{25}{4}$ of the FWHM under consideration

\(^{11}\) which was uncommon
Results

For a linear chirp neglecting spontaneous emission, it often proved to be the case that the highest possible excited population came at the cost of a greater delay (Fig. 27). In these situations and in those in which any correlation between \( maxpop, t_{\text{maxrel}}, \) and \( \alpha \) was unclear (Fig. 29), I found a range of chirp rates that were optimal\(^{12} \) for a given pair of pulse parameters\(^{13} \). For situations in which \( maxpop \) had a positive correlation with \( \alpha \) and \( t_{\text{maxrel}} \) had a negative correlation (or vice versa), there was in fact one chirp rate that was optimal (Fig. 28). It happens that this only occurred for (most of) the simulations that used a peak intensity of 100 \( \text{W/cm}^2 \).

Figure 27: \( maxpop \) (blue) and \( t_{\text{maxrel}} \) (red) versus \( \alpha \) for a linear chirp, \( \Gamma = 0, \ FWHM = 26.2 \text{ ns}, \ I_m = 0.01 \text{ W/cm}^2 \). Both horizontal axes are chirp rates in \( \text{Hz/s} \); both vertical axes are dimensionless because of the definitions of the quantities. This is an example of a trade-off between size and speed.

\(^{12} \)by my previously stated standards

\(^{13} \)Depending on the application of chirped excitation, one needs to weigh the importance of a high ceiling against a quick result, and may even need to define “optimal” differently than I did.
Figure 28: $maxpop$ and $t_{maxrel}$ versus $\alpha$ for a linear chirp, $\Gamma = 0$, $FWHM = 26.2$ ns, $I_m = 100 \, \text{W}/\text{cm}^2$. These plots use the same units and colors as Fig. 27. This is an example of a pulse parameter pair with one optimal chirp rate ($1 \, \text{GHz}/\text{ns}$).

Figure 29: $maxpop$ and $t_{maxrel}$ versus $\alpha$ for a linear chirp, $\Gamma = 0$, $FWHM = 40$ ns, $I_m = 1 \, \text{W}/\text{cm}^2$. These plots use the same units and colors as Figs. 27 and 28. This is an example of the frequent lack of a crystal-clear correlation between neither $maxpop$ and $\alpha$ nor $t_{maxrel}$ and $\alpha$.

The following tables list the optimal chirp rate ranges for each of the pulse widths from Table 3 and the resulting maxima and minima of $maxpop$ and $t_{maxrel}$, with each table dedicated to a unique peak intensity from Table 3. Each chirp rate is listed in “ordinary” frequency units, meaning that each of these rates multiplied by $2\pi$ yields the value of $\alpha$ as an angular frequency used in each simulation. Omitted pulse widths had no optimal chirp rates for the peak intensity under consideration.

Tables 4.1-4.5: The results for a linear chirp neglecting spontaneous emission.
Table 4.1: The results for a linear chirp, $I_m = 0.01 \text{ W/cm}^2$. The ceiling of $\text{maxpop}$ for this peak intensity was 100%, therefore the minimum acceptable value of $\text{maxpop}$ was 90%.

<table>
<thead>
<tr>
<th>FWHM (ns)</th>
<th>Minimum optimal Chirp (GHz/ns)</th>
<th>Maximum optimal Chirp (GHz/ns)</th>
<th>Maximum $\text{maxpop}$ (%)</th>
<th>Minimum $t_{\text{maxrel}}$</th>
<th>Maximum $t_{\text{maxrel}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>26.2</td>
<td>0</td>
<td>2.40E-04</td>
<td>92.9</td>
<td>1.8</td>
<td>4</td>
</tr>
<tr>
<td>40</td>
<td>0</td>
<td>5.90E-04</td>
<td>100</td>
<td>0.48</td>
<td>2.7</td>
</tr>
<tr>
<td>100</td>
<td>0</td>
<td>7.6</td>
<td>100</td>
<td>0.29</td>
<td>1.6</td>
</tr>
</tbody>
</table>

Table 4.2: The results for a linear chirp, $I_m = 0.1 \text{ W/cm}^2$. The ceiling of $\text{maxpop}$ for this peak intensity was 100%, therefore the minimum acceptable value of $\text{maxpop}$ was 90%.

