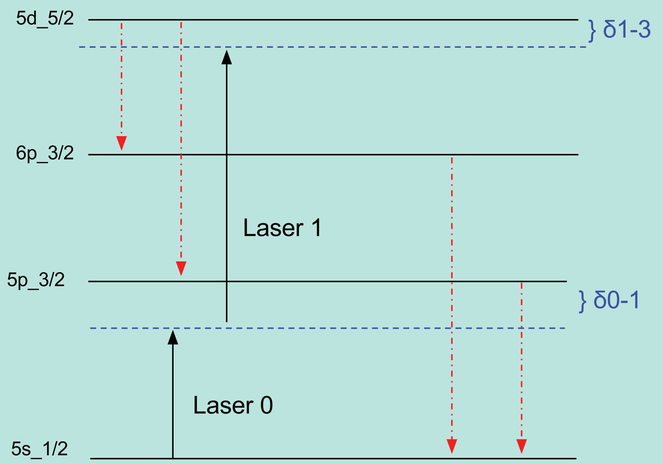
COMPUTATIONAL LIGHT-MATTER INTERACTIONS

Daniel C. Keylon, Department of Physics, Kansas State University: Home University: Union University
Mentor: Dr. Brett Depaola, Professor, Ph.D. Physics

Introduction [3]

In AMO physics, a frequent field of study is laser-matter interactions. Lasers are used to probe the energy structure of atoms to determine the relative electron populations. However, experiments can be time consuming to set up with parameters that are difficult to vary during runtime. The goal of this project is to build a software package to solve theoretical equations that predict population evolution. This software will be used to quickly test different experimental setups and locate parameters that produce interesting results. The initial version of this program will focus on solving the population evolutions for Rubidium and its isotopes.



The graph above represents a 4-level energy scheme for a Rb-87 atom.

Each solid black line represents an energy level. The blue dotted lines represent the detuning of the laser from resonance. The δ's represent this detuning in units of Hz. The solid vertical arrows represent the lasers and demonstrate which levels will undergo stimulated absorption and stimulated emission. The red dotted lines represent possible energy transitions due to spontaneous emission.

Development of the Hamiltonian [1]

$$-\hbar\dot{c}_1 = -i[(E_l^0 - \hbar\dot{\xi}_l)c_l + \sum_n c_n V_{ln} e^{-i(\xi_n - \xi_l)}]$$

The equation above is used to build the Hamiltonian that helps determine the rates of population change. The l subscript on the c-dot is an iterative variable that ranges from the first energy level of the atomic system to the last level. The n subscript on the summation also ranges from the first energy level to the last.

An equivalent form to the summation notation above is the matrix formulation. This formulation becomes more useful the larger our system grows as we'll see later.

$$\hbar\dot{c} = -i\begin{pmatrix} E_1^0 + V_{11} - \hbar\dot{\xi}_1 & V_{12}e^{-i(\xi_2-\xi_1)} \\ V_{12}^* e^{i(\xi_2-\xi_1)} & E_2^0 + V_{22} - \hbar\dot{\xi}_2 \end{pmatrix} c$$

Development of the Hamiltonian [cont.]

$$\hbar\dot{c} = -i\begin{pmatrix} E_1 - \hbar\dot{\xi}_1 & \frac{\hbar\Omega}{2}\left(e^{-i(\xi_2-\xi_1-\omega t)} + e^{-i(\xi_2-\xi_1+\omega t)}\right) \\ \frac{\hbar\Omega^*}{2}\left(e^{i(\xi_2-\xi_1-\omega t)} + e^{i(\xi_2-\xi_1+\omega t)}\right) & E_2 - \hbar\dot{\xi}_2 \end{pmatrix} c$$

Applying the dipole approximation, we find that we can replace the V12 term with the more easily dealt with exponential form shown above.

$$\hbar\dot{c} = -i\begin{pmatrix} 2\hbar\Delta_1 & \hbar\Omega \\ \hbar\Omega^* & 2\hbar\Delta_2 \end{pmatrix} c \qquad \hbar\dot{c} = \frac{-i}{2}\begin{pmatrix} 0 & \Omega \\ \Omega^* & 2\Delta_2 \end{pmatrix} c$$

With yet more approximations, we get the form on the left. By setting the energy of our ground state equal to zero, which we can do by simply scaling the rest of our energies, we arrive at the form to the right.

$$H = \frac{\hbar}{2}\begin{pmatrix} 0 & \Omega \\ \Omega^* & 2\Delta \end{pmatrix}$$

With a slight change of scalars, we see that what we have actually determined is our Hamiltonian.