<table>
<thead>
<tr>
<th>FWHM (ns)</th>
<th>Minimum optimal Chirp (GHz/ns)</th>
<th>Maximum optimal Chirp (GHz/ns)</th>
<th>Excitation Ceiling</th>
<th>Minimum $t_{\text{maxrel}}$</th>
<th>Maximum $t_{\text{maxrel}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0</td>
<td>5.10E-03</td>
<td>100</td>
<td>1.1</td>
<td>5.8</td>
</tr>
<tr>
<td>40</td>
<td>0</td>
<td>7.80E-03</td>
<td>100</td>
<td>-0.41</td>
<td>1.4</td>
</tr>
<tr>
<td>100</td>
<td>0</td>
<td>7.80E-04</td>
<td>100</td>
<td>-0.77</td>
<td>2.3</td>
</tr>
</tbody>
</table>

Table 4.3: The results for a linear chirp, $I_m = 1 \text{ W/cm}^2$. The ceiling of $\text{maxpop}$ for this peak intensity was 100%; therefore the minimum acceptable value of $\text{maxpop}$ was 90%.

<table>
<thead>
<tr>
<th>FWHM (ns)</th>
<th>Minimum optimal Chirp (GHz/ns)</th>
<th>Maximum optimal Chirp (GHz/ns)</th>
<th>Excitation Ceiling</th>
<th>Minimum $t_{\text{maxrel}}$</th>
<th>Maximum $t_{\text{maxrel}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0</td>
<td>0.0375</td>
<td>100</td>
<td>0.98</td>
<td>2.4</td>
</tr>
<tr>
<td>26.2</td>
<td>0.009375</td>
<td>0.046875</td>
<td>100</td>
<td>0.38</td>
<td>3.4</td>
</tr>
<tr>
<td>40</td>
<td>0</td>
<td>0.075</td>
<td>100</td>
<td>0.072</td>
<td>5.7</td>
</tr>
<tr>
<td>100</td>
<td>0</td>
<td>0.075</td>
<td>100</td>
<td>0.029</td>
<td>1.2</td>
</tr>
</tbody>
</table>

Table 4.4: The results for a linear chirp, $I_m = 10 \text{ W/cm}^2$. The ceiling of $\text{maxpop}$ for this peak intensity was 100%, therefore the minimum acceptable value of $\text{maxpop}$ was 90%.

<table>
<thead>
<tr>
<th>FWHM (ns)</th>
<th>Minimum optimal Chirp (GHz/ns)</th>
<th>Maximum optimal Chirp (GHz/ns)</th>
<th>Excitation Ceiling</th>
<th>Minimum $t_{\text{maxrel}}$</th>
<th>Maximum $t_{\text{maxrel}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0.49</td>
<td>100</td>
<td>1.1</td>
<td>5.9</td>
</tr>
<tr>
<td>10</td>
<td>0.0125</td>
<td>0.48</td>
<td>100</td>
<td>0.11</td>
<td>3.1</td>
</tr>
<tr>
<td>26.2</td>
<td>0.0125</td>
<td>0.46</td>
<td>100</td>
<td>0.35</td>
<td>5.9</td>
</tr>
<tr>
<td>40</td>
<td>0.0016</td>
<td>0.46</td>
<td>100</td>
<td>1.2</td>
<td>2.4</td>
</tr>
<tr>
<td>100</td>
<td>0.0031</td>
<td>0.48</td>
<td>100</td>
<td>1.7</td>
<td>5.3</td>
</tr>
</tbody>
</table>

Table 4.5: The results for a linear chirp, $I_m = 100 \text{ W/cm}^2$. The ceiling of $\text{maxpop}$ for this peak intensity was 100%, therefore the minimum acceptable value of $\text{maxpop}$ was 90%.
When accounting for spontaneous emission with a linear chirp, it was often the case again that optimizing two of the three goal quantities $maxpop$, $t_{maxrel}$, and $d$ came at the expense of the third, or the correlations were not obvious (Fig. 30). The situations with one optimal chirp rate were like those in Figs. 31 and 32, in which $maxpop$ and $d$ both had the same correlation to $\alpha$ (either both positive or both negative), and $t_{maxrel}$ had the opposite correlation.
Figure 30: \( \text{maxpop} \) (blue), \( t_{\text{maxrel}} \) (red), and \( d \) (green) versus \( \alpha \) for a linear chirp, \( \Gamma = \frac{1}{T'} \), \( \text{FWHM} = 10 \text{ ns} \), \( I_m = 10 \text{ W/cm}^2 \). All horizontal axes are chirp rates in \( \text{Hz/s} \); the first vertical axis is probability, the second is dimensionless, and the third is time in seconds. This is an example of complex relations between the three quantities.
Figure 31: $maxpop$, $t_{maxrel}$, and $d$ versus $\alpha$ for a linear chirp, $\Gamma = \frac{1}{t}$, $FWHM = 40$ ns, $I_m = 0.01$ $W/cm^2$. All three of these plots have the same units as those of Fig. 30. In this case there is only one optimal chirp rate (zero).
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Figure 32: maxpop, $t_{\text{maxrel}}$, and $d$ versus $\alpha$ for a linear chirp, $\Gamma = \frac{1}{\tau}$, FWHM = 10 ns, $I_m = 100$ W/cm$^2$. All three of these plots have the same units as those of Fig. 30. In this case there is only one optimal chirp rate ($1$ GHz/\text{ns}).

On occasion it was not only the case that there was not one optimal chirp rate for a given pulse parameter pair, but there was more than one interval of optimal chirp rates. This was not uncommon because usually maxpop, $t_{\text{maxrel}}$, and $d$ were not monotonic with respect to the chirp rate. In many of the non-monotonic situations for which there was only one optimal interval, there was only one hill in a target quantity that stood above my threshold for that quantity, such as the hill for maxpop in Fig. 29. On other occasions, there was more than one hill, and each hill...
corresponded to another interval. Some of these intervals were very short compared to my absolute maximum chirp rate for analysis, but the plots I observed of \textit{maxpop} suggested that they could not be ignored.

In my simulations only the behavior of \textit{maxpop} determined when there occurred more than one optimal interval of chirp rates. I believe that this is because I set a relatively stringent standard for my results as concerned \textit{maxpop}, and my standards as to \( t_{\text{maxrel}} \) and \( d \) were relatively loose-I did not even have standards regarding \( d \). I suspect this because the red and green lines in Figs. 30-33 have hills and valleys as often and in the same manner as all of the blue lines. The only differences in principle between the three quantities were the thresholds that I set for each of them.
Figure 33: \( \text{maxpop}, t_{\text{maxrel}}, \) and \( d \) versus \( \alpha \) for a linear chirp, \( \Gamma = \frac{1}{\tau}, FWHM = 26.2 \) ns, \( I_m = 10 \) \( W/cm^2 \). All three of these plots have the same units as those of Fig. 30. This is an example (as was Fig. 30) of a situation in which there are multiple, separate intervals of optimal chirp rates. The endpoints of these intervals are the points of intersection of the excitation threshold \( I \) set (87.7\% in this case) with the graph of \( \text{maxpop} \).

The following tables give my results for a linear chirp when including spontaneous emission. In addition to the extrema for \( \text{maxpop} \) and \( t_{\text{maxrel}} \), these results include extrema for \( d \).

Table 5.1-5.5: The results for a linear chirp (accounting for spontaneous emission).

Table 5.1: The results for a linear chirp, \( I_m = 0.01 \) \( W/cm^2 \). The ceiling of \( \text{maxpop} \) for this peak intensity was 50.6\%, therefore the minimum acceptable value of \( \text{maxpop} \) was 45.5\%.
Table 5.2: The results for a linear chirp, $I_m = 0.1 \ W/\ cm^2$. The ceiling of $maxpop$ for this peak intensity was 78.6%, therefore the minimum acceptable value of $maxpop$ was 70.7%.

<table>
<thead>
<tr>
<th>FWHM (ns)</th>
<th>Minimum optimal Chirp (GHz/ns)</th>
<th>Maximum optimal Chirp (GHz/ns)</th>
<th>Excitation Ceiling</th>
<th>Minimum t_maxrel</th>
<th>Maximum t_maxrel</th>
<th>Minimum d (ns)</th>
<th>Maximum d (ns)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0</td>
<td>0</td>
<td>74.7</td>
<td>0.71</td>
<td>0.71</td>
<td>19</td>
<td>19</td>
</tr>
<tr>
<td>26.2</td>
<td>0</td>
<td>0.00045</td>
<td>78.6</td>
<td>0.95</td>
<td>0.99</td>
<td>12</td>
<td>13</td>
</tr>
<tr>
<td>26.2</td>
<td>0.0024</td>
<td>0.0077</td>
<td>77.0</td>
<td>0.32</td>
<td>0.44</td>
<td>16</td>
<td>21</td>
</tr>
</tbody>
</table>

Table 5.3: The results for a linear chirp, $I_m = 1 \ W/\ cm^2$. The ceiling of $maxpop$ for this peak intensity was 91.7%, therefore the minimum acceptable value of $maxpop$ was 82.5%.