Formulation of the Density Matrix [1]

$$\rho = \begin{pmatrix} \rho 00 & \rho 01 & \rho 02 & \rho 03 \\ \rho 10 & \rho 11 & \rho 12 & \rho 13 \\ \rho 20 & \rho 21 & \rho 22 & \rho 23 \\ \rho 30 & \rho 31 & \rho 32 & \rho 33 \end{pmatrix}$$

The matrix above is known as the density matrix. The diagonal values are the populations of each level. For example, ρ00 is the electron population of the ground state. The off-diagonal values are related to the decay rates for each transition. Generating the numerical values for this matrix is the central goal of this project.

$$i\hbar\dot{\rho} = H\rho - \rho H = [H, \rho]$$

To create the density matrix, we first build equations for the rate of population change. The equation above is true only for theoretical systems without spontaneous emission. This form also lets us define the central commutator.

$$i\hbar\dot{\rho}_{ij} = [H, \rho]_{ij} - i\hbar[\Gamma\rho]_{ij}$$

This form includes spontaneous emission though use of the gamma-rho term. This is the form that was used to build the rho-dot equations in our code.

$$[\Gamma\rho]_{ij} \equiv \rho_{ij}\sum_k \frac{1}{2}(\gamma_{ik} + \gamma_{jk}) - \delta_{ij}\sum_k \rho \quad \gamma ki$$

This is the equation that builds the gamma-rho matrix. Note that the delta in the equation is the Kronecker delta and is equal to zero unless i = j. Another point to note is that each gamma term is equal to zero in the case that the first subscript is less than or equal to the second subscript.

Wigner Relationships and Decay Rates [2]

$$\langle \alpha' l' j' m_j' | x_q | \alpha l j m_j \rangle = (-1)^{j'-m_{j'}} \begin{pmatrix} j' & 1 & j \\ -m_{j'} & q & m_j \end{pmatrix} \langle \alpha' l' j' || x || \alpha l j \rangle$$

$$\langle \alpha' l' j' I F' m_F' | x_q | \alpha l j I F m_F \rangle = (-1)^{F'-m_{F'}} \begin{pmatrix} F' & 1 & F \\ -m_{F'} & q & m_F \end{pmatrix} \langle \alpha' l' I F' || x || \alpha l I F \rangle$$

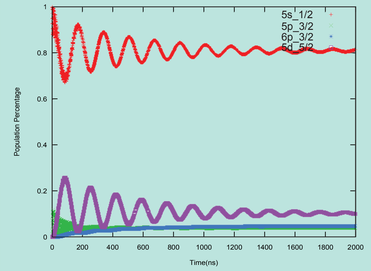
The equations above give the probability that an electron will make certain energy transitions.

The term that resembles a matrix is called a Wigner 3J symbol and stands for a much more complex calculation.

The right-most term of the expression is known as the reduced matrix element. Physically, when squared, it is proportional to the probability of an electron transition from one energy level to another. We read in this value from a pre-built database of values.

Also note that alpha here stands for any quantum numbers that are non-important for calculations. q is the polarization of the laser enabling the transition. The 1 specifies that this is a dipole transition.The rest of the values are standard quantum numbers.

Selected Evolution Graphs

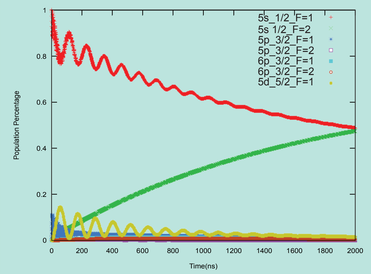


The graph to the left was created with the following parameters:

Energy Levels: $5s\frac{1}{2}$, $5p\frac{3}{2}$, $6p\frac{3}{2}$, $5d\frac{5}{2}$
No Hyper-Fine splitting
2 Laser Transitions

The first:
$5s\frac{1}{2}$ to $5p\frac{3}{2}$
q = 0 (The laser is linearly polarized)
Detuning = 1 GHz
Intensity = 1000 $\frac{mW}{cm^2}$

The second:
$5p\frac{3}{2}$ to $5d\frac{5}{2}$
q = 0 (The laser is linearly polarized)
Detuning = 0 GHz
Intensity = 1000 $\frac{mW}{cm^2}$



The graph to the left was created with the following parameters:

Energy Levels: $5s\frac{1}{2}$, $5p\frac{3}{2}$, $6p\frac{3}{2}$, $5d\frac{5}{2}$
All Hyper-Fine splitting
2 Laser Transitions

The first:
$5s\frac{1}{2}$_F=1 to $5p\frac{3}{2}$_F=1
q = 0 (The laser is linearly polarized)
Detuning = 1 GHz
Intensity = 1000 $\frac{mW}{cm^2}$

The second:
$5p\frac{3}{2}$_F=1 to $5d\frac{5}{2}$_F=1
q = 0 (The laser is linearly polarized)
Detuning = 0 GHz
Intensity = 1000 $\frac{mW}{cm^2}$

Acknowledgements

1. B. D. Depoala, *Notes for Lectures on Coherent Excitation*
2. B. D. Depoala, Wigner *Relationships Connecting Fully Differential Dipole Matrix Elements to Reduced Matrix Elements*, (Department of Physics, Kansas State University, Manhattan, Kansas 66506-2601), June 26, 2015
3. B. D. Depoala, personal communication

This material is based upon work supported by National Science Foundation Grant: Kansas State University: Interactions of Matter, light, and learning; NSF Grant number: PHYS-1461251