<table>
<thead>
<tr>
<th>FWHM (ns)</th>
<th>Minimum optimal Chirp (GHz/ns)</th>
<th>Maximum optimal Chirp (GHz/ns)</th>
<th>Excitation Ceiling</th>
<th>Minimum t_maxrel</th>
<th>Maximum t_maxrel</th>
<th>Minimum d (ns)</th>
<th>Maximum d (ns)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0.020</td>
<td>0.081</td>
<td>91.7</td>
<td>0.27</td>
<td>0.63</td>
<td>16</td>
<td>21</td>
</tr>
<tr>
<td>26.2</td>
<td>0.0742042</td>
<td>0.080</td>
<td>85.2</td>
<td>0.10</td>
<td>0.11</td>
<td>18.1</td>
<td>18.6</td>
</tr>
</tbody>
</table>

Table 5.4: The results for a linear chirp, $I_m = 10 \ W/\ cm^2$. The ceiling of $maxpop$ for this peak intensity was 97.4%, therefore the minimum acceptable value of $maxpop$ was 87.7%.

<table>
<thead>
<tr>
<th>FWHM (ns)</th>
<th>Minimum optimal Chirp (GHz/ns)</th>
<th>Maximum optimal Chirp (GHz/ns)</th>
<th>Excitation Ceiling</th>
<th>Minimum t_maxrel</th>
<th>Maximum t_maxrel</th>
<th>Minimum d (ns)</th>
<th>Maximum d (ns)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0.53</td>
<td>96.2</td>
<td>1.0</td>
<td>1.2</td>
<td>4.1</td>
<td>4.6</td>
</tr>
<tr>
<td>10</td>
<td>0.15</td>
<td>0.33</td>
<td>92.6</td>
<td>0.26</td>
<td>0.35</td>
<td>21.1</td>
<td>21.5</td>
</tr>
<tr>
<td>10</td>
<td>0.36</td>
<td>0.44</td>
<td>96.7</td>
<td>0.11</td>
<td>0.33</td>
<td>20</td>
<td>22</td>
</tr>
<tr>
<td>10</td>
<td>0.51</td>
<td>0.525</td>
<td>96.6</td>
<td>0.104</td>
<td>0.105</td>
<td>20.2</td>
<td>20.4</td>
</tr>
<tr>
<td>10</td>
<td>0.544</td>
<td>0.548</td>
<td>95.5</td>
<td>0.1025</td>
<td>0.1028</td>
<td>19.95</td>
<td>20</td>
</tr>
<tr>
<td>10</td>
<td>0.5929</td>
<td>0.61</td>
<td>94.7</td>
<td>0.098</td>
<td>0.099</td>
<td>19.2</td>
<td>19.4</td>
</tr>
<tr>
<td>26.2</td>
<td>0.1625</td>
<td>0.28</td>
<td>93.3</td>
<td>0.11</td>
<td>0.18</td>
<td>23</td>
<td>24</td>
</tr>
<tr>
<td>26.2</td>
<td>0.3</td>
<td>0.4</td>
<td>97.3</td>
<td>0.037</td>
<td>0.10</td>
<td>23.6</td>
<td>24.7</td>
</tr>
<tr>
<td>26.2</td>
<td>0.41</td>
<td>0.4118</td>
<td>97.4</td>
<td>0.042</td>
<td>0.043</td>
<td>23.7</td>
<td>23.8</td>
</tr>
<tr>
<td>26.2</td>
<td>0.421</td>
<td>0.429</td>
<td>97.4</td>
<td>0.039</td>
<td>0.043</td>
<td>23.5</td>
<td>23.7</td>
</tr>
<tr>
<td>40</td>
<td>0.16875</td>
<td>0.2875</td>
<td>92.5</td>
<td>0.033</td>
<td>0.11</td>
<td>23</td>
<td>25</td>
</tr>
<tr>
<td>40</td>
<td>0.3007</td>
<td>0.33</td>
<td>92.8</td>
<td>0.031</td>
<td>0.032</td>
<td>24.6</td>
<td>24.9</td>
</tr>
<tr>
<td>40</td>
<td>0.368</td>
<td>0.387</td>
<td>96.9</td>
<td>0.0292</td>
<td>0.0298</td>
<td>24.1</td>
<td>24.3</td>
</tr>
</tbody>
</table>
Numerical Simulations of Chirped Excitation
Ben Iannitelli

<table>
<thead>
<tr>
<th>FWHM (ns)</th>
<th>Minimum optimal Chirp (GHz/ns)</th>
<th>Maximum optimal Chirp (GHz/ns)</th>
<th>Excitation Ceiling</th>
<th>Minimum t_maxrel</th>
<th>Maximum t_maxrel</th>
<th>Minimum d (ns)</th>
<th>Maximum d (ns)</th>
</tr>
</thead>
<tbody>
<tr>
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<td>0.077</td>
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<tr>
<td>100</td>
<td>0.625</td>
<td>1</td>
<td>89.9</td>
<td>0.022</td>
<td>0.031</td>
<td>24.6</td>
<td>25.0</td>
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</tbody>
</table>

Table 5.5: The results for a linear chirp, \( I_m = 100 \text{ W/cm}^2 \). The ceiling of max pop for this peak intensity was 97.0%, therefore the minimum acceptable value of max pop was 87.3%.

For a hyperbolic-tangent-chirp

\[ \omega_t = \delta_m \tanh \left( \frac{t}{\tau_f} \right) + \omega_a, \] (29)

with a hyperbolic-secant Rabi pulse

\[ \Omega = \Omega_m \text{ sech} \left( \frac{t}{\tau_f} \right), \] (30)

there is an analytical solution to the Bloch equations so long as one neglects spontaneous emission [5, 8]. In terms of the excited fraction, this analytical solution is [5]

\[ \rho_{22} = \frac{1}{2} \tanh \left( \frac{t}{\tau_f} \right) + \frac{1}{2}. \] (31)
Figure 34: The detuning and Rabi pulse described by Eqs. 29-30, with a frequency sweep of 600 MHz, $\tau_l$ set to $\tau$, and a peak intensity of $10^6 W/cm^2$.

Figure 35: The excited fraction described by Eq. 31, predicted to correspond to the chirp and Rabi pulse described by Eqs. 29-30, simulated with the same laser parameters as in Fig. 34.

As another test of the validity of my simulations, I compared the solution in Eq. 31 to that produced by my numerical solution to the Bloch equations, with $\tau_l$ set to $\tau$. My resources specifically discussed leaving the arguments of the hyperbolic trigonometric functions as shown in Eqs. 29 and 30, and qualified their assertions by only supposing $\delta_m$, half of the frequency range that one wishes the chirp to span, and $\Omega_m$, the peak Rabi frequency, to be arbitrary\(^{14}\). It is also worth noting that this prediction does not show any dependence upon specific values of $\delta_m$ or $\Omega_m$. In principle these conditions required fixing the FWHM of the intensity pulse at 46.2 ns, and left me free to vary the remaining two parameters when comparing my simulations.

For a thorough comparison I varied $\delta_m$ from 0 to $2\pi*1$ GHz by increments of $2\pi*50$ MHz, and $I_m$ by the powers of ten prescribed in Table 3. For each setting of the parameters I calculated the time average of the difference between the excited fraction predicted by the analytical solution and that predicted by my numerical solution over the entire time window used in each simulation. This average prediction difference ranged from 0.3% to as high as 47.2% depending on the specific parameters, and averaged to 11.4%.

\(^{14}\) as opposed to letting all of the laser parameters be arbitrary, say by replacing $\tau_l$ with an arbitrary parameter $T_{\delta}$ in Eq. 29 and with a separate parameter $T_{\Omega}$ in Eq. 30.
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At first glance, one might guess that the disagreement stems from finite errors in the numerical solution. Actually, the reason is that the analytical solution offered by my resources assumes that the intensity of the laser changes slowly enough that the Bloch vector precesses about the generalized Rabi vector [5]. This approximation is referred to as “adiabatic following,” and does not hold for frequency sweeps near (or equal to) zero. This compelled me to conduct another test to see how well my simulations agreed with theory, specifically for small frequency sweeps. A frequency sweep of zero allowed me to derive a single, uncoupled second-order equation for $w(t)$ from the Bloch equations (Eqs. 18). I then graphed the numerical solution to this equation for all five peak intensities, and found perfect agreement with my simulations for a hyperbolic-tangent chirp and the Bloch equations in their typical coupled form. Apparently my numerical solutions obeyed the Bloch equations more often than the analytical solution presented in Eqs. 29-31. Rather than a sign of some flaw in my simulations, the average difference of 11.4% between my numerical solutions and the provided analytical solution is a validation of the “adiabatic following” approximation.

For my simulations of a hyperbolic-tangent chirp with spontaneous emission, I faced the option either to vary all of the chirp parameters, or to follow the precedent implied by the analytical solution provided to me and only vary the frequency sweep. I was faced with this decision because for full generality, rather than a laser described by Eqs. 29-30, one should consider a laser of the form

$$\omega_t = \delta_m \tanh \left( \frac{t}{T_\delta} \right) + \omega_a, \quad (32)$$

$$\Omega = \Omega_m \sech \left( \frac{t}{T_\Omega} \right), \quad (33)$$

I chose to fix $T_\delta$ at $r$ and to only vary the chirp amplitude, because I encountered challenges adapting the tools that I had already employed for a linear chirp (which has only one parameter)
to a chirp with two parameters. Having chosen this course, I varied $\delta_m$ from zero to $2\pi \times 500$ MHz, which is equivalent to varying the frequency sweep from zero to 1 GHz. As for the pulse parameters, I found the formula for the parameter $T_\Omega$ as a function of the FWHM of the intensity pulse:

$$T_\Omega = \frac{FWHM}{2 \text{ sech}^{-1}\left(\frac{\sqrt{2}}{2}\right)} \quad (34)$$

Armed with Eq. 34, I was free to vary the pulse parameters in the same manner as for the previous numerical solutions, albeit with a different pulse shape.

Not unlike simulations with the linear chirp, there were pulse parameter sets that had multiple optimal chirp parameter intervals\(^{15}\) and others that had a single optimal chirp. Optimal intervals had all sorts of lengths\(^{16}\) and occurred for the hyperbolic-tangent chirp simulations for the same reasons as for the linear-chirp simulations, though for this new chirp shape there were generally fewer. These results are presented in Tables 6.1-6.5 in the same manner as for the linear chirp.

Table 6.1: The results for a hyperbolic-tangent chirp including spontaneous emission.

<table>
<thead>
<tr>
<th>FWHM (ns)</th>
<th>Minimum optimal sweep (GHz)</th>
<th>Maximum optimal sweep(GHz)</th>
<th>Excitation Ceiling</th>
<th>Minimum $t_{\text{max rel}}$</th>
<th>Maximum $t_{\text{max rel}}$</th>
<th>Minimum $d$ (ns)</th>
<th>Maximum $d$ (ns)</th>
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</thead>
<tbody>
<tr>
<td>40</td>
<td>0</td>
<td>0</td>
<td>51.3</td>
<td>0.33</td>
<td>0.33</td>
<td>24</td>
<td>24</td>
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<tr>
<td>100</td>
<td>0</td>
<td>0.0035</td>
<td>47.1</td>
<td>-0.13</td>
<td>-0.088</td>
<td>53</td>
<td>57</td>
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<tr>
<td>100</td>
<td>0.011</td>
<td>0.0345</td>
<td>49.2</td>
<td>0.26</td>
<td>0.30</td>
<td>14</td>
<td>29</td>
</tr>
<tr>
<td>100</td>
<td>0.0394</td>
<td>0.041</td>
<td>47.0</td>
<td>0.24</td>
<td>0.25</td>
<td>12.7</td>
<td>13.0</td>
</tr>
</tbody>
</table>

\(^{15}\) This time they were intervals of frequency sweeps instead of chirp rates.

\(^{16}\) including length zero (single optimal chirp parameter values)
Table 6.2: The results for a hyperbolic-tangent chirp, $I_m = 0.1 \text{ W/cm}^2$. The ceiling of $maxpop$ for this peak intensity was 78.6%, therefore the minimum acceptable value of $maxpop$ was 70.7%.

<table>
<thead>
<tr>
<th>FWHM (ns)</th>
<th>Minimum optimal sweep (GHz)</th>
<th>Maximum optimal sweep (GHz)</th>
<th>Excitation Ceiling</th>
<th>Minimum $t_{\text{maxrel}}$</th>
<th>Maximum $t_{\text{maxrel}}$</th>
<th>Minimum $d$ (ns)</th>
<th>Maximum $d$ (ns)</th>
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<tbody>
<tr>
<td>10</td>
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<td>0.175</td>
<td>77.1</td>
<td>0.62</td>
<td>0.85</td>
<td>17</td>
<td>20</td>
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<tr>
<td>26.2</td>
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<td>0.4</td>
<td>76.9</td>
<td>0.32</td>
<td>0.44</td>
<td>16</td>
<td>21</td>
</tr>
<tr>
<td>40</td>
<td>0.1125</td>
<td>0.4</td>
<td>77.9</td>
<td>0.21</td>
<td>0.31</td>
<td>16</td>
<td>21</td>
</tr>
<tr>
<td>100</td>
<td>0.10625</td>
<td>0.44375</td>
<td>78.6</td>
<td>0.08</td>
<td>0.13</td>
<td>15</td>
<td>25</td>
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Table 6.3: The results for a hyperbolic-tangent chirp, $I_m = 1 \text{ W/cm}^2$. The ceiling of $maxpop$ for this peak intensity was 81.5%, therefore the minimum acceptable value of $maxpop$ was 73.4%.

<table>
<thead>
<tr>
<th>FWHM (ns)</th>
<th>Minimum optimal sweep (GHz)</th>
<th>Maximum optimal sweep (GHz)</th>
<th>Excitation Ceiling</th>
<th>Minimum $t_{\text{maxrel}}$</th>
<th>Maximum $t_{\text{maxrel}}$</th>
<th>Minimum $d$ (ns)</th>
<th>Maximum $d$ (ns)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0</td>
<td>0.0625</td>
<td>76.9</td>
<td>0.68</td>
<td>0.74</td>
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<td>17</td>
</tr>
<tr>
<td>10</td>
<td>0.2</td>
<td>1</td>
<td>81.5</td>
<td>0.65</td>
<td>1.1</td>
<td>18</td>
<td>20</td>
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<tr>
<td>26.2</td>
<td>0.6</td>
<td>1</td>
<td>80.9</td>
<td>0.19</td>
<td>0.30</td>
<td>22.7</td>
<td>24.0</td>
</tr>
<tr>
<td>40</td>
<td>0.65</td>
<td>1</td>
<td>80.8</td>
<td>0.12</td>
<td>0.16</td>
<td>24.0</td>
<td>24.4</td>
</tr>
<tr>
<td>100</td>
<td>0.675</td>
<td>1</td>
<td>80.8</td>
<td>0.05</td>
<td>0.06</td>
<td>25.0</td>
<td>25.5</td>
</tr>
</tbody>
</table>

Table 6.4: The results for a hyperbolic-tangent chirp, $I_m = 10 \text{ W/cm}^2$. The ceiling of $maxpop$ for this peak intensity was 97.3%, therefore the minimum acceptable value of $maxpop$ was 87.6%.

<table>
<thead>
<tr>
<th>FWHM (ns)</th>
<th>Minimum optimal sweep (GHz)</th>
<th>Maximum optimal sweep (GHz)</th>
<th>Excitation Ceiling</th>
<th>Minimum $t_{\text{maxrel}}$</th>
<th>Maximum $t_{\text{maxrel}}$</th>
<th>Minimum $d$ (ns)</th>
<th>Maximum $d$ (ns)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>97.3</td>
<td>0.76</td>
<td>0.76</td>
<td>4.574</td>
<td>4.574</td>
</tr>
</tbody>
</table>

Table 6.5: The results for a hyperbolic-tangent chirp, $I_m = 100 \text{ W/cm}^2$. The ceiling of $maxpop$ for this peak intensity was 97.1%, therefore the minimum acceptable value of $maxpop$ was 87.4%.

<table>
<thead>
<tr>
<th>FWHM (ns)</th>
<th>Minimum optimal sweep (GHz)</th>
<th>Maximum optimal sweep (GHz)</th>
<th>Excitation Ceiling</th>
<th>Minimum $t_{\text{maxrel}}$</th>
<th>Maximum $t_{\text{maxrel}}$</th>
<th>Minimum $d$ (ns)</th>
<th>Maximum $d$ (ns)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>97.1</td>
<td>0.645</td>
<td>0.645</td>
<td>1.59</td>
<td>1.59</td>
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</tbody>
</table>
Conclusion

For all of the simulations in which the decay constant was its proper value (regardless of the chirp shape), whenever there was one single optimal value of the chirp parameter that value was zero. Put more plainly, whenever there was a single optimal chirp that optimal chirp was no chirp at all, with $\omega_f$ locked at $\omega_a$.

I tabulated the lengths of the optimal chirp parameter intervals from the data presented in Tables 4-6, found the mean of the lengths in each case featured in Tables 4-6, and divided this mean by the maximum chirp parameter value originally under consideration. Table 7 compares this quantity, the average relative optimal interval length, for the different simulations.

Table 7: Average relative optimal interval length for a linear chirp and both values of $\Gamma$ and for a hyperbolic-tangent chirp and $\Gamma = \frac{1}{\tau}$.

<table>
<thead>
<tr>
<th>Case</th>
<th>Average Relative Optimal Interval Length</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linear chirp, $\Gamma = 0$</td>
<td>0.56</td>
</tr>
<tr>
<td>Linear chirp, $\Gamma = \frac{1}{\tau}$</td>
<td>0.16</td>
</tr>
<tr>
<td>Hyperbolic-tangent chirp, $\Gamma = \frac{1}{\tau}$</td>
<td>0.20</td>
</tr>
</tbody>
</table>

Table 7 shows that on average, for each pair of pulse parameters which had an interval of optimal chirp parameter values, that interval was about one-third as long as what one would expect based on the pie-in-the-sky simulations that ignored spontaneous emission. While examples exist of two-state phenomena for which spontaneous emission is negligible, evidently for the transition of $^{87}\text{Rb}$ from $5^2S_{1/2}$ to $5^2P_{3/2}$ the effect of spontaneous emission cannot be ignored [1]. Otherwise, one is very likely to mistakenly use a chirp rate or frequency sweep that

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17I viewed cases in which there was only a single optimal chirp parameter value to have optimal intervals of length zero, and thus they contributed to this mean.

181 GHz/ns for $\alpha$, and 1 GHz for $\delta_m$. 
does not excite at least 90% of all the atoms that one could hope to excite, and in all likelihood
one is seriously mistaken as to what that limit even happens to be.

The ceilings of excitation for a linear chirp and the general nature of the results also
testify to the importance of spontaneous emission to the behavior of $^{87}$Rb. Ignoring spontaneous
emission, my simulations predicted twenty opportunities for excitation higher than 92%,
somewhat evenly distributed amongst the different values of $I_m$ that I used. Acknowledging
spontaneous emission there are instead seventeen, and none of them involve a peak intensity of
0.01 or 0.1 $\text{W/cm}^2$. By the standards that I established for an optimal excitation, the simulations
with spontaneous emission show dramatically more opportunities for optimal excitement at a
peak intensity of 10 $\text{W/cm}^2$ (17, versus 5 for the next most fruitful peak intensity, which was
100 $\text{W/cm}^2$).

For the hyperbolic-tangent chirp, which I only optimized while including spontaneous
emission, I generally found less pulse parameter pairs that had an interval of optimal chirp
parameter values than I had with the linear chirp and spontaneous emission. The hyperbolic-
tangent chirp also behaved somewhat oppositely with respect to peak intensity; it is more even,
and only offers one opportunity each for 10 and 100 $\text{W/cm}^2$. It happens to slightly favor
$I_m = 1 \text{W/cm}^2$ with a total of 5 chirp parameter intervals for 4 pulse parameter pairs, compared
to 4 chirp intervals for each of the remaining peak intensities.

By the standards that I established earlier for all three of the target quantities $\text{maxpop}$,
$t_{\text{maxrel}}$, and $d$, a linear chirp is superior in every way to a hyperbolic-tangent chirp, albeit not by
much. On average, the optimal chirps for a linear chirp bring the atoms to their maximum
excitation at $t_{\text{maxrel}}$ of 0.25, and result in a duration of 20.7 ns. For the hyperbolic-tangent chirp,
these averages were 0.38 and 20.1 ns, respectively. The absolute best ceiling was 97.4% for the linear chirp, and 97.3% for the hyperbolic-tangent chirp. Specifically, the best excitation that I have found uses a linear chirp that has a chirp rate between 0.2 and 0.65 GHz/\text{ns} and with a Gaussian intensity pulse that has a FWHM of 100 ns and a peak intensity of 10 W/\text{cm}^2.

References


